Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:22 PM EST

PDB ID	:	5B66
Title	:	Crystal structure analysis of Photosystem II complex
Authors	:	Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on	:	2016-05-25
Resolution	:	1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

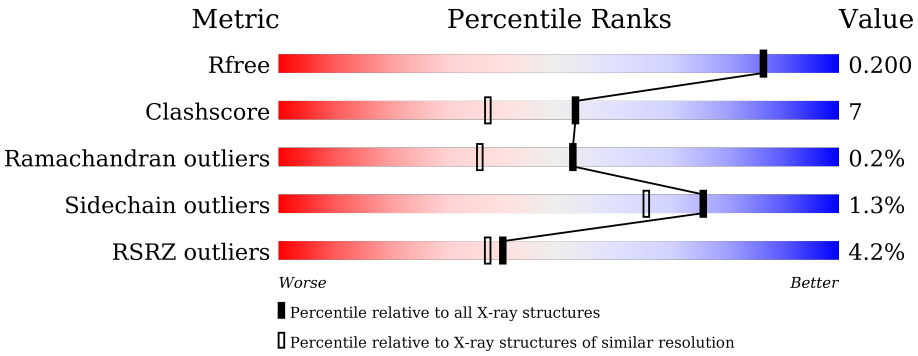
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	87% 10%
1	a	344	2% 95%
2	B	505	4% 87% 13%
2	b	505	4% 95%
3	C	455	2% 87% 12%
3	c	455	97%

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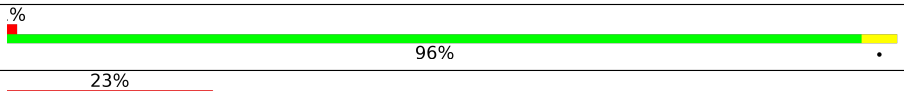
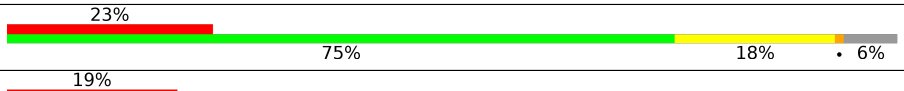
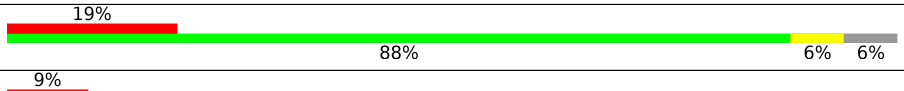
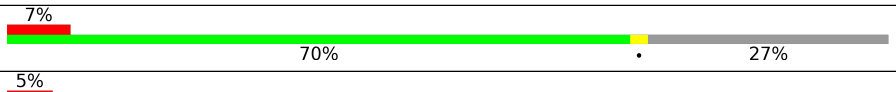
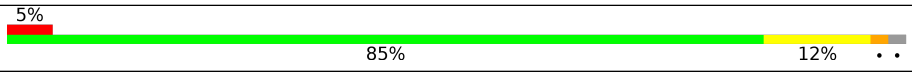
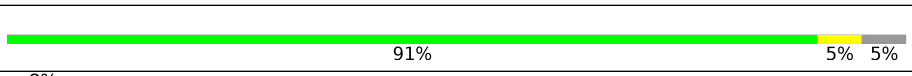
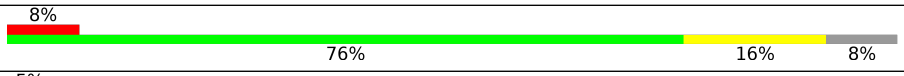
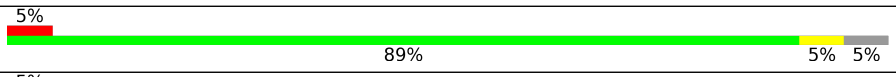
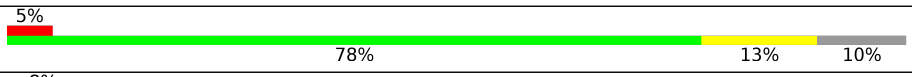
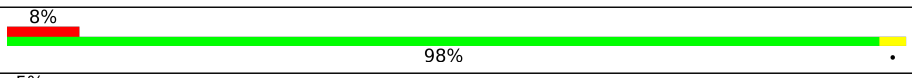
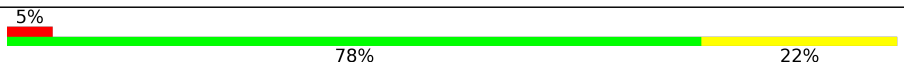
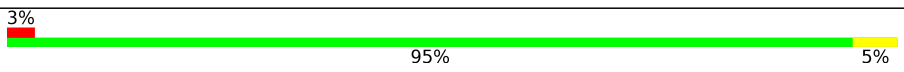
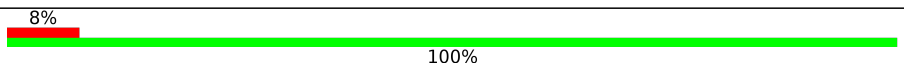
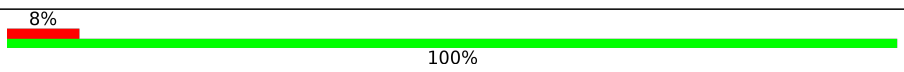
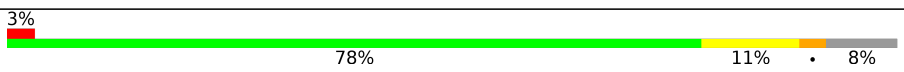
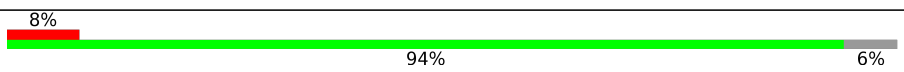
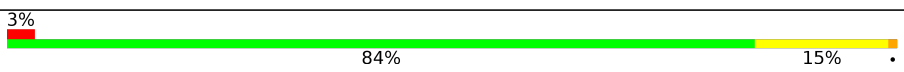
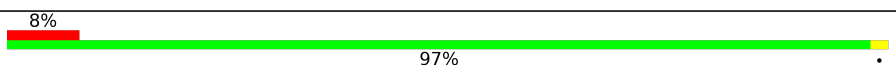
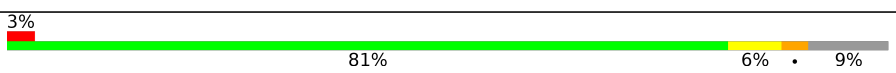
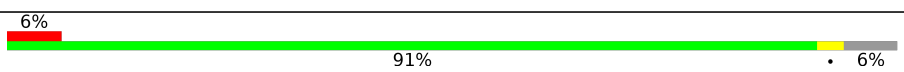
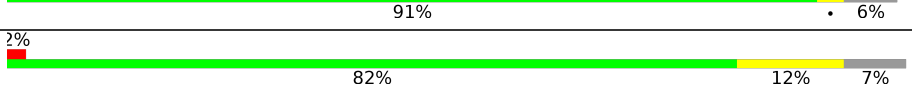
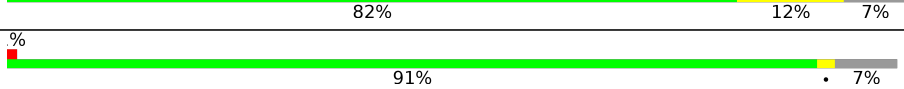
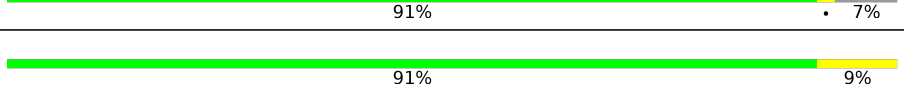
Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	4% 99%
17	Y	30	20% 70% 27%
17	y	30	17% 97%
18	X	40	13% 90% 5% 5%
18	x	40	5% 88% 13%
19	Z	62	23% 77% 18% 5%
19	z	62	19% 90% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	401	X	-	-	-
20	CLA	A	402	X	-	-	-
20	CLA	A	404	X	-	-	-
20	CLA	B	601	X	-	-	-
20	CLA	B	602	X	-	-	X
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	609	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	C	504	X	-	-	-
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	511	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	C	513	X	-	-	-
20	CLA	D	401	X	-	-	-
20	CLA	D	402	X	-	-	-
20	CLA	D	404	X	-	-	X
20	CLA	a	403	X	-	-	-
20	CLA	a	404	X	-	-	X
20	CLA	a	407	X	-	-	-
20	CLA	b	603	X	-	-	X
20	CLA	b	604	X	-	-	-
20	CLA	b	605	X	-	-	-
20	CLA	b	606	X	-	-	-
20	CLA	b	607	X	-	-	-
20	CLA	b	608	X	-	-	-
20	CLA	b	609	X	-	-	-
20	CLA	b	610	X	-	-	-
20	CLA	b	611	X	-	-	-
20	CLA	b	612	X	-	-	-
20	CLA	b	613	X	-	-	-
20	CLA	b	614	X	-	-	-
20	CLA	b	615	X	-	-	-
20	CLA	b	616	X	-	-	-
20	CLA	b	617	X	-	-	-
20	CLA	b	618	X	-	-	-
20	CLA	c	501	X	-	-	-
20	CLA	c	502	X	-	-	-
20	CLA	c	503	X	-	-	-
20	CLA	c	504	X	-	-	-
20	CLA	c	505	X	-	-	-
20	CLA	c	506	X	-	-	-
20	CLA	c	507	X	-	-	-
20	CLA	c	508	X	-	-	-
20	CLA	c	509	X	-	-	-
20	CLA	c	510	X	-	-	-
20	CLA	c	511	X	-	-	-
20	CLA	c	512	X	-	-	-
20	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	402	X	-	-	-
20	CLA	d	403	X	-	-	-
20	CLA	d	404	X	-	-	-
22	BCR	K	102	-	-	-	X
23	SQD	a	401	-	-	-	X
23	SQD	b	622	-	-	-	X
23	SQD	f	101	-	-	-	X
23	SQD	l	101	-	-	-	X
24	LMG	A	407	-	-	-	X
24	LMG	B	620	-	-	-	X
24	LMG	C	524	-	-	-	X
24	LMG	a	410	-	-	-	X
24	LMG	b	623	-	-	-	X
24	LMG	c	518	-	-	-	X
26	UNL	A	410	-	-	-	X
26	UNL	B	630	-	-	-	X
26	UNL	B	633	-	-	-	X
26	UNL	C	523	-	-	-	X
26	UNL	D	410	-	-	-	X
26	UNL	D	411	-	-	-	X
26	UNL	E	102	-	-	-	X
26	UNL	J	105	-	-	-	X
26	UNL	T	103	-	-	-	X
26	UNL	U	901	-	-	X	X
26	UNL	X	101	-	-	-	X
26	UNL	b	630	-	-	-	X
26	UNL	d	409	-	-	-	X
26	UNL	d	410	-	-	-	X
26	UNL	d	411	-	-	-	X
26	UNL	h	103	-	-	-	X
26	UNL	j	106	-	-	-	X
26	UNL	t	102	-	-	-	X
27	PL9	A	411	-	-	-	X
27	PL9	a	415	-	-	-	X
28	DMS	A	416	-	-	-	X
28	DMS	A	417	-	-	-	X
28	DMS	A	418	-	-	-	X
28	DMS	B	634	-	-	-	X
28	DMS	B	637	-	-	-	X
28	DMS	B	638	-	-	-	X
28	DMS	B	639	-	-	X	X
28	DMS	B	641	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	DMS	B	642	-	-	X	X
28	DMS	B	644	-	-	X	-
28	DMS	C	525[A]	-	-	-	X
28	DMS	C	525[B]	-	-	-	X
28	DMS	C	526	-	-	-	X
28	DMS	C	527	-	-	-	X
28	DMS	C	530	-	-	X	X
28	DMS	C	531	-	-	X	X
28	DMS	C	532	-	-	X	X
28	DMS	D	413	-	-	-	X
28	DMS	D	414	-	-	X	-
28	DMS	D	415	-	-	-	X
28	DMS	O	304	-	-	-	X
28	DMS	O	305	-	-	-	X
28	DMS	O	306	-	-	-	X
28	DMS	O	307	-	-	X	-
28	DMS	O	309	-	-	-	X
28	DMS	O	310	-	-	-	X
28	DMS	U	902	-	-	-	X
28	DMS	U	903[A]	-	-	-	X
28	DMS	U	903[B]	-	-	X	X
28	DMS	V	205	-	-	-	X
28	DMS	V	206	-	-	X	-
28	DMS	b	631	-	-	-	X
28	DMS	b	633	-	-	-	X
28	DMS	b	636	-	-	-	X
28	DMS	c	528	-	-	-	X
28	DMS	c	530	-	-	-	X
28	DMS	c	535	-	-	-	X
28	DMS	c	536	-	-	-	X
28	DMS	d	413	-	-	-	X
28	DMS	d	414	-	-	-	X
28	DMS	o	304	-	-	-	X
28	DMS	o	306	-	-	-	X
28	DMS	o	307	-	-	-	X
28	DMS	u	202	-	-	-	X
28	DMS	v	202	-	-	-	X
28	DMS	v	206	-	-	-	X
31	BCT	A	421	-	-	X	-
32	HTG	B	621	-	-	-	X
32	HTG	B	622	-	-	-	X
32	HTG	C	521	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	HTG	C	522	-	-	-	X
32	HTG	D	417	-	-	-	X
32	HTG	O	302	-	-	-	X
32	HTG	V	202	-	-	-	X
32	HTG	b	625	-	-	-	X
32	HTG	c	521	-	-	-	X
32	HTG	d	401	-	-	-	X
32	HTG	v	210	-	-	-	X
34	LMT	B	626	-	-	-	X
34	LMT	B	627	-	-	-	X
34	LMT	E	101	-	-	-	X
34	LMT	J	103	-	-	-	X
34	LMT	T	102	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	b	627	-	-	-	X
34	LMT	b	628	-	-	-	X
34	LMT	f	102	-	-	-	X
34	LMT	m	101	-	-	-	X
35	DGD	D	406	-	-	-	X
35	DGD	H	102	-	-	-	X
35	DGD	d	416	-	-	-	X
35	DGD	h	101	-	-	-	X
36	LHG	D	409	-	-	-	X
36	LHG	E	103	-	-	-	X
36	LHG	d	407	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 54996 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2626	1721	430	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2622	1719	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	11	0
			4012	2632	668	699	13			
2	b	495	Total	C	N	O	S	0	4	0
			3884	2550	650	671	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	1	0
			3483	2280	582	608	13			
3	c	455	Total	C	N	O	S	0	1	0
			3523	2305	591	614	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2728	1808	446	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	78	Total	C	N	O	0	1	0
			632	413	101	118			
5	e	78	Total	C	N	O	0	2	0
			636	419	99	118			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			508	339	81	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			284	194	45	44	1			
8	i	36	Total	C	N	O	S	0	1	0
			300	203	49	47	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			272	183	41	47	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			285	199	42	44			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	1	0
			296	200	45	51			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			259	175	37	46	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	6	0
			1870	1172	309	384	5			
13	o	243	Total	C	N	O	S	0	2	0
			1838	1153	305	376	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	1	0
			257	181	35	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			766	486	128	152			
15	u	97	Total	C	N	O	0	0	0
			770	489	129	152			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	3	0
			1080	685	181	210	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			213	140	37	33	3			

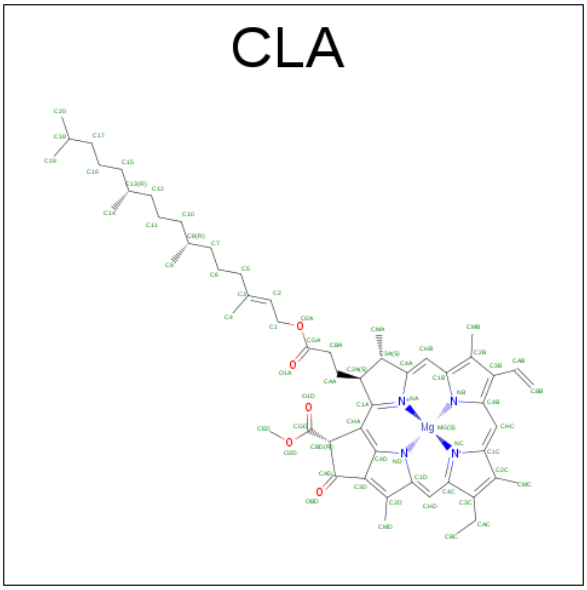
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			274	183	44	47			
18	x	35	Total	C	N	O	0	0	0
			252	171	38	43			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			450	308	67	73	2			
19	z	61	Total	C	N	O	S	0	0	0
			433	297	66	69	1			

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 60 50 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	C	1	Total C Mg N O 55 45 1 4 5	0	0
20	C	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	D	1	Total C Mg N O 65 55 1 4 5	0	0
20	a	1	Total C Mg N O 65 55 1 4 5	0	0
20	a	1	Total C Mg N O 60 50 1 4 5	0	0
20	a	1	Total C Mg N O 47 37 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	b	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 60 50 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0
20	c	1	Total C Mg N O 65 55 1 4 5	0	0

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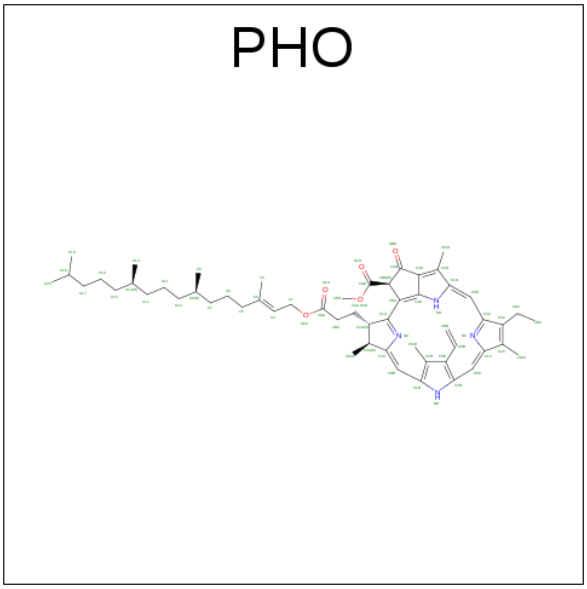
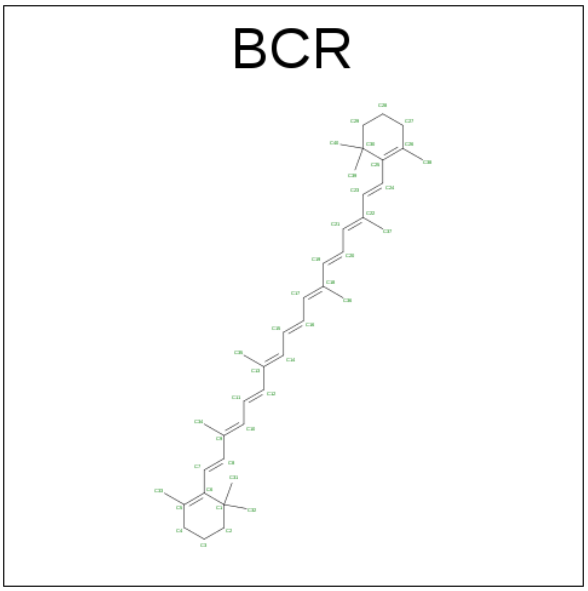
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	D	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	D	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	T	1	Total C 40 40	0	0
22	a	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0

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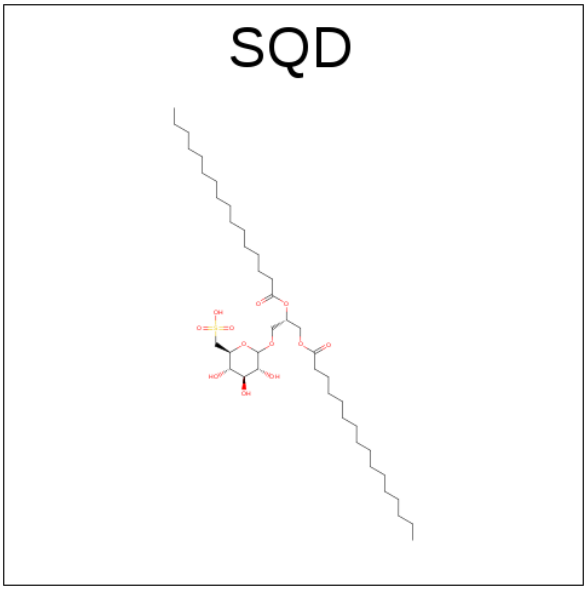
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	c	1	Total C 40 40	0	0
22	d	1	Total C 40 40	0	0
22	j	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	t	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 54 41 12 1	0	0
23	A	1	Total C O S 54 41 12 1	0	0
23	F	1	Total C O S 35 23 11 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0

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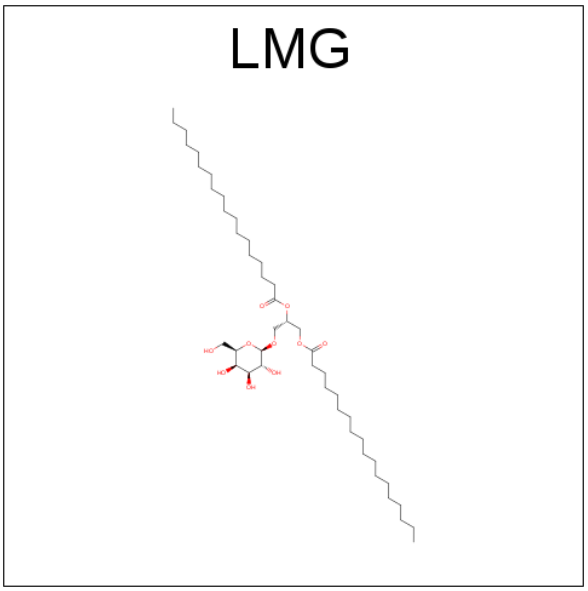
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	b	1	Total C O S 54 41 12 1	0	0
23	f	1	Total C O S 40 27 12 1	0	0
23	l	1	Total C O S 54 41 12 1	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C O 51 41 10	0	0
24	B	1	Total C O 51 41 10	0	0
24	C	1	Total C O 51 41 10	0	0
24	C	1	Total C O 45 35 10	0	0
24	J	1	Total C O 45 35 10	0	0
24	a	1	Total C O 51 41 10	0	0
24	b	1	Total C O 49 39 10	0	0
24	c	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C O 51 41 10	0	0
24	j	1	Total C O 45 35 10	0	0

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	2	Total Cl 2 2	0	0
25	a	2	Total Cl 2 2	0	0

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	h	1	Total C 16 16	0	0
26	B	6	Total C 84 84	0	0
26	c	3	Total C O 48 43 5	0	0
26	t	1	Total C 16 16	0	0
26	X	1	Total C 16 16	0	0
26	J	4	Total C 33 33	0	0
26	E	1	Total C 15 15	0	0
26	b	7	Total C 68 68	0	0
26	A	2	Total C O 40 35 5	0	0
26	x	1	Total C 9 9	0	0
26	M	1	Total C 12 12	0	0
26	j	2	Total C 22 22	0	0
26	D	2	Total C O 53 48 5	0	0

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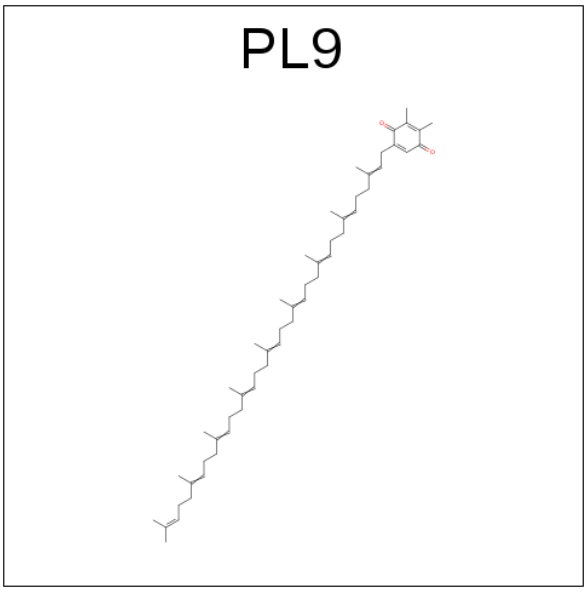
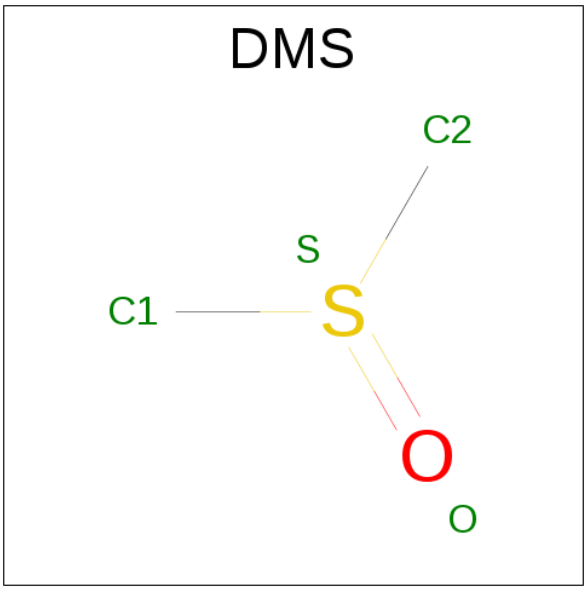
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	e	1	Total C 7 7	0	0
26	I	5	Total C 61 61	0	0
26	Z	1	Total C 4 4	0	0
26	a	3	Total C O 45 40 5	0	0
26	U	1	Total C 14 14	0	0
26	L	1	Total C 14 14	0	0
26	d	3	Total C O 68 63 5	0	0
26	H	2	Total C 10 10	0	0
26	i	3	Total C 38 38	0	0
26	C	1	Total C O 34 29 5	0	0
26	z	1	Total C 6 6	0	0
26	T	1	Total C 13 13	0	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

- Molecule 28 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 8	C 4	O 2	S 2	0	1
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	C	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	D	1	Total C O S 4 2 1 1	0	0
28	F	1	Total C O S 4 2 1 1	0	0
28	H	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	O	1	Total C O S 4 2 1 1	0	0
28	U	1	Total C O S 4 2 1 1	0	0
28	U	1	Total C O S 8 4 2 2	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	U	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	V	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	b	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	c	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	d	1	Total C O S 4 2 1 1	0	0
28	h	1	Total C O S 4 2 1 1	0	0
28	i	1	Total C O S 4 2 1 1	0	0
28	j	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	o	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0

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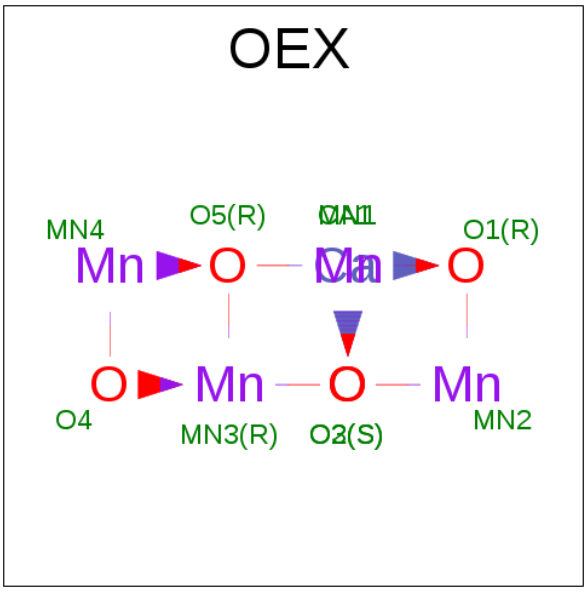
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	u	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

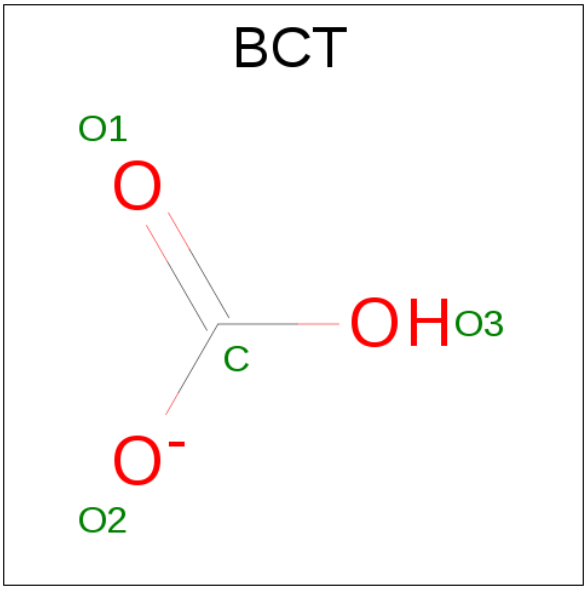
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Fe 1 1	0	0
29	a	1	Total Fe 1 1	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



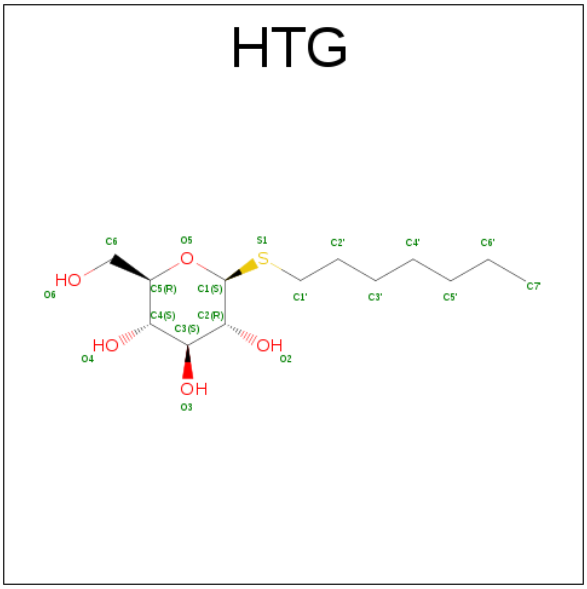
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	B	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	C	1	Total C O S 19 13 5 1	0	0
32	D	1	Total C O S 19 13 5 1	0	0
32	O	1	Total C O S 19 13 5 1	0	0
32	V	1	Total C O S 13 7 5 1	0	0

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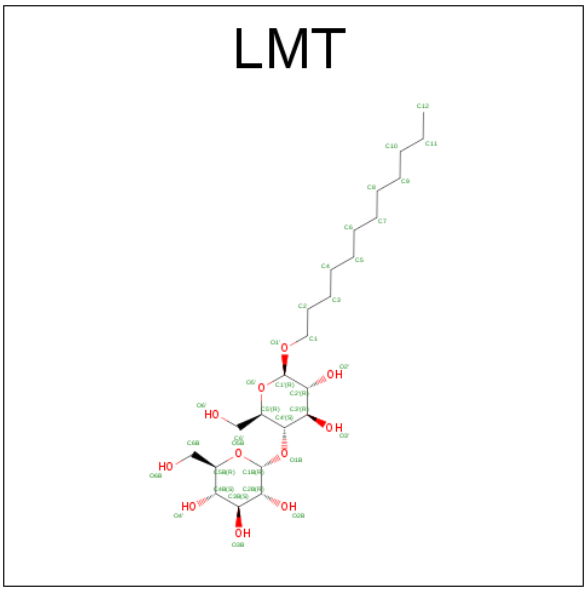
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	d	1	Total C O S 19 13 5 1	0	0
32	u	1	Total C S 8 7 1	0	0
32	v	1	Total C O S 14 8 5 1	0	0

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	V	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			16	14	2		
34	E	1	Total	C	O	0	0
			24	18	6		
34	I	1	Total	C	O	0	0
			35	24	11		
34	J	1	Total	C	O	0	0
			24	18	6		
34	M	1	Total	C	O	0	0
			35	24	11		
34	T	1	Total	C	O	0	0
			24	18	6		
34	Z	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			32	21	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	c	1	Total	C	O	0	0
			35	24	11		
34	f	1	Total	C	O	0	0
			24	18	6		

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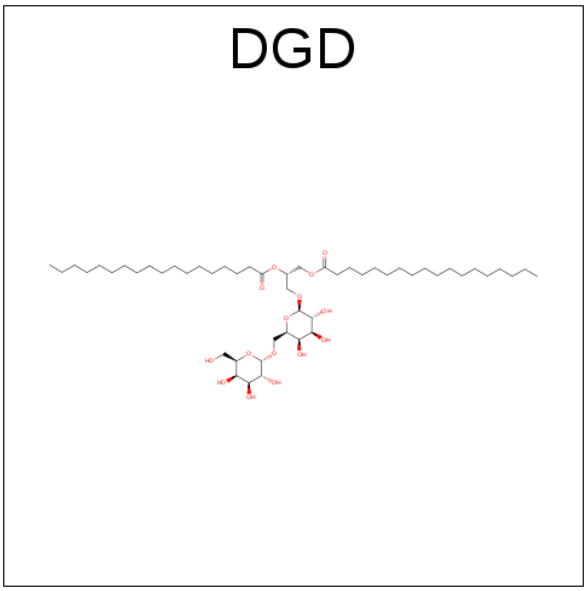
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	m	1	Total C O 35 24 11	0	0
34	m	1	Total C O 35 24 11	0	0
34	z	1	Total C O 35 24 11	0	0

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 62 47 15	0	0
35	C	1	Total C O 55 40 15	0	0
35	C	1	Total C O 62 47 15	0	0
35	D	1	Total C O 51 41 10	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 62 47 15	0	0
35	c	1	Total C O 57 42 15	0	0
35	c	1	Total C O 62 47 15	0	0

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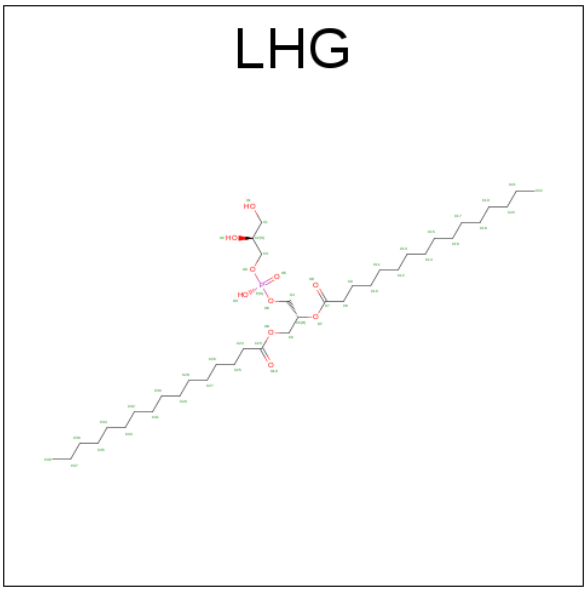
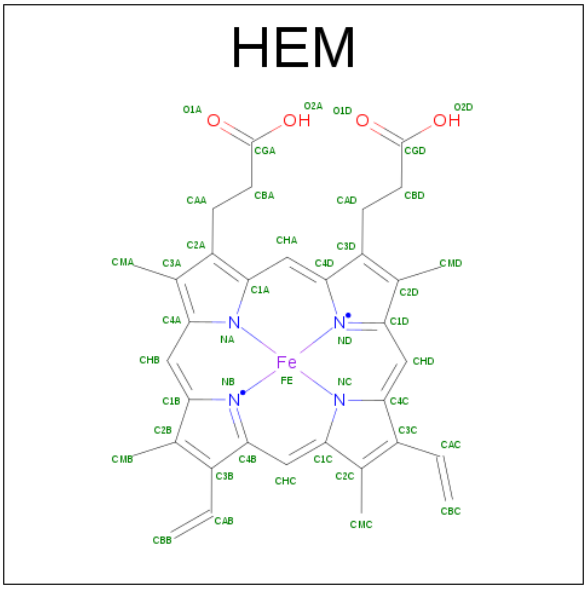
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	d	1	Total C O 51 41 10	0	0
35	h	1	Total C O 62 47 15	0	0

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



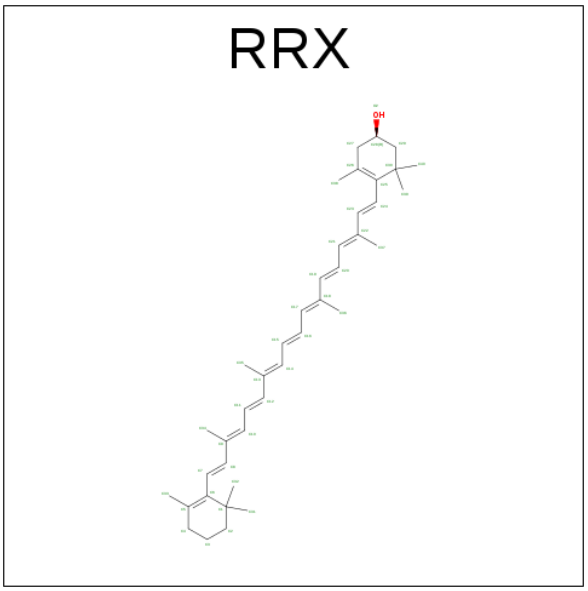
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	D	1	Total C O P 49 38 10 1	0	0
36	E	1	Total C O P 48 37 10 1	0	0
36	L	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	d	1	Total C O P 49 38 10 1	0	0
36	l	1	Total C O P 49 38 10 1	0	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
37	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
37	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
37	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	H	1	Total C O 41 40 1	0	0
38	x	1	Total C O 41 40 1	0	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	J	1	Total Mg 1 1	0	0
39	j	1	Total Mg 1 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	177	Total O 182 182	0	5
40	B	447	Total O 473 473	0	25
40	C	317	Total O 324 324	0	7
40	D	175	Total O 180 180	0	5
40	E	62	Total O 66 66	0	4

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	F	8	Total O 8 8	0	0
40	H	62	Total O 65 65	0	3
40	I	16	Total O 16 16	0	0
40	J	23	Total O 23 23	0	0
40	K	12	Total O 12 12	0	0
40	L	19	Total O 21 21	0	2
40	M	12	Total O 12 12	0	0
40	O	263	Total O 273 273	0	10
40	T	19	Total O 20 20	0	1
40	U	133	Total O 136 136	0	3
40	V	177	Total O 183 183	0	6
40	Y	7	Total O 7 7	0	0
40	X	22	Total O 22 22	0	0
40	Z	5	Total O 5 5	0	0
40	a	182	Total O 185 185	0	3
40	b	451	Total O 465 465	0	14
40	c	362	Total O 374 374	0	12
40	d	176	Total O 182 182	0	6
40	e	48	Total O 49 49	0	1
40	f	15	Total O 16 16	0	1
40	h	68	Total O 70 70	0	2

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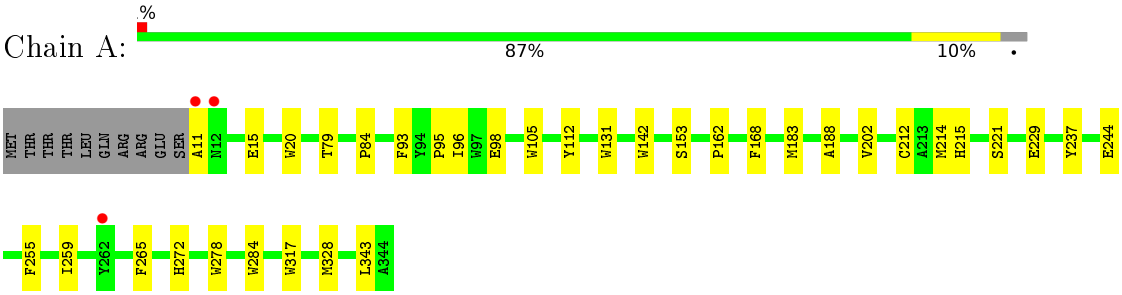
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	i	19	Total O 21 21	0	2
40	j	23	Total O 24 24	0	1
40	k	11	Total O 12 12	0	1
40	l	22	Total O 24 24	0	2
40	m	23	Total O 24 24	0	1
40	o	214	Total O 230 230	0	15
40	t	19	Total O 20 20	0	1
40	u	146	Total O 150 150	0	4
40	v	144	Total O 147 147	0	3
40	y	7	Total O 7 7	0	0
40	x	25	Total O 26 26	0	1
40	z	12	Total O 12 12	0	0

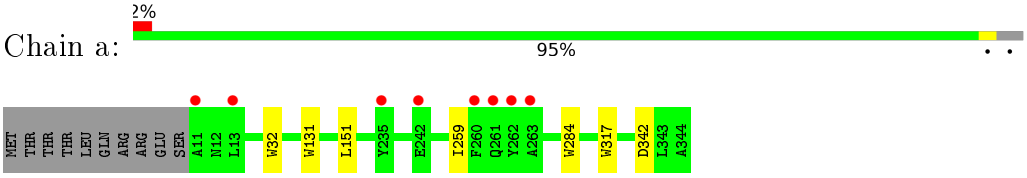
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

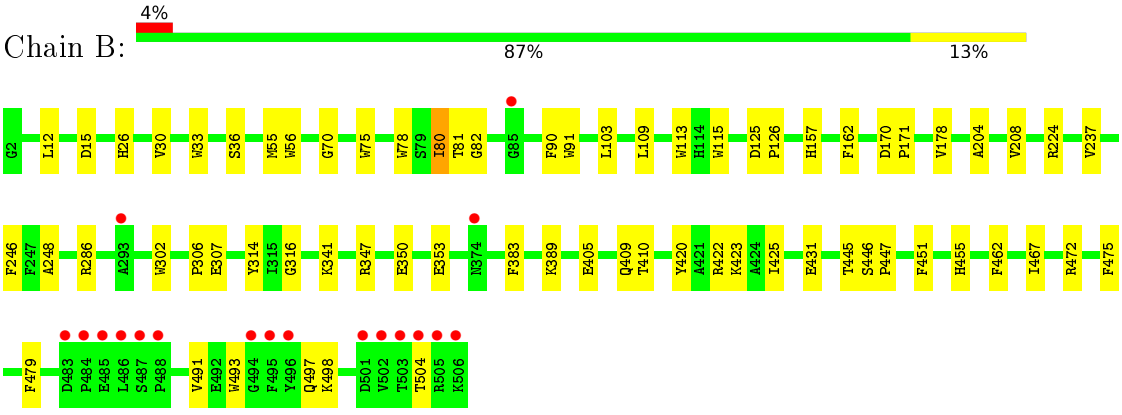
• Molecule 1: Photosystem II protein D1



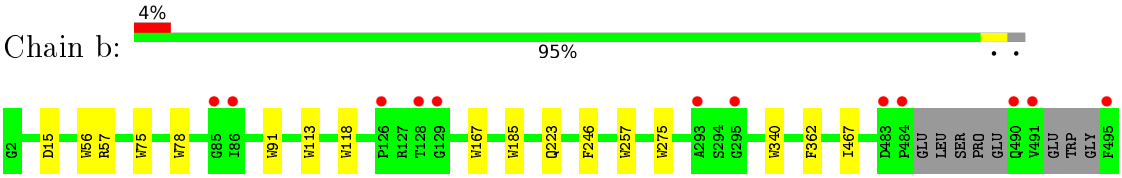
• Molecule 1: Photosystem II protein D1

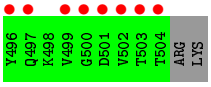


• Molecule 2: Photosystem II CP47 reaction center protein



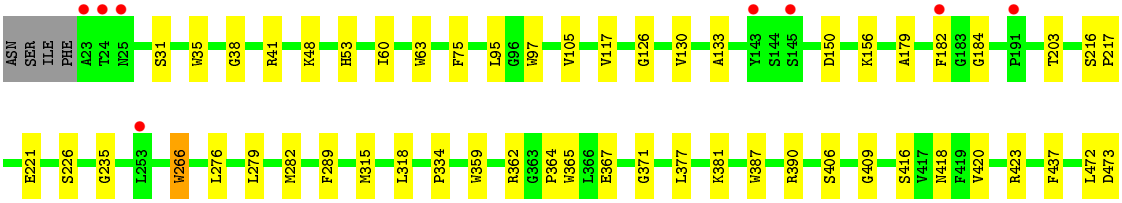
• Molecule 2: Photosystem II CP47 reaction center protein





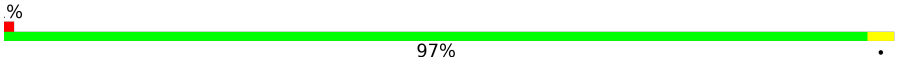
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



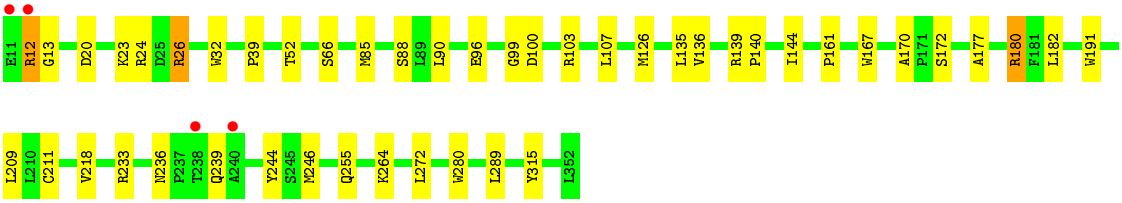
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



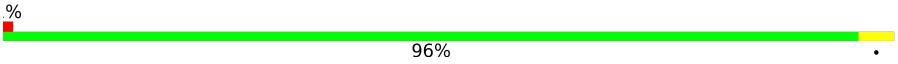
• Molecule 4: Photosystem II D2 protein

Chain D:



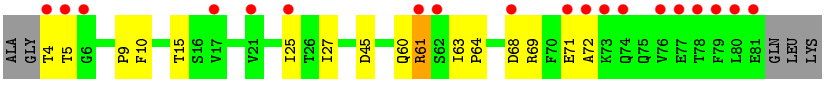
• Molecule 4: Photosystem II D2 protein

Chain d:



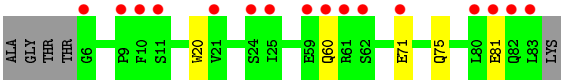
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

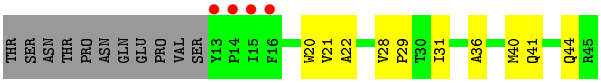


• Molecule 5: Cytochrome b559 subunit alpha

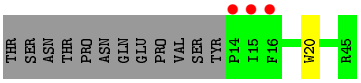
Chain e:



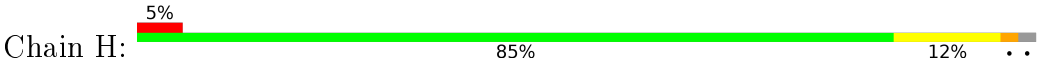
• Molecule 6: Cytochrome b559 subunit beta

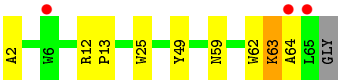


• Molecule 6: Cytochrome b559 subunit beta

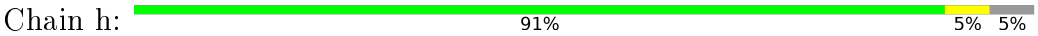


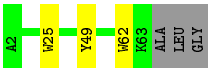
• Molecule 7: Photosystem II reaction center protein H



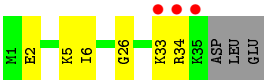


• Molecule 7: Photosystem II reaction center protein H

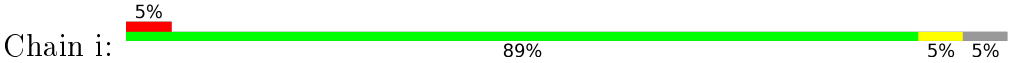


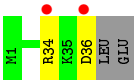


• Molecule 8: Photosystem II reaction center protein I

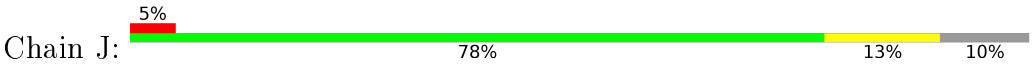


• Molecule 8: Photosystem II reaction center protein I



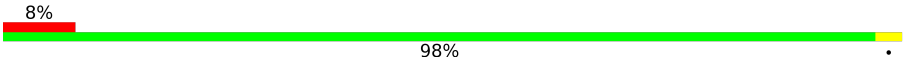


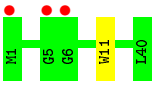
• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J

Chain j:



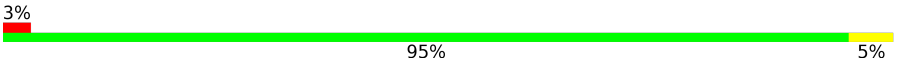


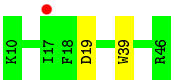
• Molecule 10: Photosystem II reaction center protein K

Chain K:

• Molecule 10: Photosystem II reaction center protein K

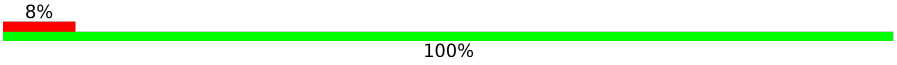
Chain k:





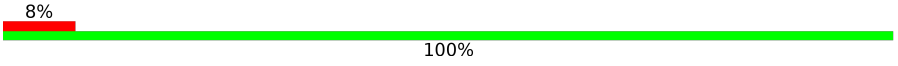
• Molecule 11: Photosystem II reaction center protein L

Chain L:



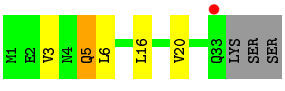
• Molecule 11: Photosystem II reaction center protein L

Chain l:



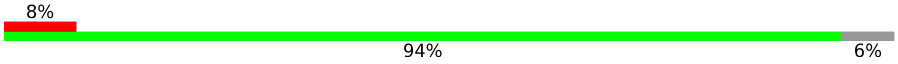
• Molecule 12: Photosystem II reaction center protein M

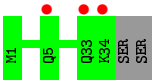
Chain M:



• Molecule 12: Photosystem II reaction center protein M

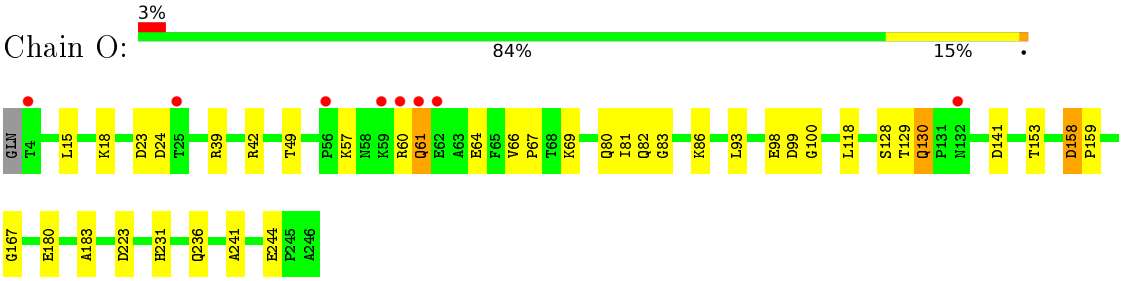
Chain m:





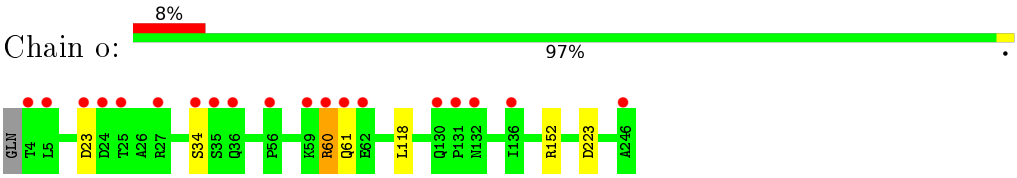
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



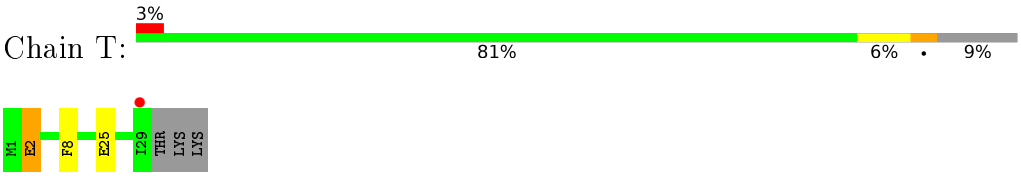
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



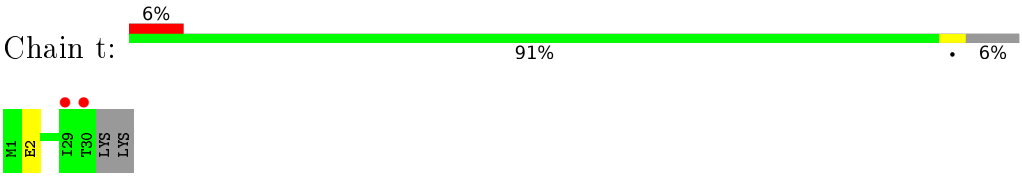
• Molecule 14: Photosystem II reaction center protein T

Chain T:



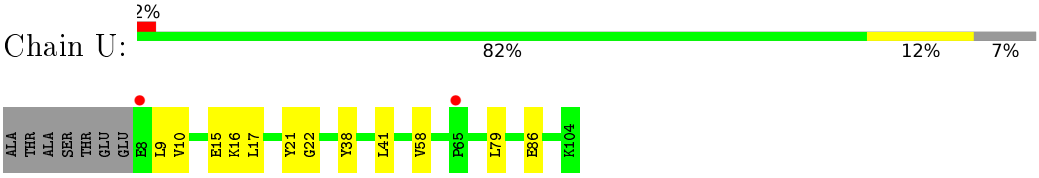
• Molecule 14: Photosystem II reaction center protein T

Chain t:



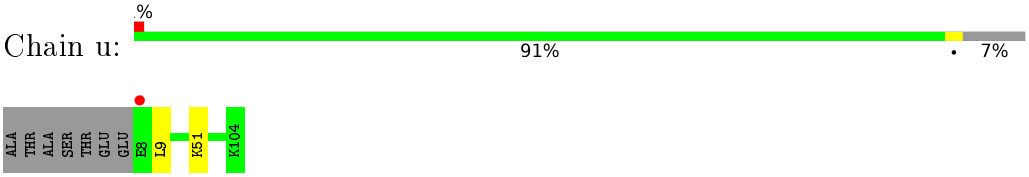
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



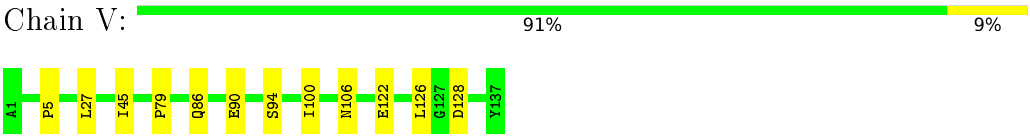
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



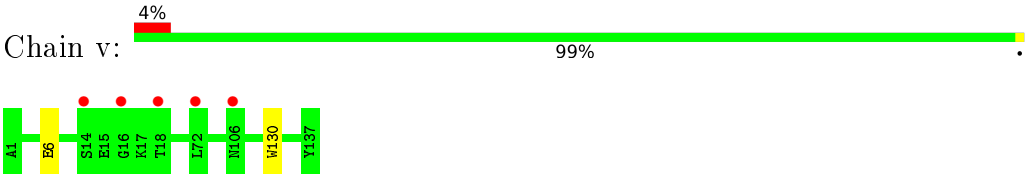
• Molecule 16: Cytochrome c-550

Chain V:



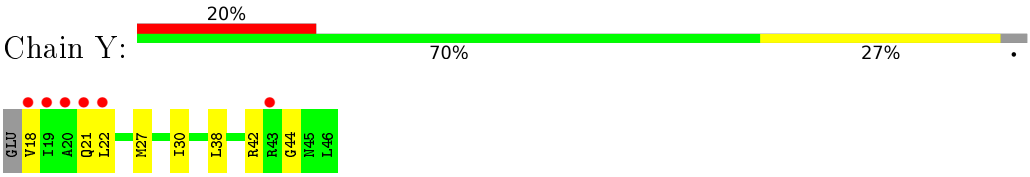
• Molecule 16: Cytochrome c-550

Chain v:



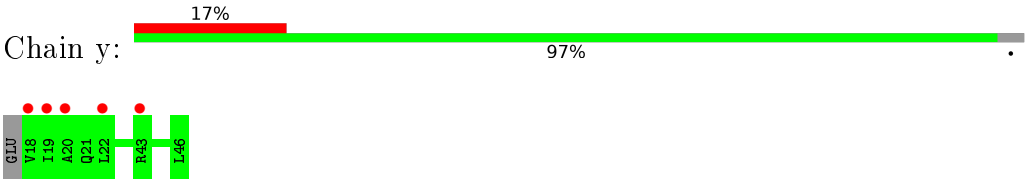
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



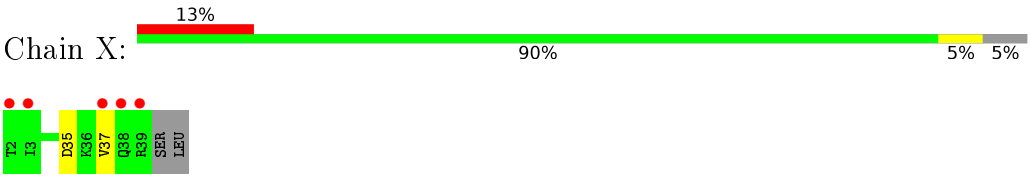
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



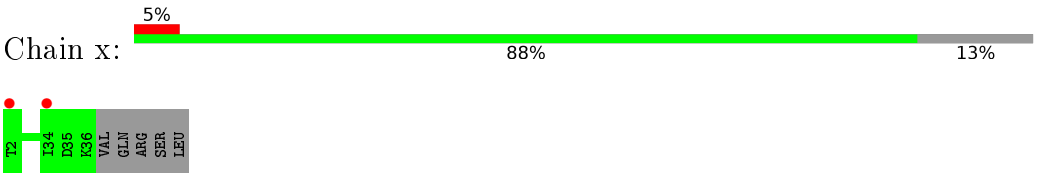
• Molecule 18: Photosystem II reaction center protein X

Chain X:



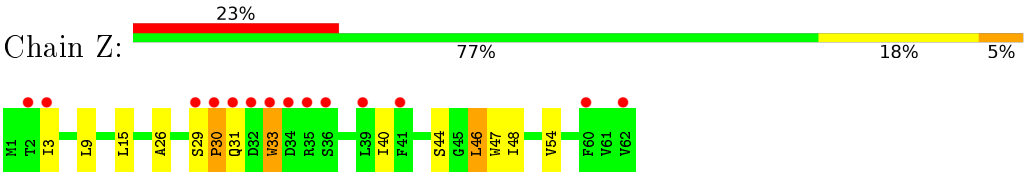
• Molecule 18: Photosystem II reaction center protein X

Chain x:



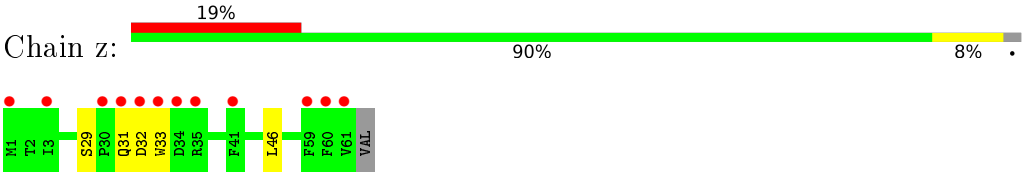
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:


19%
90%
8%
M1
T2
I3
S29
P30
Q31
D32
W33
D34
R35
F41
L46
F59
F60
V61
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.47Å 228.18Å 286.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-1.85) 100.0 (19.99-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	33616 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 70.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, HTG, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, DMS, FE2, RRX, BCT, HEM, FME, UNL, LMG, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.95	5/2717 (0.2%)	0.77	1/3707 (0.0%)
1	a	0.93	4/2718 (0.1%)	0.79	2/3707 (0.1%)
2	B	0.90	9/4181 (0.2%)	0.77	1/5700 (0.0%)
2	b	0.91	11/4029 (0.3%)	0.78	2/5490 (0.0%)
3	C	0.87	7/3599 (0.2%)	0.74	2/4901 (0.0%)
3	c	0.86	8/3640 (0.2%)	0.72	2/4956 (0.0%)
4	D	0.95	3/2826 (0.1%)	0.78	1/3850 (0.0%)
4	d	0.95	8/2817 (0.3%)	0.78	1/3839 (0.0%)
5	E	0.71	0/654	0.68	0/896
5	e	0.69	1/661 (0.2%)	0.72	0/904
6	F	0.79	1/278 (0.4%)	0.60	0/379
6	f	0.81	1/265 (0.4%)	0.62	0/360
7	H	0.84	2/524 (0.4%)	0.75	0/715
7	h	0.86	2/517 (0.4%)	0.71	0/704
8	I	0.63	0/281	0.69	0/380
8	i	0.61	0/300	0.62	0/405
9	J	0.82	1/257 (0.4%)	0.61	0/349
9	j	0.81	1/278 (0.4%)	0.62	0/378
10	K	0.70	1/303 (0.3%)	0.65	0/416
10	k	0.72	1/295 (0.3%)	0.64	0/407
11	L	0.88	0/312	0.76	0/425
11	l	0.91	0/306	0.76	0/418
12	M	0.70	0/265	0.74	0/362
12	m	0.70	0/270	0.76	0/369
13	O	0.72	0/1919	0.80	1/2607 (0.0%)
13	o	0.69	0/1875	0.77	2/2548 (0.1%)
14	T	0.78	0/259	0.77	0/352
14	t	0.79	0/257	0.73	0/349
15	U	0.77	0/777	0.78	0/1055
15	u	0.76	0/781	0.77	0/1059
16	V	0.80	0/1110	0.80	1/1506 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.71	1/1073 (0.1%)	0.75	0/1461
17	Y	0.50	0/213	0.63	0/285
17	y	0.45	0/214	0.60	0/286
18	X	0.54	0/277	0.69	0/375
18	x	0.57	0/255	0.66	0/345
19	Z	0.70	2/461 (0.4%)	0.56	0/632
19	z	0.61	1/444 (0.2%)	0.57	0/611
All	All	0.85	70/42208 (0.2%)	0.75	16/57488 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.13	1.50	1.41
1	A	343	LEU	C-N	6.74	1.49	1.34
1	a	131	TRP	CD2-CE2	6.46	1.49	1.41
3	C	266	TRP	CD2-CE2	6.43	1.49	1.41
2	B	33	TRP	CD2-CE2	6.27	1.48	1.41
9	j	11	TRP	CD2-CE2	6.26	1.48	1.41
10	k	39	TRP	CD2-CE2	6.25	1.48	1.41
2	B	56	TRP	CD2-CE2	6.21	1.48	1.41
3	c	35	TRP	CD2-CE2	6.21	1.48	1.41
2	B	78	TRP	CD2-CE2	6.18	1.48	1.41
4	D	280	TRP	CD2-CE2	6.11	1.48	1.41
2	b	113	TRP	CD2-CE2	6.08	1.48	1.41
1	a	284	TRP	CD2-CE2	6.00	1.48	1.41
16	v	130	TRP	CD2-CE2	5.96	1.48	1.41
3	c	443	TRP	CD2-CE2	5.93	1.48	1.41
1	A	278	TRP	CD2-CE2	5.90	1.48	1.41
2	b	56	TRP	CD2-CE2	5.90	1.48	1.41
19	Z	47	TRP	CD2-CE2	5.86	1.48	1.41
6	f	20	TRP	CD2-CE2	5.85	1.48	1.41
3	c	97	TRP	CD2-CE2	5.76	1.48	1.41
1	A	284	TRP	CD2-CE2	5.74	1.48	1.41
2	b	275	TRP	CD2-CE2	5.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	387	TRP	CD2-CE2	5.69	1.48	1.41
9	J	11	TRP	CD2-CE2	5.68	1.48	1.41
2	B	113	TRP	CD2-CE2	5.67	1.48	1.41
6	F	20	TRP	CD2-CE2	5.60	1.48	1.41
7	H	62	TRP	CD2-CE2	5.60	1.48	1.41
7	h	62	TRP	CD2-CE2	5.60	1.48	1.41
4	D	32	TRP	CD2-CE2	5.59	1.48	1.41
4	D	167	TRP	CD2-CE2	5.58	1.48	1.41
3	C	35	TRP	CD2-CE2	5.48	1.48	1.41
10	K	39	TRP	CD2-CE2	5.47	1.48	1.41
19	Z	33	TRP	CD2-CE2	5.47	1.48	1.41
4	d	48	TRP	CD2-CE2	5.45	1.47	1.41
4	d	111	TRP	CD2-CE2	5.44	1.47	1.41
2	b	185	TRP	CD2-CE2	5.44	1.47	1.41
1	A	20	TRP	CD2-CE2	5.43	1.47	1.41
1	a	32	TRP	CD2-CE2	5.42	1.47	1.41
2	b	340	TRP	CD2-CE2	5.41	1.47	1.41
1	a	317	TRP	CD2-CE2	5.41	1.47	1.41
3	c	250	TRP	CD2-CE2	5.40	1.47	1.41
2	b	78	TRP	CD2-CE2	5.37	1.47	1.41
3	C	365	TRP	CD2-CE2	5.37	1.47	1.41
2	B	302	TRP	CD2-CE2	5.35	1.47	1.41
7	h	25	TRP	CD2-CE2	5.35	1.47	1.41
3	C	97	TRP	CD2-CE2	5.32	1.47	1.41
4	d	93	TRP	CD2-CE2	5.32	1.47	1.41
4	d	58	TRP	CD2-CE2	5.32	1.47	1.41
19	z	33	TRP	CD2-CE2	5.29	1.47	1.41
2	b	91	TRP	CD2-CE2	5.29	1.47	1.41
3	c	365	TRP	CG-CD1	5.26	1.44	1.36
4	d	104	TRP	CD2-CE2	5.25	1.47	1.41
5	e	20	TRP	CD2-CE2	5.25	1.47	1.41
2	b	75	TRP	CD2-CE2	5.23	1.47	1.41
4	d	21	TRP	CD2-CE2	5.22	1.47	1.41
1	A	142	TRP	CD2-CE2	5.21	1.47	1.41
4	d	32	TRP	CD2-CE2	5.21	1.47	1.41
3	C	359	TRP	CD2-CE2	5.20	1.47	1.41
2	B	91	TRP	CD2-CE2	5.17	1.47	1.41
4	d	14	TRP	CD2-CE2	5.15	1.47	1.41
2	B	75	TRP	CD2-CE2	5.14	1.47	1.41
3	C	63	TRP	CD2-CE2	5.14	1.47	1.41
2	B	115	TRP	CD2-CE2	5.13	1.47	1.41
2	b	167	TRP	CD2-CE2	5.13	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	239	TRP	CD2-CE2	5.09	1.47	1.41
2	B	493	TRP	CD2-CE2	5.07	1.47	1.41
2	b	118	TRP	CD2-CE2	5.06	1.47	1.41
3	c	223	TRP	CD2-CE2	5.04	1.47	1.41
7	H	25	TRP	CD2-CE2	5.03	1.47	1.41
2	b	257	TRP	CD2-CE2	5.01	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	342	ASP	CB-CG-OD1	6.34	124.01	118.30
16	V	128	ASP	CB-CG-OD1	6.14	123.82	118.30
3	C	473	ASP	CB-CG-OD2	5.92	123.63	118.30
13	o	152	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	c	423	ARG	NE-CZ-NH2	-5.79	117.41	120.30
4	D	100	ASP	CB-CG-OD1	5.70	123.43	118.30
2	b	57	ARG	NE-CZ-NH1	5.47	123.04	120.30
13	O	158	ASP	CB-CG-OD1	5.38	123.14	118.30
2	B	15	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	131	TRP	CA-CB-CG	-5.31	103.61	113.70
3	c	423	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	b	15	ASP	CB-CG-OD1	5.21	122.98	118.30
3	C	423	ARG	NE-CZ-NH2	-5.11	117.75	120.30
13	o	223	ASP	CB-CG-OD1	5.04	122.84	118.30
1	a	151	LEU	CB-CG-CD2	-5.04	102.44	111.00
4	d	297	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	60	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2626	0	2515	27	0
1	a	2622	0	2529	0	0
2	B	4012	0	3860	82	0
2	b	3884	0	3743	0	0
3	C	3483	0	3397	50	0
3	c	3523	0	3439	0	0
4	D	2728	0	2636	52	0
4	d	2722	0	2623	0	0
5	E	632	0	605	14	0
5	e	636	0	612	0	0
6	F	269	0	277	6	0
6	f	257	0	269	0	0
7	H	508	0	524	7	0
7	h	501	0	526	0	0
8	I	284	0	303	6	0
8	i	300	0	320	0	0
9	J	251	0	257	3	0
9	j	272	0	271	0	0
10	K	293	0	305	6	0
10	k	285	0	290	0	0
11	L	302	0	316	0	0
11	l	296	0	305	0	0
12	M	259	0	281	22	0
12	m	264	0	283	0	0
13	O	1870	0	1836	41	0
13	o	1838	0	1789	0	0
14	T	257	0	260	2	0
14	t	258	0	261	0	0
15	U	766	0	758	21	0
15	u	770	0	769	0	0
16	V	1080	0	1097	15	0
16	v	1052	0	1040	0	0
17	Y	212	0	237	6	0
17	y	213	0	239	0	0
18	X	274	0	297	2	0
18	x	252	0	277	0	0
19	Z	450	0	455	8	0
19	z	433	0	422	0	0
20	A	189	0	202	11	0
20	B	1040	0	1152	54	0
20	C	830	0	900	51	0
20	D	195	0	216	7	0
20	a	172	0	166	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	b	1040	0	1152	0	0
20	c	840	0	923	0	0
20	d	195	0	216	0	0
21	A	64	0	74	2	0
21	D	64	0	74	2	0
21	a	128	0	148	0	0
22	A	40	0	56	4	0
22	B	120	0	168	6	0
22	C	80	0	112	5	0
22	D	40	0	56	3	0
22	K	80	0	112	8	0
22	T	40	0	56	7	0
22	a	40	0	56	0	0
22	b	120	0	168	0	0
22	c	40	0	56	0	0
22	d	40	0	56	0	0
22	j	40	0	56	0	0
22	k	80	0	112	0	0
22	t	40	0	56	0	0
23	A	108	0	156	5	0
23	F	35	0	40	3	0
23	a	108	0	156	0	0
23	b	54	0	78	0	0
23	f	40	0	47	0	0
23	l	54	0	78	0	0
24	A	51	0	72	4	0
24	B	51	0	72	0	0
24	C	96	0	132	5	0
24	J	45	0	60	0	0
24	a	51	0	72	0	0
24	b	49	0	68	0	0
24	c	102	0	144	0	0
24	j	45	0	60	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	40	0	0	0	0
26	B	84	0	0	2	0
26	C	34	0	0	0	0
26	D	53	0	0	0	0
26	E	15	0	0	0	0
26	H	10	0	0	0	0
26	I	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	J	33	0	0	1	0
26	L	14	0	0	0	0
26	M	12	0	0	0	0
26	T	13	0	0	0	0
26	U	14	0	0	3	0
26	X	16	0	0	0	0
26	Z	4	0	0	0	0
26	a	45	0	0	0	0
26	b	68	0	0	0	0
26	c	48	0	0	0	0
26	d	68	0	0	0	0
26	e	7	0	0	0	0
26	h	16	0	0	0	0
26	i	38	0	0	0	0
26	j	22	0	0	0	0
26	t	16	0	0	0	0
26	x	9	0	0	0	0
26	z	6	0	0	0	0
27	A	55	0	80	11	0
27	D	55	0	80	0	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	20	0	30	1	0
28	B	48	0	72	29	0
28	C	40	0	60	20	0
28	D	16	0	24	16	0
28	F	4	0	6	3	0
28	H	4	0	6	0	0
28	O	36	0	54	17	0
28	U	16	0	24	16	0
28	V	24	0	36	7	0
28	b	44	0	66	0	0
28	c	40	0	60	0	0
28	d	12	0	18	0	0
28	h	4	0	6	0	0
28	i	4	0	6	0	0
28	j	4	0	6	0	0
28	o	28	0	42	0	0
28	u	12	0	18	0	0
28	v	32	0	48	0	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	4	0	0	5	0
31	a	4	0	0	0	0
32	B	95	0	130	11	0
32	C	76	0	104	3	0
32	D	19	0	26	3	0
32	O	19	0	26	0	0
32	V	13	0	11	0	0
32	b	76	0	104	0	0
32	c	38	0	52	0	0
32	d	19	0	26	0	0
32	u	8	0	15	0	0
32	v	14	0	13	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	V	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	64	0	95	3	0
34	E	24	0	35	0	0
34	I	35	0	46	2	0
34	J	24	0	35	1	0
34	M	35	0	46	0	0
34	T	24	0	35	0	0
34	Z	35	0	46	0	0
34	a	35	0	46	0	0
34	b	57	0	72	0	0
34	c	35	0	46	0	0
34	f	24	0	35	0	0
34	m	70	0	92	0	0
34	z	35	0	46	0	0
35	C	179	0	232	3	0
35	D	51	0	71	5	0
35	H	62	0	82	2	0
35	c	181	0	236	0	0
35	d	51	0	71	0	0
35	h	62	0	82	0	0
36	D	147	0	222	37	0
36	E	48	0	71	6	0
36	L	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	d	147	0	222	0	0
36	l	49	0	74	0	0
37	E	43	0	30	2	0
37	V	43	0	30	0	0
37	e	43	0	30	0	0
37	v	43	0	30	0	0
38	H	41	0	56	0	0
38	x	41	0	56	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	182	0	0	5	0
40	B	473	0	0	25	0
40	C	324	0	0	10	0
40	D	180	0	0	1	0
40	E	66	0	0	1	0
40	F	8	0	0	0	0
40	H	65	0	0	3	0
40	I	16	0	0	1	0
40	J	23	0	0	0	0
40	K	12	0	0	0	0
40	L	21	0	0	0	0
40	M	12	0	0	1	0
40	O	273	0	0	20	0
40	T	20	0	0	0	0
40	U	136	0	0	3	0
40	V	183	0	0	3	0
40	X	22	0	0	1	0
40	Y	7	0	0	1	0
40	Z	5	0	0	1	0
40	a	185	0	0	0	0
40	b	465	0	0	0	0
40	c	374	0	0	0	0
40	d	182	0	0	0	0
40	e	49	0	0	0	0
40	f	16	0	0	0	0
40	h	70	0	0	0	0
40	i	21	0	0	0	0
40	j	24	0	0	0	0
40	k	12	0	0	0	0
40	l	24	0	0	0	0
40	m	24	0	0	0	0
40	o	230	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	t	20	0	0	0	0
40	u	150	0	0	0	0
40	v	147	0	0	0	0
40	x	26	0	0	0	0
40	y	7	0	0	0	0
40	z	12	0	0	0	0
All	All	54996	0	51554	535	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (535) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:HD11	2.58	1.58
12:M:16[B]:LEU:HD22	12:M:16[B]:LEU:CD1	2.65	1.45
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:CD1	2.45	1.19
15:U:22:GLY:HA2	28:U:903[B]:DMS:H12	1.24	1.19
2:B:347[B]:ARG:NH1	40:B:1031[B]:HOH:O	1.81	1.14
2:B:350:GLU:HG3	28:B:639:DMS:H11	41.70	1.12
12:M:16[B]:LEU:HD13	12:M:16[B]:LEU:HD13	0.00	1.12
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:CD2	0.97	1.12
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:HD21	0.00	1.11
1:A:214:MET:HG2	27:A:411:PL9:H102	1.10	1.10
36:D:409:LHG:H132	36:D:409:LHG:H382	1.25	1.09
36:D:409:LHG:C13	36:D:409:LHG:H382	1.81	1.09
5:E:61:ARG:NH2	40:E:201:HOH:O	1.83	1.08
3:C:362:ARG:HH11	28:C:530:DMS:H11	2.42	1.06
20:C:510:CLA:H41	36:D:408:LHG:H383	29.60	1.05
4:D:233:ARG:HH11	4:D:233:ARG:HG2	4.60	1.02
15:U:86:GLU:HG2	26:U:901:UNL:C16	1.88	1.02
36:D:409:LHG:H302	36:D:409:LHG:H342	1.36	1.02
15:U:22:GLY:HA2	28:U:903[B]:DMS:C1	1.90	1.02
36:D:408:LHG:H132	36:D:408:LHG:C37	11.46	1.00
20:D:404:CLA:HMB1	20:D:404:CLA:HBB1	1.89	0.99
28:B:642:DMS:H22	40:B:755:HOH:O	1.63	0.96
3:C:362:ARG:NH1	28:C:530:DMS:H11	3.02	0.94
2:B:350:GLU:HG3	28:B:639:DMS:C1	41.66	0.93
16:V:90:GLU:HB2	28:V:206:DMS:C1	41.77	0.93
2:B:405:GLU:HG2	40:B:1060:HOH:O	1.68	0.93
36:D:409:LHG:H132	36:D:409:LHG:C38	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:17:LEU:HD23	28:U:903[B]:DMS:H13	1.51	0.92
31:A:421:BCT:O1	4:D:264[A]:LYS:NZ	2.03	0.92
13:O:130[A]:GLN:HE21	13:O:130[A]:GLN:H	1.17	0.91
1:A:214:MET:CG	27:A:411:PL9:H102	2.02	0.89
1:A:214:MET:HG2	27:A:411:PL9:C10	1.99	0.89
20:C:510:CLA:H41	36:D:408:LHG:C38	30.48	0.88
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:HD11	2.35	0.88
2:B:350:GLU:H	28:B:639:DMS:H13	38.66	0.88
20:C:510:CLA:H41	36:D:409:LHG:H381	1.56	0.88
12:M:16[B]:LEU:CD1	12:M:16[B]:LEU:HD13	0.97	0.87
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:CG	2.06	0.86
3:C:362:ARG:HD3	28:C:530:DMS:C1	4.04	0.86
12:M:16[B]:LEU:CD1	12:M:16[B]:LEU:CD1	0.00	0.86
20:A:401:CLA:HBB1	20:A:401:CLA:HMB1	1.57	0.86
20:C:504:CLA:H201	36:D:409:LHG:H352	1.58	0.85
20:C:513:CLA:HMB1	20:C:513:CLA:HBB1	1.96	0.85
3:C:362:ARG:HD3	28:C:530:DMS:H11	3.62	0.83
15:U:9:LEU:HA	28:U:904:DMS:S	2.19	0.83
2:B:389:LYS:HE3	40:B:987:HOH:O	1.79	0.83
31:A:421:BCT:C	4:D:264[A]:LYS:NZ	2.42	0.82
40:C:745:HOH:O	8:I:33:LYS:HE2	1.78	0.82
12:M:16[B]:LEU:HD22	12:M:16[B]:LEU:HD11	2.87	0.82
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.06	0.81
36:E:103:LHG:H321	36:E:103:LHG:H271	1.61	0.81
16:V:90:GLU:HB2	28:V:206:DMS:H13	40.90	0.81
20:C:509:CLA:HBB1	20:C:509:CLA:HMB1	1.64	0.80
36:D:408:LHG:H132	36:D:408:LHG:H372	11.99	0.80
15:U:22:GLY:CA	28:U:903[B]:DMS:H12	2.08	0.80
36:D:408:LHG:H372	36:D:408:LHG:H332	5.71	0.79
13:O:49[A]:THR:HG22	40:O:613:HOH:O	1.82	0.79
2:B:350:GLU:CG	28:B:639:DMS:H11	41.60	0.78
36:D:409:LHG:H302	36:D:409:LHG:C34	2.14	0.78
40:A:511:HOH:O	4:D:139:ARG:HD2	31.41	0.78
12:M:16[B]:LEU:CG	12:M:16[B]:LEU:HD11	2.06	0.78
31:A:421:BCT:C	4:D:264[A]:LYS:HZ3	1.97	0.77
20:C:508:CLA:HBC2	36:D:409:LHG:H371	1.65	0.77
13:O:64:GLU:HG3	40:O:595:HOH:O	1.83	0.77
28:B:634:DMS:H22	40:B:1015:HOH:O	18.03	0.76
2:B:350:GLU:H	28:B:639:DMS:C1	39.54	0.76
2:B:423:LYS:HG3	32:B:622:HTG:H1'2	1.66	0.76
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:CG	1.52	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:D:409:LHG:C30	36:D:409:LHG:H342	2.16	0.75
13:O:231:HIS:HD2	40:O:568:HOH:O	1.70	0.75
28:B:641:DMS:H12	40:B:1079:HOH:O	1.86	0.75
2:B:178:VAL:H	28:B:642:DMS:C2	2.00	0.75
2:B:423:LYS:HE2	40:O:444:HOH:O	57.05	0.74
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.86	0.74
28:O:307:DMS:H23	40:O:515:HOH:O	14.37	0.73
35:D:406:DGD:HD4	5:E:45:ASP:HB3	1.71	0.73
36:D:409:LHG:H131	36:D:409:LHG:H382	1.69	0.73
4:D:12:ARG:HG3	4:D:13:GLY:N	2.04	0.72
15:U:17:LEU:HD23	28:U:903[B]:DMS:C1	2.19	0.72
20:B:614:CLA:HBB1	20:B:614:CLA:HMB1	1.71	0.72
20:C:508:CLA:HBB1	20:C:508:CLA:HMB1	1.88	0.71
4:D:233:ARG:HG2	4:D:233:ARG:NH1	4.75	0.71
4:D:144:ILE:CD1	28:D:414:DMS:O	2.39	0.71
12:M:16[B]:LEU:CD2	12:M:16[B]:LEU:CD2	0.00	0.71
1:A:183:MET:HA	20:A:401:CLA:HMD2	1.73	0.70
20:B:612:CLA:HMB1	20:B:612:CLA:HBB1	1.74	0.70
40:B:755:HOH:O	13:O:57:LYS:HD2	61.41	0.70
2:B:423:LYS:CG	32:B:622:HTG:H1'2	2.23	0.69
7:H:63:LYS:HG3	40:H:257:HOH:O	12.69	0.69
13:O:130[A]:GLN:NE2	13:O:130[A]:GLN:H	1.90	0.69
2:B:82:GLY:O	28:O:308:DMS:S	89.06	0.68
20:A:404:CLA:HBB1	20:A:404:CLA:HMB1	2.16	0.68
36:D:408:LHG:H132	36:D:408:LHG:H371	11.31	0.68
21:A:403:PHO:HMB1	21:A:403:PHO:HBB1	1.76	0.68
3:C:362:ARG:HH11	28:C:530:DMS:C1	3.09	0.68
31:A:421:BCT:O3	4:D:264[A]:LYS:NZ	2.27	0.68
4:D:12:ARG:HG3	4:D:13:GLY:H	1.56	0.68
13:O:49[A]:THR:HG23	40:O:437:HOH:O	1.93	0.68
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.74	0.67
20:B:604:CLA:HMB1	20:B:604:CLA:HBB1	1.97	0.67
20:C:508:CLA:CBC	36:D:409:LHG:H371	2.25	0.67
20:C:508:CLA:HBC2	36:D:408:LHG:H361	27.86	0.67
7:H:59:ASN:HD22	7:H:64:ALA:HB3	1.60	0.67
2:B:409:GLN:HE21	28:B:644:DMS:C1	2.08	0.66
13:O:15:LEU:HD23	13:O:18:LYS:HD2	1.76	0.66
15:U:17:LEU:CD2	28:U:903[B]:DMS:C1	2.74	0.66
2:B:462:PHE:CE1	20:B:615:CLA:HMB3	14.78	0.66
28:C:532:DMS:H22	40:C:603:HOH:O	1.95	0.66
20:C:510:CLA:HBB1	20:C:510:CLA:HMB1	1.88	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:367:GLU:HB2	28:C:531:DMS:C2	2.26	0.65
2:B:341:LYS:NZ	32:B:622:HTG:S1	2.62	0.65
2:B:472:ARG:HG2	28:D:414:DMS:C1	2.26	0.65
2:B:405:GLU:OE1	2:B:431[A]:GLU:OE1	2.14	0.65
20:B:615:CLA:HBB1	20:B:615:CLA:HMB1	2.11	0.65
2:B:178:VAL:H	28:B:642:DMS:H21	1.60	0.65
16:V:90:GLU:CB	28:V:206:DMS:C1	41.68	0.65
20:B:601:CLA:H43	20:B:601:CLA:HED2	1.79	0.65
20:B:602:CLA:H42	40:B:1029:HOH:O	1.97	0.65
21:D:403:PHO:HMB1	21:D:403:PHO:HBB1	1.77	0.65
2:B:409:GLN:HE21	28:B:644:DMS:H11	1.62	0.64
36:D:409:LHG:H362	36:D:409:LHG:H152	1.80	0.64
20:C:506:CLA:HMC2	20:C:507:CLA:H102	1.79	0.64
5:E:15:THR:HB	9:J:8:ILE:O	1.97	0.64
3:C:362:ARG:HD3	28:C:530:DMS:H13	4.96	0.64
3:C:367:GLU:HB2	28:C:531:DMS:H21	1.80	0.64
20:B:606:CLA:C14	20:B:611:CLA:HED2	2.28	0.63
22:T:101:BCR:HC8	22:T:101:BCR:H321	1.80	0.63
20:C:506:CLA:HBB1	20:C:506:CLA:HMB1	1.78	0.63
5:E:10:PHE:H	36:E:103:LHG:HC32	1.64	0.63
3:C:117:VAL:CG1	24:C:524:LMG:H202	2.28	0.63
40:B:980:HOH:O	28:D:414:DMS:C2	2.46	0.63
2:B:472:ARG:HG2	28:D:414:DMS:H13	1.79	0.63
20:B:616:CLA:HMB1	20:B:616:CLA:HBB1	1.80	0.63
22:T:101:BCR:HC8	22:T:101:BCR:H311	2.12	0.62
1:A:98[A]:GLU:OE2	40:A:501:HOH:O	2.11	0.62
22:B:618:BCR:H331	22:B:618:BCR:C8	2.29	0.62
13:O:231:HIS:HD2	28:O:306:DMS:O	17.57	0.62
20:C:505:CLA:HBB1	20:C:505:CLA:HMB1	1.85	0.61
1:A:265:PHE:HE2	27:A:411:PL9:H122	1.64	0.61
20:B:606:CLA:HMD2	20:B:614:CLA:H203	18.94	0.61
36:D:409:LHG:C30	36:D:409:LHG:C34	2.75	0.61
2:B:248:ALA:HA	20:B:605:CLA:H42	11.32	0.61
20:B:601:CLA:H201	26:B:628:UNL:C15	2.31	0.61
28:C:527:DMS:H22	40:C:797:HOH:O	2.01	0.61
12:M:16[B]:LEU:CG	12:M:16[B]:LEU:CD1	1.52	0.61
20:D:402:CLA:HBB1	20:D:402:CLA:HMB1	1.82	0.61
20:B:601:CLA:HMB1	20:B:601:CLA:HBB1	1.82	0.60
28:F:102:DMS:C1	16:V:27:LEU:HD21	2.31	0.60
13:O:49[B]:THR:HG23	13:O:236:GLN:HB2	1.81	0.60
24:A:407:LMG:H422	24:A:407:LMG:C25	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:86:GLU:H	26:U:901:UNL:C16	2.15	0.60
28:F:102:DMS:H11	16:V:27:LEU:HD21	1.84	0.60
20:C:506:CLA:H92	34:I:101:LMT:H111	1.84	0.60
40:A:511:HOH:O	4:D:139:ARG:CD	31.87	0.59
13:O:231:HIS:CD2	40:O:568:HOH:O	2.50	0.59
2:B:410:THR:H	28:B:640:DMS:H22	84.48	0.59
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.84	0.59
27:A:411:PL9:H162	36:E:103:LHG:H322	1.84	0.59
2:B:350:GLU:N	28:B:639:DMS:C1	39.55	0.59
20:C:504:CLA:C20	36:D:409:LHG:H352	2.30	0.59
19:Z:44:SER:O	19:Z:48:ILE:HG13	2.83	0.59
3:C:117:VAL:HG12	24:C:524:LMG:H202	1.84	0.58
4:D:144:ILE:HD11	28:D:414:DMS:O	2.01	0.58
7:H:59:ASN:HD22	7:H:64:ALA:CB	2.16	0.58
20:B:613:CLA:HBB1	20:B:613:CLA:HMB1	2.00	0.58
16:V:90:GLU:HB2	28:V:206:DMS:H11	42.42	0.58
20:B:611:CLA:H203	20:B:611:CLA:H151	1.84	0.58
5:E:9:PRO:HA	36:E:103:LHG:HC32	1.84	0.58
20:B:605:CLA:H43	20:B:606:CLA:H2	1.85	0.58
13:O:42:ARG:O	13:O:241:ALA:HA	2.24	0.58
20:C:511:CLA:HMB1	20:C:511:CLA:HBB1	1.86	0.58
2:B:103:LEU:HD21	20:B:606:CLA:HMC3	1.86	0.58
20:C:508:CLA:HMD2	36:D:408:LHG:H382	27.01	0.58
27:A:411:PL9:H502	4:D:39:PRO:HG3	1.86	0.57
23:A:406:SQD:C12	23:A:406:SQD:H162	2.34	0.57
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.87	0.57
20:C:501:CLA:H192	20:C:506:CLA:C1B	2.78	0.57
16:V:106[A]:ASN:OD1	40:V:301:HOH:O	2.17	0.57
2:B:224[B]:ARG:NH2	40:B:702:HOH:O	2.37	0.57
28:B:635:DMS:H13	40:B:902:HOH:O	2.03	0.57
3:C:182:PHE:HA	32:C:520:HTG:H61	2.18	0.57
20:C:512:CLA:HMB1	20:C:512:CLA:HBB1	1.87	0.56
22:B:619:BCR:C8	22:B:619:BCR:H331	2.34	0.56
35:C:516:DGD:HAT2	35:C:517:DGD:HBH2	26.11	0.56
34:J:103:LMT:H123	26:J:107:UNL:C3	2.35	0.56
28:O:306:DMS:H23	40:O:607:HOH:O	41.06	0.56
20:B:601:CLA:C20	26:B:628:UNL:C15	2.83	0.56
2:B:178:VAL:H	28:B:642:DMS:H23	1.70	0.56
16:V:5:PRO:HD3	28:V:206:DMS:H23	1.87	0.56
20:C:501:CLA:H42	20:C:502:CLA:HMD1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:D:408:LHG:H132	36:D:408:LHG:C38	12.32	0.56
24:C:519:LMG:H221	10:K:30:VAL:HG11	1.87	0.56
15:U:17:LEU:CD2	28:U:903[B]:DMS:H13	2.28	0.55
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.88	0.55
23:F:101:SQD:H461	40:X:201:HOH:O	2.07	0.55
22:C:515:BCR:C8	22:C:515:BCR:H331	2.36	0.55
4:D:140:PRO:HD2	28:D:414:DMS:C2	2.37	0.55
24:C:519:LMG:H242	9:J:22:ILE:HD13	1.88	0.55
22:D:405:BCR:H313	35:D:406:DGD:HAW2	1.88	0.55
3:C:279:LEU:HD12	3:C:282:MET:CE	2.37	0.54
13:O:39:ARG:HH11	13:O:82:GLN:HE21	1.54	0.54
15:U:10:VAL:H	28:U:904:DMS:C2	2.20	0.54
22:D:405:BCR:H331	22:D:405:BCR:C8	2.44	0.54
7:H:2:ALA:N	40:H:201:HOH:O	2.41	0.54
28:C:530:DMS:H13	40:O:417:HOH:O	31.80	0.54
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.89	0.54
2:B:171:PRO:HB3	7:H:63:LYS:HA	1.90	0.54
3:C:409:GLY:HA2	28:C:532:DMS:S	2.48	0.54
13:O:244:GLU:HG2	28:O:307:DMS:H11	1.90	0.54
23:A:406:SQD:H162	23:A:406:SQD:H122	1.90	0.53
7:H:59:ASN:ND2	7:H:64:ALA:HB3	2.23	0.53
40:C:745:HOH:O	8:I:33:LYS:CE	2.47	0.53
27:A:411:PL9:H151	36:E:103:LHG:H331	1.90	0.53
20:B:616:CLA:H111	20:B:616:CLA:H161	5.44	0.53
20:A:404:CLA:HMD3	4:D:182:LEU:HD11	40.36	0.53
28:C:532:DMS:C2	40:C:603:HOH:O	2.55	0.53
1:A:237:TYR:CZ	4:D:264[B]:LYS:HG3	2.44	0.53
3:C:38:GLY:HA3	20:C:511:CLA:HMD3	2.05	0.53
13:O:141:ASP:HB2	28:O:310:DMS:C1	2.39	0.53
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.54	0.53
20:B:604:CLA:C4D	20:B:606:CLA:H43	2.38	0.53
19:Z:3:ILE:HA	40:Z:201:HOH:O	13.17	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.43	0.53
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.91	0.53
2:B:462:PHE:CZ	20:B:615:CLA:HMB3	14.35	0.53
3:C:150:ASP:OD2	40:C:601:HOH:O	2.19	0.53
2:B:36[A]:SER:OG	22:B:618:BCR:H362	2.08	0.52
28:O:307:DMS:C2	40:O:488:HOH:O	57.38	0.52
20:B:607:CLA:HBB1	20:B:607:CLA:HHC	4.27	0.52
2:B:237:VAL:HG12	20:B:613:CLA:HMD1	1.91	0.52
3:C:371:GLY:HA3	40:C:622:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:362:ARG:CD	28:C:530:DMS:H11	3.84	0.52
13:O:129:THR:HA	13:O:141:ASP:O	2.22	0.52
4:D:13:GLY:HA3	32:D:417:HTG:H62	1.91	0.52
31:A:421:BCT:C	4:D:264[A]:LYS:HZ1	2.12	0.52
40:B:1009[B]:HOH:O	28:D:413:DMS:H12	2.09	0.52
13:O:231:HIS:HE1	40:O:498:HOH:O	37.43	0.52
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.76	0.52
20:C:508:CLA:CBC	36:D:408:LHG:H361	27.73	0.52
3:C:126:GLY:O	3:C:130:VAL:HG23	2.53	0.51
20:C:502:CLA:H61	20:C:512:CLA:H42	2.08	0.51
2:B:410:THR:H	28:B:640:DMS:C2	83.83	0.51
3:C:179:ALA:O	3:C:184:GLY:HA2	2.30	0.51
22:T:101:BCR:H23C	22:T:101:BCR:H382	1.92	0.51
20:C:504:CLA:H202	36:D:409:LHG:H361	1.92	0.51
3:C:437:PHE:CZ	20:C:510:CLA:HMB3	2.46	0.51
4:D:99:GLY:O	35:D:406:DGD:HA21	2.10	0.51
2:B:472:ARG:CG	28:D:414:DMS:C1	3.18	0.51
17:Y:18:VAL:N	40:Y:101:HOH:O	38.27	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
20:A:402:CLA:HMD3	4:D:182:LEU:HD11	1.94	0.50
23:A:412:SQD:H442	40:A:661:HOH:O	2.11	0.50
2:B:423:LYS:HE2	40:B:886:HOH:O	2.10	0.50
2:B:462:PHE:CE1	20:B:614:CLA:HMB3	2.46	0.50
1:A:215:HIS:HA	27:A:411:PL9:O1	2.11	0.50
20:B:609:CLA:HMB1	20:B:609:CLA:HBB1	1.92	0.50
20:C:502:CLA:HBB1	20:C:502:CLA:HMB1	2.46	0.50
4:D:236:ASN:O	4:D:239:GLN:HG2	2.37	0.50
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.27	0.50
13:O:223:ASP:OD2	28:O:305:DMS:H11	2.12	0.50
20:B:607:CLA:C14	20:B:612:CLA:HED2	40.42	0.50
4:D:12:ARG:CG	4:D:13:GLY:H	2.18	0.50
20:C:504:CLA:H191	36:D:408:LHG:H362	27.75	0.50
23:A:406:SQD:H142	36:D:409:LHG:H161	1.94	0.49
15:U:16:LYS:NZ	40:U:1004:HOH:O	2.45	0.49
15:U:17:LEU:CD2	28:U:903[B]:DMS:H11	2.41	0.49
28:D:415:DMS:H23	40:O:656:HOH:O	2.12	0.49
2:B:224[B]:ARG:HH11	34:B:625:LMT:H2'	1.76	0.49
35:C:517:DGD:HBF1	36:D:408:LHG:H223	35.73	0.49
17:Y:18:VAL:O	17:Y:22:LEU:HD12	2.12	0.49
12:M:5:GLN:HE21	12:M:5:GLN:H	1.60	0.49
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:GLU:HG3	28:B:637:DMS:O	2.12	0.49
3:C:406:SER:HA	3:C:420:VAL:HG23	2.02	0.49
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.48	0.49
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.94	0.49
20:B:610:CLA:HMB2	20:B:611:CLA:C2B	2.43	0.49
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.93	0.49
20:C:510:CLA:H41	36:D:409:LHG:C38	2.35	0.49
5:E:10:PHE:H	36:E:103:LHG:C3	2.24	0.49
4:D:272:LEU:HD23	4:D:272:LEU:C	2.38	0.48
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.95	0.48
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.94	0.48
16:V:122:GLU:HG3	16:V:126:LEU:HD12	2.12	0.48
1:A:229:GLU:HG2	40:A:577:HOH:O	2.13	0.48
2:B:409:GLN:NE2	28:B:644:DMS:C1	2.76	0.48
21:A:403:PHO:NC	21:A:403:PHO:ND	2.62	0.48
24:A:407:LMG:H201	24:A:407:LMG:H231	1.56	0.48
28:C:530:DMS:C1	40:O:417:HOH:O	31.26	0.48
23:A:412:SQD:H272	2:B:109:LEU:HD13	59.85	0.48
20:C:510:CLA:H52	36:D:409:LHG:H372	1.95	0.48
4:D:13:GLY:HA3	32:D:417:HTG:C6	2.43	0.48
2:B:472:ARG:HG2	28:D:414:DMS:H11	2.20	0.48
1:A:215:HIS:ND1	27:A:411:PL9:O1	2.39	0.48
2:B:90:PHE:H	32:B:632:HTG:H62	1.78	0.48
40:B:980:HOH:O	28:D:414:DMS:H23	2.09	0.48
17:Y:44:GLY:HA2	19:Z:30:PRO:HD3	2.60	0.48
27:A:411:PL9:H403	6:F:22:ALA:HB2	1.96	0.48
2:B:472:ARG:HG3	28:D:414:DMS:C1	3.72	0.48
2:B:162:PHE:O	20:B:608:CLA:HHD	31.20	0.48
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.95	0.48
19:Z:15:LEU:HD22	19:Z:46:LEU:HD23	3.75	0.48
3:C:60:ILE:HG22	20:C:503:CLA:HHD	1.95	0.48
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.01	0.48
15:U:17:LEU:HD22	28:U:903[B]:DMS:H11	1.95	0.48
3:C:437:PHE:CE1	20:C:510:CLA:HMB3	2.51	0.47
3:C:364:PRO:HA	28:C:531:DMS:C2	2.44	0.47
20:A:401:CLA:CBD	20:D:402:CLA:HAC2	2.44	0.47
13:O:231:HIS:CD2	28:O:306:DMS:O	17.86	0.47
12:M:16[B]:LEU:HD21	12:M:16[B]:LEU:CD1	2.59	0.47
13:O:244:GLU:HG2	28:O:307:DMS:C1	2.43	0.47
36:D:408:LHG:H372	36:D:408:LHG:C33	5.08	0.47
16:V:5:PRO:HD3	28:V:206:DMS:C2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ALA:HA	20:B:604:CLA:H42	1.96	0.47
20:B:605:CLA:H93	20:B:606:CLA:HAB	1.96	0.47
20:C:502:CLA:H193	32:C:520:HTG:H3'1	1.95	0.47
5:E:68:ASP:O	5:E:72:ALA:HB2	2.15	0.47
3:C:390:ARG:HD3	16:V:100:ILE:HD12	2.11	0.47
20:C:513:CLA:C4B	22:C:514:BCR:H383	2.43	0.47
3:C:318:LEU:C	3:C:318:LEU:HD23	2.34	0.47
40:B:980:HOH:O	28:D:414:DMS:H21	2.11	0.47
28:V:205:DMS:H22	40:V:343:HOH:O	2.15	0.47
20:C:504:CLA:C19	36:D:408:LHG:H362	28.68	0.47
3:C:53:HIS:CB	20:C:512:CLA:HMD1	2.52	0.47
22:A:405:BCR:H23C	22:A:405:BCR:H382	1.97	0.46
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.50	0.46
3:C:364:PRO:HA	28:C:531:DMS:H23	1.97	0.46
13:O:39:ARG:HH11	13:O:82:GLN:NE2	2.13	0.46
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.28	0.46
36:D:408:LHG:H161	36:D:408:LHG:H331	7.32	0.46
4:D:140:PRO:HD2	28:D:414:DMS:H21	1.96	0.46
10:K:11:LEU:HD11	10:K:22:VAL:HG21	2.13	0.46
22:T:101:BCR:C23	22:T:101:BCR:H382	2.45	0.46
20:B:611:CLA:CBB	20:B:611:CLA:HHC	2.44	0.46
20:C:512:CLA:C1B	22:K:102:BCR:H401	25.06	0.46
3:C:334:PRO:HA	13:O:153:THR:OG1	2.16	0.46
13:O:49[B]:THR:CG2	13:O:236:GLN:HB2	2.46	0.46
2:B:286:ARG:HH11	2:B:286:ARG:HG2	1.80	0.46
2:B:30:VAL:HG12	20:B:606:CLA:HHD	1.98	0.46
13:O:141:ASP:HB2	28:O:310:DMS:H11	1.97	0.46
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.61	0.46
15:U:22:GLY:HA2	28:U:903[B]:DMS:H11	1.90	0.46
15:U:21:TYR:O	28:U:903[B]:DMS:H12	2.15	0.46
2:B:26:HIS:HB2	20:B:613:CLA:HMB2	1.98	0.46
28:B:641:DMS:C1	40:B:931:HOH:O	2.64	0.46
20:A:401:CLA:CAD	20:D:402:CLA:HAC2	2.46	0.46
4:D:52:THR:O	4:D:66:SER:HA	2.33	0.46
28:A:416:DMS:H12	8:I:5:LYS:NZ	2.31	0.46
2:B:306:PRO:HA	28:B:641:DMS:H11	1.97	0.46
4:D:85:MET:HE3	4:D:96:GLU:HG2	2.11	0.46
26:U:901:UNL:C15	40:U:1118:HOH:O	2.63	0.46
2:B:420:TYR:CD1	32:B:622:HTG:H1'1	2.50	0.46
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.71	0.46
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:101:BCR:C8	22:K:101:BCR:H331	3.41	0.46
1:A:96:ILE:HD12	20:A:404:CLA:HMD1	1.98	0.46
20:B:612:CLA:HHC	20:B:612:CLA:HBB1	4.59	0.45
28:B:641:DMS:H21	40:B:706:HOH:O	70.28	0.45
15:U:10:VAL:HG11	15:U:15:GLU:OE1	2.16	0.45
2:B:208:VAL:HG21	20:B:603:CLA:HMC1	1.99	0.45
4:D:103:ARG:O	4:D:107:LEU:HG	2.17	0.45
22:A:405:BCR:H371	22:A:405:BCR:H24C	1.78	0.45
2:B:204:ALA:CB	20:B:603:CLA:HAB	2.47	0.45
2:B:55:MET:CE	2:B:80:ILE:HG12	2.71	0.45
4:D:246:MET:HB2	4:D:264[B]:LYS:HE2	1.99	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45
8:I:26:GLY:HA3	34:I:101:LMT:H6'1	1.99	0.45
34:B:626:LMT:H123	14:T:8:PHE:HA	30.03	0.45
13:O:86:LYS:HD3	40:O:449:HOH:O	2.17	0.45
24:C:519:LMG:H221	10:K:30:VAL:CG1	2.46	0.45
28:C:533:DMS:H11	40:C:816:HOH:O	28.51	0.45
20:C:504:CLA:H42	35:C:516:DGD:HB31	25.40	0.45
2:B:103:LEU:HD21	20:B:607:CLA:HMC3	14.80	0.44
22:K:101:BCR:HC7	22:K:101:BCR:H331	1.67	0.44
15:U:10:VAL:H	28:U:904:DMS:H21	1.81	0.44
20:A:402:CLA:HAB	20:A:402:CLA:HHC	1.82	0.44
32:B:631:HTG:C6	40:B:829:HOH:O	2.64	0.44
22:C:514:BCR:H341	22:C:514:BCR:H11C	2.05	0.44
28:B:641:DMS:H12	40:B:941:HOH:O	20.10	0.44
19:Z:31:GLN:O	19:Z:33:TRP:N	2.79	0.44
22:A:405:BCR:C23	22:A:405:BCR:H382	2.48	0.44
2:B:497:GLN:HB2	2:B:504:THR:HB	2.00	0.44
20:C:506:CLA:HMB2	20:C:507:CLA:NB	2.36	0.44
19:Z:26:ALA:HB3	19:Z:40:ILE:HD11	2.16	0.44
1:A:15:GLU:HG3	40:I:201:HOH:O	2.16	0.44
23:F:101:SQD:H262	23:F:101:SQD:O10	3.37	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.65	0.44
20:B:606:CLA:H41	20:B:606:CLA:H62	1.79	0.44
20:B:610:CLA:H161	20:B:610:CLA:H141	2.86	0.44
28:B:635:DMS:C2	40:B:731:HOH:O	32.04	0.44
20:C:509:CLA:HMB1	20:C:509:CLA:CBB	2.43	0.44
28:O:307:DMS:H22	40:O:488:HOH:O	57.28	0.44
20:C:505:CLA:HMD2	22:C:515:BCR:H343	2.00	0.44
36:D:408:LHG:H381	36:D:408:LHG:H122	15.99	0.44
8:I:2:GLU:O	8:I:6:ILE:HG12	4.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:60:ARG:O	13:O:61:GLN:CB	3.03	0.44
20:B:612:CLA:C15	20:B:612:CLA:H203	3.67	0.44
3:C:276:LEU:HD23	20:C:509:CLA:HED1	2.00	0.44
36:D:408:LHG:H132	36:D:408:LHG:H381	13.15	0.44
12:M:5:GLN:HE21	12:M:5:GLN:N	2.14	0.44
28:O:307:DMS:H21	40:O:488:HOH:O	58.26	0.44
35:H:102:DGD:HAN2	35:H:102:DGD:HAW2	1.89	0.43
2:B:409:GLN:NE2	28:B:644:DMS:H12	2.33	0.43
20:B:606:CLA:H43	20:B:607:CLA:H2	14.96	0.43
24:A:407:LMG:H292	3:C:216:SER:HA	2.00	0.43
24:A:407:LMG:H321	3:C:217:PRO:HD3	2.01	0.43
3:C:31:SER:CB	3:C:41:ARG:HG2	2.48	0.43
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.43
4:D:26:ARG:HA	5:E:5:THR:HB	1.99	0.43
4:D:85:MET:CE	4:D:96:GLU:HG2	2.53	0.43
4:D:209:LEU:HD23	4:D:209:LEU:C	2.39	0.43
4:D:244:TYR:OH	4:D:264[A]:LYS:NZ	2.46	0.43
6:F:21:VAL:HG21	23:F:101:SQD:H241	5.29	0.43
3:C:95:LEU:HD21	20:C:501:CLA:OBD	2.18	0.43
21:D:403:PHO:HHD	21:D:403:PHO:HBC2	2.00	0.43
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.01	0.43
3:C:221:GLU:O	3:C:226:SER:HB3	2.18	0.43
32:D:417:HTG:H61	40:D:591:HOH:O	2.18	0.43
13:O:39:ARG:HB2	13:O:83:GLY:O	2.19	0.43
28:C:527:DMS:C2	40:C:797:HOH:O	2.61	0.43
3:C:409:GLY:HA2	28:C:532:DMS:C1	2.49	0.43
16:V:45:ILE:HG12	40:V:469:HOH:O	2.18	0.43
20:B:611:CLA:HBB1	20:B:611:CLA:HHC	2.00	0.43
28:B:641:DMS:H11	40:B:931:HOH:O	2.18	0.43
5:E:27:ILE:HG12	37:E:104:HEM:HMC3	2.00	0.42
40:B:732:HOH:O	13:O:57:LYS:HD2	43.77	0.42
22:B:619:BCR:C23	22:B:619:BCR:H383	2.49	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.24	0.42
2:B:472:ARG:CG	28:D:414:DMS:H12	3.27	0.42
2:B:479:PHE:HA	40:B:980:HOH:O	2.19	0.42
32:B:622:HTG:H6'2	32:B:622:HTG:H3'2	1.28	0.42
3:C:472:LEU:HD11	4:D:255:GLN:HG3	2.01	0.42
3:C:48:LYS:HG2	3:C:133:ALA:O	2.36	0.42
22:T:101:BCR:C38	22:T:101:BCR:C23	2.97	0.42
4:D:24:ARG:NH2	18:X:35:ASP:O	4.42	0.42
20:B:607:CLA:HHC	20:B:607:CLA:CBB	3.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:501:CLA:HMD2	20:C:502:CLA:H101	2.00	0.42
28:F:102:DMS:H13	16:V:27:LEU:HD21	2.01	0.42
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.08	0.42
20:B:605:CLA:HMB1	20:B:605:CLA:HBB1	2.00	0.42
2:B:341:LYS:NZ	32:B:622:HTG:O2	2.37	0.42
2:B:82:GLY:O	28:B:641:DMS:O	16.59	0.42
22:K:102:BCR:H341	22:K:102:BCR:H11C	1.95	0.42
13:O:180:GLU:O	28:O:303:DMS:H23	53.15	0.42
2:B:498:LYS:HA	4:D:24:ARG:HA	2.29	0.42
20:B:601:CLA:H41	20:B:601:CLA:H62	1.46	0.42
2:B:467:ILE:HG12	4:D:126:MET:HE1	3.71	0.42
22:B:618:BCR:H382	22:T:101:BCR:H11C	46.30	0.42
3:C:279:LEU:HD22	20:C:509:CLA:HED2	2.01	0.42
3:C:381:LYS:NZ	13:O:99:ASP:OD1	2.45	0.42
20:B:602:CLA:H161	20:B:602:CLA:H143	1.89	0.42
3:C:266:TRP:CZ3	20:C:507:CLA:HAC2	2.61	0.42
36:D:408:LHG:H141	36:D:408:LHG:H111	4.45	0.42
2:B:80:ILE:HA	2:B:80:ILE:HD12	1.80	0.42
2:B:422:ARG:O	2:B:425:ILE:HG12	2.20	0.42
2:B:157:HIS:C	2:B:157:HIS:CD2	2.94	0.41
20:B:604:CLA:H151	20:B:604:CLA:H111	3.19	0.41
20:C:501:CLA:C4D	20:C:503:CLA:H2	2.49	0.41
4:D:23:LYS:HD3	4:D:135:LEU:HD21	2.37	0.41
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.19	0.41
34:B:627:LMT:H12	12:M:6:LEU:HD11	2.01	0.41
13:O:69:LYS:HE2	40:O:480:HOH:O	2.19	0.41
2:B:445:THR:HA	40:B:709:HOH:O	19.79	0.41
35:H:102:DGD:HE5	40:H:238:HOH:O	2.19	0.41
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.67	0.41
16:V:79:PRO:HD3	16:V:94:SER:HB3	2.10	0.41
20:B:607:CLA:H202	32:B:632:HTG:H61	2.01	0.41
20:B:608:CLA:H111	20:B:608:CLA:H93	3.90	0.41
2:B:467:ILE:HG12	4:D:126:MET:CE	4.15	0.41
5:E:63:ILE:HG23	5:E:64:PRO:HD2	2.02	0.41
8:I:33:LYS:HB3	8:I:34:ARG:H	1.70	0.41
22:K:101:BCR:H371	22:K:101:BCR:H24C	1.97	0.41
37:E:104:HEM:HMC1	6:F:31:ILE:HG13	2.03	0.41
28:B:635:DMS:H12	40:B:763:HOH:O	2.21	0.41
2:B:81:THR:HG21	28:B:642:DMS:S	2.60	0.41
22:K:101:BCR:C8	22:K:101:BCR:H311	2.50	0.41
13:O:183:ALA:HB3	28:O:303:DMS:H23	50.06	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:SER:HB2	20:A:401:CLA:H43	2.03	0.41
22:D:405:BCR:HC21	35:D:406:DGD:HAT2	2.02	0.41
28:D:415:DMS:H12	40:M:205:HOH:O	2.20	0.41
10:K:17:ILE:HG23	10:K:18:PHE:CD2	2.74	0.41
28:U:902:DMS:H22	40:U:1046:HOH:O	2.21	0.41
1:A:11:ALA:HB1	1:A:15:GLU:OE1	2.20	0.41
22:B:619:BCR:H371	22:B:619:BCR:H24C	1.82	0.41
22:C:514:BCR:H351	22:C:514:BCR:H15C	1.92	0.41
1:A:221:SER:HB2	4:D:139:ARG:O	2.21	0.41
2:B:12:LEU:HB2	20:B:614:CLA:HMC2	19.64	0.41
20:B:613:CLA:H72	20:B:613:CLA:H112	4.72	0.41
20:C:509:CLA:H91	20:C:509:CLA:H111	1.89	0.41
20:C:513:CLA:HBC2	32:C:534:HTG:H6'2	2.03	0.41
36:D:409:LHG:H362	36:D:409:LHG:H332	1.81	0.41
3:C:377:LEU:HB3	13:O:80:GLN:OE1	2.21	0.41
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.50	0.41
2:B:498:LYS:HE3	4:D:20:ASP:HA	2.02	0.41
22:K:101:BCR:H361	22:K:101:BCR:H20C	2.16	0.41
3:C:406:SER:O	3:C:418:ASN:HA	2.30	0.41
5:E:60:GLN:O	5:E:61:ARG:NE	2.54	0.41
15:U:21:TYR:CD1	28:U:903[B]:DMS:H13	2.56	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.95	0.40
2:B:347[B]:ARG:HG2	2:B:353:GLU:HA	2.04	0.40
3:C:156:LYS:HE3	40:C:675:HOH:O	49.28	0.40
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.56	0.40
13:O:98:GLU:HG3	40:O:418:HOH:O	2.21	0.40
1:A:202:VAL:HG11	20:A:402:CLA:C3D	2.51	0.40
20:B:604:CLA:CMB	20:B:604:CLA:HBB1	2.69	0.40
32:B:622:HTG:C7'	40:O:407:HOH:O	2.69	0.40
3:C:38:GLY:O	3:C:41:ARG:HB2	2.22	0.40
20:D:401:CLA:HHD	20:D:401:CLA:HBC3	2.04	0.40
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.35	0.40
22:A:405:BCR:C23	22:A:405:BCR:C38	2.98	0.40
2:B:286:ARG:NH1	2:B:286:ARG:HG2	2.37	0.40
20:D:402:CLA:H162	20:D:402:CLA:H203	1.80	0.40
20:D:404:CLA:CMB	20:D:404:CLA:HBB1	2.70	0.40
13:O:183:ALA:HB3	28:O:303:DMS:C2	50.26	0.40
28:O:308:DMS:H13	40:O:648:HOH:O	2.21	0.40
16:V:45:ILE:HD12	16:V:45:ILE:C	2.59	0.40
1:A:265:PHE:HE2	27:A:411:PL9:C12	2.32	0.40
20:B:604:CLA:H111	20:B:604:CLA:H91	3.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:ARG:NH1	20:C:511:CLA:HMD1	2.40	0.40
35:D:406:DGD:C4D	5:E:45:ASP:HB3	2.47	0.40
6:F:36:ALA:O	6:F:40:MET:HG3	2.47	0.40
13:O:81:ILE:HA	13:O:100:GLY:HA3	2.05	0.40
13:O:93:LEU:O	13:O:128:SER:HA	2.34	0.40
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.93	0.40
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.04	0.40
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.57	0.40
2:B:341:LYS:HZ1	32:B:622:HTG:C2	2.30	0.40
2:B:26:HIS:HB2	20:B:614:CLA:HMB2	8.70	0.40
20:C:507:CLA:H41	20:C:507:CLA:H61	1.84	0.40
22:K:102:BCR:H24C	22:K:102:BCR:H371	1.86	0.40
22:T:101:BCR:H311	22:T:101:BCR:C8	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	46	29
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	46	29
2	B	514/505 (102%)	503 (98%)	11 (2%)	0	100	100
2	b	493/505 (98%)	485 (98%)	8 (2%)	0	100	100
3	C	450/455 (99%)	436 (97%)	13 (3%)	1 (0%)	52	36
3	c	454/455 (100%)	442 (97%)	11 (2%)	1 (0%)	52	36
4	D	341/342 (100%)	334 (98%)	6 (2%)	1 (0%)	46	29
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	78/83 (94%)	78 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	31/44 (70%)	31 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	247/244 (101%)	235 (95%)	11 (4%)	1 (0%)	39	22
13	o	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	16	4
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	138/137 (101%)	133 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	5	0
All	All	5201/5350 (97%)	5069 (98%)	120 (2%)	12 (0%)	52	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
19	z	32	ASP
3	C	416	SER
4	D	12	ARG
13	O	61	GLN
3	c	416	SER
19	z	31	GLN
19	Z	30	PRO
13	o	34	SER
13	o	61	GLN
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	269/279 (96%)	268 (100%)	1 (0%)	93 92
1	a	270/279 (97%)	270 (100%)	0	100 100
2	B	405/403 (100%)	401 (99%)	4 (1%)	82 76
2	b	390/403 (97%)	386 (99%)	4 (1%)	82 76
3	C	351/356 (99%)	349 (99%)	2 (1%)	90 87
3	c	356/356 (100%)	351 (99%)	5 (1%)	74 63
4	D	277/277 (100%)	274 (99%)	3 (1%)	80 72
4	d	276/277 (100%)	272 (99%)	4 (1%)	74 63
5	E	68/72 (94%)	65 (96%)	3 (4%)	35 15
5	e	68/72 (94%)	63 (93%)	5 (7%)	17 4
6	F	27/38 (71%)	26 (96%)	1 (4%)	41 20
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	41 20
7	h	54/54 (100%)	53 (98%)	1 (2%)	65 49
8	I	30/34 (88%)	30 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	i	32/34 (94%)	29 (91%)	3 (9%)	11 1
9	J	23/28 (82%)	22 (96%)	1 (4%)	35 16
9	j	24/28 (86%)	24 (100%)	0	100 100
10	K	30/30 (100%)	30 (100%)	0	100 100
10	k	28/30 (93%)	27 (96%)	1 (4%)	42 21
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	33/35 (94%)	33 (100%)	0	100 100
12	M	30/33 (91%)	29 (97%)	1 (3%)	45 25
12	m	30/33 (91%)	30 (100%)	0	100 100
13	O	207/207 (100%)	202 (98%)	5 (2%)	57 39
13	o	199/207 (96%)	197 (99%)	2 (1%)	82 76
14	T	26/28 (93%)	23 (88%)	3 (12%)	7 1
14	t	26/28 (93%)	25 (96%)	1 (4%)	40 19
15	U	82/89 (92%)	82 (100%)	0	100 100
15	u	83/89 (93%)	81 (98%)	2 (2%)	57 39
16	V	120/117 (103%)	119 (99%)	1 (1%)	86 82
16	v	114/117 (97%)	113 (99%)	1 (1%)	84 79
17	Y	21/23 (91%)	19 (90%)	2 (10%)	11 1
17	y	21/23 (91%)	21 (100%)	0	100 100
18	X	29/33 (88%)	29 (100%)	0	100 100
18	x	27/33 (82%)	27 (100%)	0	100 100
19	Z	44/52 (85%)	43 (98%)	1 (2%)	58 41
19	z	39/52 (75%)	37 (95%)	2 (5%)	29 11
All	All	4223/4376 (96%)	4162 (99%)	61 (1%)	76 63

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
2	B	80	ILE
2	B	246	PHE
2	B	307[A]	GLU
2	B	307[B]	GLU
3	C	289	PHE

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Mol	Chain	Res	Type
3	C	315	MET
4	D	26	ARG
4	D	90	LEU
4	D	180	ARG
5	E	4	THR
5	E	25	ILE
5	E	61	ARG
6	F	44	GLN
7	H	49	TYR
7	H	63	LYS
9	J	10	LEU
12	M	5	GLN
13	O	23	ASP
13	O	24	ASP
13	O	118	LEU
13	O	130[A]	GLN
13	O	130[B]	GLN
14	T	2	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
16	V	86	GLN
17	Y	27	MET
17	Y	30	ILE
19	Z	46	LEU
2	b	223	GLN
2	b	246	PHE
2	b	362	PHE
2	b	467	ILE
3	c	156	LYS
3	c	255	THR
3	c	289	PHE
3	c	355	THR
3	c	416	SER
4	d	180	ARG
4	d	233	ARG
4	d	237	PRO
4	d	329	MET
5	e	60[A]	GLN
5	e	60[B]	GLN
5	e	71	GLU
5	e	75	GLN
5	e	81	GLU

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Mol	Chain	Res	Type
7	h	49	TYR
8	i	34[A]	ARG
8	i	34[B]	ARG
8	i	36	ASP
10	k	19	ASP
13	o	23	ASP
13	o	118	LEU
14	t	2	GLU
15	u	9	LEU
15	u	51	LYS
16	v	6	GLU
19	z	29	SER
19	z	46	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
2	B	53	ASN
2	B	179	GLN
2	B	331	ASN
2	B	409	GLN
7	H	59	ASN
11	L	6	ASN
12	M	5	GLN
13	O	82	GLN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	331	ASN
4	d	332	GLN
13	o	82	GLN
13	o	231	HIS
15	u	73	GLN
16	v	34	GLN
16	v	118	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	FME	I	1	8	8,9,10	0.68	0	5,9,11	1.31	1 (20%)
14	FME	T	1	14	8,9,10	0.40	0	5,9,11	1.95	2 (40%)
8	FME	i	1	8	8,9,10	0.47	0	5,9,11	1.77	2 (40%)
14	FME	t	1	14	8,9,10	0.48	0	5,9,11	1.93	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	O-C-CA	-2.69	118.34	125.69
14	t	1	FME	O-C-CA	-2.48	118.90	125.69
8	i	1	FME	O1-CN-N	-2.43	121.08	124.80
8	i	1	FME	O-C-CA	-2.17	119.76	125.69
8	I	1	FME	O-C-CA	-2.12	119.91	125.69
14	t	1	FME	CG-CB-CA	2.21	119.72	113.07
14	t	1	FME	CE-SD-CG	2.31	108.38	100.36
14	T	1	FME	CE-SD-CG	2.68	109.68	100.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 349 ligands modelled in this entry, 55 are unknown and 14 are monoatomic - leaving 280 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	CLA	A	401	-	57,73,73	1.68	11 (19%)	61,113,113	2.06	19 (31%)
20	CLA	A	402	40	51,67,73	1.50	10 (19%)	53,105,113	2.37	14 (26%)
21	PHO	A	403	-	67,69,69	1.66	11 (16%)	86,99,99	2.08	23 (26%)
20	CLA	A	404	-	57,73,73	1.78	12 (21%)	61,113,113	1.80	16 (26%)
22	BCR	A	405	-	41,41,41	0.94	3 (7%)	56,56,56	1.27	6 (10%)
23	SQD	A	406	-	53,54,54	1.45	3 (5%)	62,65,65	2.01	15 (24%)
24	LMG	A	407	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	3 (5%)
27	PL9	A	411	-	54,55,55	0.71	2 (3%)	68,69,69	1.74	17 (25%)
23	SQD	A	412	-	53,54,54	1.52	3 (5%)	62,65,65	2.08	10 (16%)
28	DMS	A	414	-	3,3,3	1.98	1 (33%)	3,3,3	0.51	0
28	DMS	A	415	-	3,3,3	2.76	1 (33%)	3,3,3	0.92	0
28	DMS	A	416	-	3,3,3	2.69	1 (33%)	3,3,3	0.70	0
28	DMS	A	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.41	0
28	DMS	A	418	-	3,3,3	2.80	1 (33%)	3,3,3	0.68	0
30	OEX	A	420	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
31	BCT	A	421	29	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	B	601	-	57,73,73	1.72	12 (21%)	61,113,113	2.02	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	602	40	57,73,73	1.92	13 (22%)	61,113,113	2.27	17 (27%)
20	CLA	B	603	-	57,73,73	1.84	12 (21%)	61,113,113	2.05	17 (27%)
20	CLA	B	604	-	57,73,73	1.73	12 (21%)	61,113,113	2.40	18 (29%)
20	CLA	B	605	-	57,73,73	1.59	12 (21%)	61,113,113	2.07	15 (24%)
20	CLA	B	606	-	57,73,73	1.67	9 (15%)	61,113,113	2.21	20 (32%)
20	CLA	B	607	-	57,73,73	1.93	12 (21%)	61,113,113	1.98	16 (26%)
20	CLA	B	608	40	57,73,73	1.61	11 (19%)	61,113,113	2.09	15 (24%)
20	CLA	B	609	-	57,73,73	1.67	10 (17%)	61,113,113	2.17	21 (34%)
20	CLA	B	610	-	57,73,73	1.69	10 (17%)	61,113,113	2.08	17 (27%)
20	CLA	B	611	40	57,73,73	1.83	13 (22%)	61,113,113	2.03	15 (24%)
20	CLA	B	612	-	57,73,73	1.53	10 (17%)	61,113,113	2.06	19 (31%)
20	CLA	B	613	-	57,73,73	1.65	11 (19%)	61,113,113	2.23	17 (27%)
20	CLA	B	614	-	57,73,73	1.69	14 (24%)	61,113,113	2.07	15 (24%)
20	CLA	B	615	-	57,73,73	1.68	11 (19%)	61,113,113	1.92	16 (26%)
20	CLA	B	616	-	57,73,73	1.75	12 (21%)	61,113,113	1.96	15 (24%)
22	BCR	B	617	-	41,41,41	0.96	0	56,56,56	1.61	10 (17%)
22	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.26	7 (12%)
22	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.60	9 (16%)
24	LMG	B	620	-	51,51,55	0.99	2 (3%)	59,59,63	1.30	5 (8%)
32	HTG	B	621	-	19,19,19	1.35	3 (15%)	22,24,24	1.93	6 (27%)
32	HTG	B	622	-	19,19,19	1.26	3 (15%)	22,24,24	2.19	5 (22%)
32	HTG	B	623	-	19,19,19	0.90	1 (5%)	22,24,24	2.01	2 (9%)
34	LMT	B	625	-	24,24,36	0.51	0	29,29,47	1.24	4 (13%)
34	LMT	B	626	-	24,24,36	0.52	0	29,29,47	1.23	3 (10%)
34	LMT	B	627	-	15,15,36	0.50	0	14,14,47	1.16	1 (7%)
32	HTG	B	631	-	19,19,19	0.88	1 (5%)	22,24,24	2.52	4 (18%)
32	HTG	B	632	-	19,19,19	0.95	1 (5%)	22,24,24	1.44	2 (9%)
28	DMS	B	634	-	3,3,3	1.94	1 (33%)	3,3,3	0.29	0
28	DMS	B	635	-	3,3,3	2.64	1 (33%)	3,3,3	0.41	0
28	DMS	B	636	-	3,3,3	2.77	1 (33%)	3,3,3	0.71	0
28	DMS	B	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.68	0
28	DMS	B	638	-	3,3,3	2.76	1 (33%)	3,3,3	0.75	0
28	DMS	B	639	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
28	DMS	B	640	-	3,3,3	2.55	1 (33%)	3,3,3	0.87	0
28	DMS	B	641	-	3,3,3	2.66	1 (33%)	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	B	642	-	3,3,3	2.80	1 (33%)	3,3,3	0.69	0
28	DMS	B	643	-	3,3,3	2.78	1 (33%)	3,3,3	0.67	0
28	DMS	B	644	-	3,3,3	2.88	1 (33%)	3,3,3	1.15	0
28	DMS	B	645	-	3,3,3	2.73	1 (33%)	3,3,3	0.85	0
20	CLA	C	501	-	57,73,73	1.73	11 (19%)	61,113,113	2.11	13 (21%)
20	CLA	C	502	-	57,73,73	1.78	12 (21%)	61,113,113	1.98	16 (26%)
20	CLA	C	503	-	57,73,73	1.89	11 (19%)	61,113,113	1.97	17 (27%)
20	CLA	C	504	40	57,73,73	1.76	9 (15%)	61,113,113	2.15	17 (27%)
20	CLA	C	505	-	57,73,73	1.85	13 (22%)	61,113,113	1.97	17 (27%)
20	CLA	C	506	-	57,73,73	1.95	13 (22%)	61,113,113	1.98	18 (29%)
20	CLA	C	507	40	57,73,73	1.88	13 (22%)	61,113,113	2.03	16 (26%)
20	CLA	C	508	-	52,68,73	2.03	13 (25%)	55,107,113	1.91	14 (25%)
20	CLA	C	509	-	57,73,73	1.81	11 (19%)	61,113,113	2.12	17 (27%)
20	CLA	C	510	-	57,73,73	1.80	12 (21%)	61,113,113	2.20	17 (27%)
20	CLA	C	511	3	57,73,73	1.85	13 (22%)	61,113,113	1.93	14 (22%)
20	CLA	C	512	-	47,63,73	2.21	12 (25%)	49,101,113	2.15	16 (32%)
20	CLA	C	513	-	57,73,73	1.98	12 (21%)	61,113,113	1.97	15 (24%)
22	BCR	C	514	-	41,41,41	0.84	0	56,56,56	1.31	6 (10%)
22	BCR	C	515	-	41,41,41	0.96	0	56,56,56	1.21	6 (10%)
35	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.21	6 (7%)
35	DGD	C	517	-	56,56,67	0.95	2 (3%)	70,70,81	0.94	4 (5%)
35	DGD	C	518	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	4 (5%)
24	LMG	C	519	-	51,51,55	1.00	2 (3%)	59,59,63	1.23	7 (11%)
32	HTG	C	520	-	19,19,19	0.83	1 (5%)	22,24,24	1.92	1 (4%)
32	HTG	C	521	-	19,19,19	0.92	1 (5%)	22,24,24	2.34	4 (18%)
32	HTG	C	522	-	19,19,19	0.99	2 (10%)	22,24,24	2.10	1 (4%)
24	LMG	C	524	-	45,45,55	1.07	3 (6%)	53,53,63	1.41	6 (11%)
28	DMS	C	525[A]	-	3,3,3	2.80	1 (33%)	3,3,3	0.77	0
28	DMS	C	525[B]	-	3,3,3	2.59	1 (33%)	3,3,3	0.73	0
28	DMS	C	526	-	3,3,3	2.56	1 (33%)	3,3,3	0.77	0
28	DMS	C	527	-	3,3,3	2.57	1 (33%)	3,3,3	0.45	0
28	DMS	C	528	-	3,3,3	2.32	1 (33%)	3,3,3	0.55	0
28	DMS	C	529	-	3,3,3	2.69	1 (33%)	3,3,3	0.73	0
28	DMS	C	530	-	3,3,3	2.62	1 (33%)	3,3,3	0.94	0
28	DMS	C	531	-	3,3,3	2.66	1 (33%)	3,3,3	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	C	532	-	3,3,3	3.29	1 (33%)	3,3,3	1.19	0
28	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.44	0
32	HTG	C	534	-	19,19,19	1.01	1 (5%)	22,24,24	1.58	5 (22%)
20	CLA	D	401	-	57,73,73	1.58	11 (19%)	61,113,113	2.33	20 (32%)
20	CLA	D	402	40	57,73,73	1.69	13 (22%)	61,113,113	2.25	19 (31%)
21	PHO	D	403	-	67,69,69	1.88	14 (20%)	86,99,99	1.90	22 (25%)
20	CLA	D	404	-	57,73,73	1.77	14 (24%)	61,113,113	1.85	20 (32%)
22	BCR	D	405	-	41,41,41	1.01	3 (7%)	56,56,56	1.74	13 (23%)
35	DGD	D	406	-	51,51,67	1.09	2 (3%)	59,59,81	1.23	6 (10%)
36	LHG	D	407	-	48,48,48	0.85	1 (2%)	49,54,54	1.28	5 (10%)
36	LHG	D	408	-	48,48,48	0.80	2 (4%)	49,54,54	1.04	1 (2%)
36	LHG	D	409	-	48,48,48	0.93	2 (4%)	49,54,54	1.05	3 (6%)
27	PL9	D	412	-	54,55,55	1.00	2 (3%)	68,69,69	1.62	11 (16%)
28	DMS	D	413	-	3,3,3	2.74	1 (33%)	3,3,3	0.62	0
28	DMS	D	414	-	3,3,3	2.53	1 (33%)	3,3,3	0.21	0
28	DMS	D	415	-	3,3,3	2.93	1 (33%)	3,3,3	0.66	0
28	DMS	D	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
32	HTG	D	417	-	19,19,19	0.99	1 (5%)	22,24,24	1.79	2 (9%)
34	LMT	E	101	-	24,24,36	0.60	1 (4%)	29,29,47	1.01	3 (10%)
36	LHG	E	103	-	46,46,48	1.03	3 (6%)	48,50,54	1.16	5 (10%)
37	HEM	E	104	5,6	24,50,50	2.16	8 (33%)	16,82,82	2.47	6 (37%)
23	SQD	F	101	-	34,35,54	1.55	2 (5%)	42,45,65	1.92	8 (19%)
28	DMS	F	102	-	3,3,3	2.64	1 (33%)	3,3,3	0.57	0
38	RRX	H	101	-	42,42,42	0.75	0	57,58,58	1.49	7 (12%)
35	DGD	H	102	-	63,63,67	1.01	3 (4%)	77,77,81	1.27	8 (10%)
28	DMS	H	103	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
34	LMT	I	101	-	36,36,36	0.64	1 (2%)	47,47,47	1.31	5 (10%)
24	LMG	J	101	39	45,45,55	0.98	2 (4%)	53,53,63	0.98	2 (3%)
34	LMT	J	103	-	24,24,36	0.63	1 (4%)	29,29,47	1.17	2 (6%)
22	BCR	K	101	-	41,41,41	0.81	1 (2%)	56,56,56	1.50	11 (19%)
22	BCR	K	102	-	41,41,41	0.90	0	56,56,56	1.48	7 (12%)
36	LHG	L	101	-	48,48,48	0.88	3 (6%)	49,54,54	0.90	1 (2%)
34	LMT	M	101	-	36,36,36	0.62	0	47,47,47	0.98	4 (8%)
32	HTG	O	302	-	19,19,19	1.22	2 (10%)	22,24,24	1.21	2 (9%)
28	DMS	O	303	-	3,3,3	2.62	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	O	304	-	3,3,3	2.62	1 (33%)	3,3,3	0.56	0
28	DMS	O	305	-	3,3,3	2.64	1 (33%)	3,3,3	0.74	0
28	DMS	O	306	-	3,3,3	2.54	1 (33%)	3,3,3	0.59	0
28	DMS	O	307	-	3,3,3	2.69	1 (33%)	3,3,3	0.38	0
28	DMS	O	308	-	3,3,3	2.76	1 (33%)	3,3,3	0.73	0
28	DMS	O	309	-	3,3,3	2.68	1 (33%)	3,3,3	1.12	0
28	DMS	O	310	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0
28	DMS	O	311	-	3,3,3	2.88	1 (33%)	3,3,3	0.83	0
22	BCR	T	101	-	41,41,41	0.80	0	56,56,56	1.50	11 (19%)
34	LMT	T	102	-	24,24,36	0.44	0	29,29,47	1.19	2 (6%)
28	DMS	U	902	-	3,3,3	2.66	1 (33%)	3,3,3	1.53	0
28	DMS	U	903[A]	-	3,3,3	2.57	1 (33%)	3,3,3	0.71	0
28	DMS	U	903[B]	-	3,3,3	2.45	1 (33%)	3,3,3	0.16	0
28	DMS	U	904	-	3,3,3	2.86	1 (33%)	3,3,3	0.64	0
37	HEM	V	201	16	24,50,50	2.07	10 (41%)	16,82,82	2.07	5 (31%)
32	HTG	V	202	-	13,13,19	0.69	0	16,18,24	2.31	6 (37%)
28	DMS	V	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.71	0
28	DMS	V	205	-	3,3,3	2.72	1 (33%)	3,3,3	0.48	0
28	DMS	V	206	-	3,3,3	2.68	1 (33%)	3,3,3	0.62	0
28	DMS	V	207	-	3,3,3	2.59	1 (33%)	3,3,3	0.42	0
28	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.69	0
28	DMS	V	209	-	3,3,3	2.61	1 (33%)	3,3,3	0.58	0
34	LMT	Z	101	-	36,36,36	0.66	1 (2%)	47,47,47	1.03	5 (10%)
23	SQD	a	401	-	53,54,54	1.57	3 (5%)	62,65,65	1.55	9 (14%)
20	CLA	a	403	-	57,73,73	1.66	13 (22%)	61,113,113	1.98	18 (29%)
20	CLA	a	404	40	52,68,73	1.71	11 (21%)	55,107,113	2.38	17 (30%)
21	PHO	a	405	-	67,69,69	1.77	12 (17%)	86,99,99	1.84	19 (22%)
21	PHO	a	406	-	67,69,69	1.86	14 (20%)	86,99,99	1.90	24 (27%)
20	CLA	a	407	-	39,55,73	2.22	11 (28%)	42,91,113	2.69	19 (45%)
22	BCR	a	408	-	41,41,41	1.18	3 (7%)	56,56,56	1.45	10 (17%)
23	SQD	a	409	-	53,54,54	1.62	3 (5%)	62,65,65	2.69	11 (17%)
24	LMG	a	410	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
31	BCT	a	413	29	0,3,3	0.00	-	0,3,3	0.00	-
27	PL9	a	415	-	54,55,55	0.70	2 (3%)	68,69,69	1.75	19 (27%)
34	LMT	a	418	-	36,36,36	0.66	1 (2%)	47,47,47	1.59	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	OEX	a	419	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
32	HTG	b	601	-	19,19,19	0.98	2 (10%)	22,24,24	1.46	1 (4%)
32	HTG	b	602	-	19,19,19	0.94	2 (10%)	22,24,24	1.45	1 (4%)
20	CLA	b	603	40	57,73,73	2.02	14 (24%)	61,113,113	1.99	16 (26%)
20	CLA	b	604	-	57,73,73	1.68	13 (22%)	61,113,113	2.24	21 (34%)
20	CLA	b	605	-	57,73,73	1.69	10 (17%)	61,113,113	2.41	20 (32%)
20	CLA	b	606	-	57,73,73	1.62	10 (17%)	61,113,113	2.25	18 (29%)
20	CLA	b	607	-	57,73,73	1.52	9 (15%)	61,113,113	2.33	15 (24%)
20	CLA	b	608	-	57,73,73	1.85	12 (21%)	61,113,113	1.97	13 (21%)
20	CLA	b	609	40	57,73,73	1.65	12 (21%)	61,113,113	2.09	20 (32%)
20	CLA	b	610	-	57,73,73	1.79	11 (19%)	61,113,113	2.21	17 (27%)
20	CLA	b	611	-	57,73,73	1.96	12 (21%)	61,113,113	1.79	14 (22%)
20	CLA	b	612	40	57,73,73	1.73	12 (21%)	61,113,113	1.92	16 (26%)
20	CLA	b	613	-	57,73,73	1.61	8 (14%)	61,113,113	2.04	15 (24%)
20	CLA	b	614	-	57,73,73	1.55	11 (19%)	61,113,113	2.34	18 (29%)
20	CLA	b	615	-	57,73,73	1.66	12 (21%)	61,113,113	1.97	17 (27%)
20	CLA	b	616	-	57,73,73	1.70	11 (19%)	61,113,113	1.99	19 (31%)
20	CLA	b	617	-	57,73,73	1.84	12 (21%)	61,113,113	2.10	20 (32%)
20	CLA	b	618	-	57,73,73	1.80	11 (19%)	61,113,113	2.29	19 (31%)
22	BCR	b	619	-	41,41,41	0.93	0	56,56,56	1.76	8 (14%)
22	BCR	b	620	-	41,41,41	1.05	1 (2%)	56,56,56	1.23	4 (7%)
22	BCR	b	621	-	41,41,41	0.79	1 (2%)	56,56,56	1.48	7 (12%)
23	SQD	b	622	-	53,54,54	1.49	3 (5%)	62,65,65	1.85	11 (17%)
24	LMG	b	623	-	49,49,55	0.93	2 (4%)	57,57,63	1.31	5 (8%)
32	HTG	b	624	-	19,19,19	1.08	2 (10%)	22,24,24	1.96	2 (9%)
32	HTG	b	625	-	19,19,19	1.16	2 (10%)	22,24,24	1.27	4 (18%)
34	LMT	b	627	-	33,33,36	0.85	1 (3%)	44,44,47	1.82	10 (22%)
34	LMT	b	628	-	25,25,36	0.53	0	30,30,47	1.21	2 (6%)
28	DMS	b	631	-	3,3,3	2.89	1 (33%)	3,3,3	1.18	0
28	DMS	b	632	-	3,3,3	2.72	1 (33%)	3,3,3	0.50	0
28	DMS	b	633	-	3,3,3	2.55	1 (33%)	3,3,3	0.97	0
28	DMS	b	634	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
28	DMS	b	635	-	3,3,3	2.69	1 (33%)	3,3,3	0.70	0
28	DMS	b	636	-	3,3,3	2.72	1 (33%)	3,3,3	0.71	0
28	DMS	b	637	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	b	638	-	3,3,3	2.79	1 (33%)	3,3,3	0.87	0
28	DMS	b	639	-	3,3,3	2.82	1 (33%)	3,3,3	0.52	0
28	DMS	b	640	-	3,3,3	2.77	1 (33%)	3,3,3	1.33	1 (33%)
28	DMS	b	641	-	3,3,3	2.79	1 (33%)	3,3,3	1.01	0
20	CLA	c	501	-	57,73,73	1.84	12 (21%)	61,113,113	2.27	16 (26%)
20	CLA	c	502	-	57,73,73	1.75	12 (21%)	61,113,113	2.10	20 (32%)
20	CLA	c	503	-	57,73,73	1.86	13 (22%)	61,113,113	1.94	13 (21%)
20	CLA	c	504	40	57,73,73	1.77	11 (19%)	61,113,113	1.91	14 (22%)
20	CLA	c	505	-	57,73,73	1.72	11 (19%)	61,113,113	1.99	17 (27%)
20	CLA	c	506	-	57,73,73	1.72	12 (21%)	61,113,113	1.90	18 (29%)
20	CLA	c	507	40	57,73,73	1.75	11 (19%)	61,113,113	2.21	17 (27%)
20	CLA	c	508	-	52,68,73	1.95	12 (23%)	55,107,113	1.87	13 (23%)
20	CLA	c	509	-	57,73,73	1.94	13 (22%)	61,113,113	1.90	17 (27%)
20	CLA	c	510	-	57,73,73	1.73	11 (19%)	61,113,113	1.94	17 (27%)
20	CLA	c	511	3	57,73,73	1.98	14 (24%)	61,113,113	1.95	15 (24%)
20	CLA	c	512	-	57,73,73	1.99	12 (21%)	61,113,113	1.97	16 (26%)
20	CLA	c	513	-	57,73,73	1.84	11 (19%)	61,113,113	2.03	16 (26%)
22	BCR	c	514	-	41,41,41	0.84	0	56,56,56	1.49	7 (12%)
35	DGD	c	515	-	63,63,67	0.83	3 (4%)	77,77,81	1.21	8 (10%)
35	DGD	c	516	-	58,58,67	0.84	2 (3%)	72,72,81	1.12	6 (8%)
35	DGD	c	517	-	63,63,67	1.02	4 (6%)	77,77,81	1.20	8 (10%)
24	LMG	c	518	-	51,51,55	1.08	3 (5%)	59,59,63	1.37	6 (10%)
24	LMG	c	519	-	51,51,55	0.98	3 (5%)	59,59,63	1.20	8 (13%)
32	HTG	c	520	-	19,19,19	0.84	2 (10%)	22,24,24	1.58	2 (9%)
32	HTG	c	521	-	19,19,19	0.90	1 (5%)	22,24,24	2.56	3 (13%)
34	LMT	c	523	-	36,36,36	0.78	1 (2%)	47,47,47	1.63	6 (12%)
28	DMS	c	527	-	3,3,3	2.32	1 (33%)	3,3,3	0.46	0
28	DMS	c	528	-	3,3,3	2.58	1 (33%)	3,3,3	0.39	0
28	DMS	c	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.50	0
28	DMS	c	530	-	3,3,3	2.80	1 (33%)	3,3,3	0.96	0
28	DMS	c	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.43	0
28	DMS	c	532	-	3,3,3	2.60	1 (33%)	3,3,3	0.44	0
28	DMS	c	533	-	3,3,3	2.74	1 (33%)	3,3,3	0.77	0
28	DMS	c	534	-	3,3,3	2.70	1 (33%)	3,3,3	0.71	0
28	DMS	c	535	-	3,3,3	2.78	1 (33%)	3,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	c	536	-	3,3,3	2.85	1 (33%)	3,3,3	1.18	0
32	HTG	d	401	-	19,19,19	1.01	1 (5%)	22,24,24	3.16	2 (9%)
20	CLA	d	402	-	57,73,73	1.73	11 (19%)	61,113,113	2.05	19 (31%)
20	CLA	d	403	40	57,73,73	1.65	9 (15%)	61,113,113	2.22	19 (31%)
20	CLA	d	404	-	57,73,73	1.72	12 (21%)	61,113,113	2.01	15 (24%)
22	BCR	d	405	-	41,41,41	0.94	0	56,56,56	1.85	11 (19%)
36	LHG	d	406	-	48,48,48	0.92	2 (4%)	49,54,54	1.21	4 (8%)
36	LHG	d	407	-	48,48,48	0.72	2 (4%)	49,54,54	0.98	2 (4%)
36	LHG	d	408	-	48,48,48	0.91	3 (6%)	49,54,54	1.00	5 (10%)
27	PL9	d	412	-	54,55,55	0.93	2 (3%)	68,69,69	1.69	18 (26%)
28	DMS	d	413	-	3,3,3	2.58	1 (33%)	3,3,3	0.84	0
28	DMS	d	414	-	3,3,3	2.51	1 (33%)	3,3,3	0.22	0
28	DMS	d	415	-	3,3,3	2.72	1 (33%)	3,3,3	0.49	0
35	DGD	d	416	-	51,51,67	1.08	3 (5%)	59,59,81	1.24	6 (10%)
37	HEM	e	102	5,6	24,50,50	2.22	10 (41%)	16,82,82	2.79	7 (43%)
23	SQD	f	101	-	39,40,54	1.77	3 (7%)	48,51,65	5.16	12 (25%)
34	LMT	f	102	-	24,24,36	0.76	1 (4%)	29,29,47	0.99	2 (6%)
35	DGD	h	101	-	63,63,67	0.95	3 (4%)	77,77,81	1.07	6 (7%)
28	DMS	h	102	-	3,3,3	2.76	1 (33%)	3,3,3	0.51	0
28	DMS	i	104	-	3,3,3	2.63	1 (33%)	3,3,3	0.30	0
24	LMG	j	101	39	45,45,55	0.98	2 (4%)	53,53,63	1.05	6 (11%)
22	BCR	j	102	-	41,41,41	0.84	0	56,56,56	1.37	8 (14%)
28	DMS	j	105	-	3,3,3	2.81	1 (33%)	3,3,3	0.77	0
22	BCR	k	101	-	41,41,41	0.92	0	56,56,56	1.11	6 (10%)
22	BCR	k	102	-	41,41,41	0.77	0	56,56,56	1.27	8 (14%)
23	SQD	l	101	-	53,54,54	1.36	4 (7%)	62,65,65	2.11	9 (14%)
36	LHG	l	102	-	48,48,48	0.77	2 (4%)	49,54,54	1.01	2 (4%)
34	LMT	m	101	-	36,36,36	0.60	0	47,47,47	0.99	2 (4%)
34	LMT	m	102	-	36,36,36	0.57	0	47,47,47	1.20	5 (10%)
28	DMS	o	302	-	3,3,3	2.76	1 (33%)	3,3,3	0.83	0
28	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.48	0
28	DMS	o	304	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
28	DMS	o	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.72	0
28	DMS	o	306	-	3,3,3	2.79	1 (33%)	3,3,3	0.95	0
28	DMS	o	307	-	3,3,3	2.66	1 (33%)	3,3,3	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DMS	o	308	-	3,3,3	2.86	1 (33%)	3,3,3	0.74	0
22	BCR	t	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.73	19 (33%)
32	HTG	u	201	-	7,7,19	0.43	0	5,6,24	0.86	0
28	DMS	u	202	-	3,3,3	2.66	1 (33%)	3,3,3	1.21	0
28	DMS	u	203	-	3,3,3	2.57	1 (33%)	3,3,3	0.71	0
28	DMS	u	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.45	0
37	HEM	v	201	16	24,50,50	2.30	9 (37%)	16,82,82	2.14	3 (18%)
28	DMS	v	202	-	3,3,3	2.50	1 (33%)	3,3,3	0.53	0
28	DMS	v	203	-	3,3,3	2.59	1 (33%)	3,3,3	0.81	0
28	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.77	0
28	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.48	0
28	DMS	v	206	-	3,3,3	2.67	1 (33%)	3,3,3	0.60	0
28	DMS	v	207	-	3,3,3	2.76	1 (33%)	3,3,3	0.50	0
28	DMS	v	208	-	3,3,3	2.64	1 (33%)	3,3,3	0.59	0
28	DMS	v	209	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
32	HTG	v	210	-	14,14,19	0.59	0	17,19,24	1.70	3 (17%)
38	RRX	x	101	-	42,42,42	0.80	0	57,58,58	1.21	5 (8%)
34	LMT	z	102	-	36,36,36	0.74	1 (2%)	47,47,47	1.53	8 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	401	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	A	402	40	2/2/18/25	0/30/128/135	0/0/9/9
21	PHO	A	403	-	-	0/53/103/103	0/1/6/6
20	CLA	A	404	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	A	405	-	-	0/29/63/63	0/2/2/2
23	SQD	A	406	-	-	0/49/69/69	0/1/1/1
24	LMG	A	407	-	-	0/46/66/70	0/1/1/1
27	PL9	A	411	-	-	0/53/73/73	0/1/1/1
23	SQD	A	412	-	-	0/49/69/69	0/1/1/1
28	DMS	A	414	-	-	0/0/0/0	0/0/0/0
28	DMS	A	415	-	-	0/0/0/0	0/0/0/0
28	DMS	A	416	-	-	0/0/0/0	0/0/0/0
28	DMS	A	417	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DMS	A	418	-	-	0/0/0/0	0/0/0/0
30	OEX	A	420	1,3,40	-	0/0/68/68	0/0/6/6
31	BCT	A	421	29	-	0/0/0/0	0/0/0/0
20	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	602	40	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	BCR	B	617	-	-	0/29/63/63	0/2/2/2
22	BCR	B	618	-	-	0/29/63/63	0/2/2/2
22	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	LMG	B	620	-	-	0/46/66/70	0/1/1/1
32	HTG	B	621	-	-	0/10/30/30	0/1/1/1
32	HTG	B	622	-	-	0/10/30/30	0/1/1/1
32	HTG	B	623	-	-	0/10/30/30	0/1/1/1
34	LMT	B	625	-	-	0/15/35/61	0/1/1/2
34	LMT	B	626	-	-	0/15/35/61	0/1/1/2
34	LMT	B	627	-	-	0/13/13/61	0/0/0/2
32	HTG	B	631	-	-	0/10/30/30	0/1/1/1
32	HTG	B	632	-	-	0/10/30/30	0/1/1/1
28	DMS	B	634	-	-	0/0/0/0	0/0/0/0
28	DMS	B	635	-	-	0/0/0/0	0/0/0/0
28	DMS	B	636	-	-	0/0/0/0	0/0/0/0
28	DMS	B	637	-	-	0/0/0/0	0/0/0/0
28	DMS	B	638	-	-	0/0/0/0	0/0/0/0
28	DMS	B	639	-	-	0/0/0/0	0/0/0/0
28	DMS	B	640	-	-	0/0/0/0	0/0/0/0
28	DMS	B	641	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DMS	B	642	-	-	0/0/0/0	0/0/0/0
28	DMS	B	643	-	-	0/0/0/0	0/0/0/0
28	DMS	B	644	-	-	0/0/0/0	0/0/0/0
28	DMS	B	645	-	-	0/0/0/0	0/0/0/0
20	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	504	40	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	505	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	507	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	508	-	3/3/19/25	0/31/129/135	0/0/9/9
20	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	C	512	-	3/3/18/25	0/25/123/135	0/0/9/9
20	CLA	C	513	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	C	514	-	-	0/29/63/63	0/2/2/2
22	BCR	C	515	-	-	0/29/63/63	0/2/2/2
35	DGD	C	516	-	-	0/51/91/95	0/2/2/2
35	DGD	C	517	-	-	0/44/84/95	0/2/2/2
35	DGD	C	518	-	-	0/51/91/95	0/2/2/2
24	LMG	C	519	-	-	0/46/66/70	0/1/1/1
32	HTG	C	520	-	-	0/10/30/30	0/1/1/1
32	HTG	C	521	-	-	0/10/30/30	0/1/1/1
32	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	LMG	C	524	-	-	0/40/60/70	0/1/1/1
28	DMS	C	525[A]	-	-	0/0/0/0	0/0/0/0
28	DMS	C	525[B]	-	-	0/0/0/0	0/0/0/0
28	DMS	C	526	-	-	0/0/0/0	0/0/0/0
28	DMS	C	527	-	-	0/0/0/0	0/0/0/0
28	DMS	C	528	-	-	0/0/0/0	0/0/0/0
28	DMS	C	529	-	-	0/0/0/0	0/0/0/0
28	DMS	C	530	-	-	0/0/0/0	0/0/0/0
28	DMS	C	531	-	-	0/0/0/0	0/0/0/0
28	DMS	C	532	-	-	0/0/0/0	0/0/0/0
28	DMS	C	533	-	-	0/0/0/0	0/0/0/0
32	HTG	C	534	-	-	0/10/30/30	0/1/1/1
20	CLA	D	401	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	D	402	40	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PHO	D	403	-	-	0/53/103/103	0/1/6/6
20	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	BCR	D	405	-	-	0/29/63/63	0/2/2/2
35	DGD	D	406	-	-	0/46/66/95	0/1/1/2
36	LHG	D	407	-	-	0/53/53/53	0/0/0/0
36	LHG	D	408	-	-	0/53/53/53	0/0/0/0
36	LHG	D	409	-	-	0/53/53/53	0/0/0/0
27	PL9	D	412	-	-	0/53/73/73	0/1/1/1
28	DMS	D	413	-	-	0/0/0/0	0/0/0/0
28	DMS	D	414	-	-	0/0/0/0	0/0/0/0
28	DMS	D	415	-	-	0/0/0/0	0/0/0/0
28	DMS	D	416	-	-	0/0/0/0	0/0/0/0
32	HTG	D	417	-	-	0/10/30/30	0/1/1/1
34	LMT	E	101	-	-	0/15/35/61	0/1/1/2
36	LHG	E	103	-	-	0/45/45/53	0/0/0/0
37	HEM	E	104	5,6	-	0/6/54/54	0/0/8/8
23	SQD	F	101	-	-	0/28/48/69	0/1/1/1
28	DMS	F	102	-	-	0/0/0/0	0/0/0/0
38	RRX	H	101	-	-	0/29/65/65	0/2/2/2
35	DGD	H	102	-	-	0/51/91/95	0/2/2/2
28	DMS	H	103	-	-	0/0/0/0	0/0/0/0
34	LMT	I	101	-	-	0/21/61/61	0/2/2/2
24	LMG	J	101	39	-	0/40/60/70	0/1/1/1
34	LMT	J	103	-	-	0/15/35/61	0/1/1/2
22	BCR	K	101	-	-	0/29/63/63	0/2/2/2
22	BCR	K	102	-	-	0/29/63/63	0/2/2/2
36	LHG	L	101	-	-	0/53/53/53	0/0/0/0
34	LMT	M	101	-	-	0/21/61/61	0/2/2/2
32	HTG	O	302	-	-	0/10/30/30	0/1/1/1
28	DMS	O	303	-	-	0/0/0/0	0/0/0/0
28	DMS	O	304	-	-	0/0/0/0	0/0/0/0
28	DMS	O	305	-	-	0/0/0/0	0/0/0/0
28	DMS	O	306	-	-	0/0/0/0	0/0/0/0
28	DMS	O	307	-	-	0/0/0/0	0/0/0/0
28	DMS	O	308	-	-	0/0/0/0	0/0/0/0
28	DMS	O	309	-	-	0/0/0/0	0/0/0/0
28	DMS	O	310	-	-	0/0/0/0	0/0/0/0
28	DMS	O	311	-	-	0/0/0/0	0/0/0/0
22	BCR	T	101	-	-	0/29/63/63	0/2/2/2
34	LMT	T	102	-	-	0/15/35/61	0/1/1/2
28	DMS	U	902	-	-	0/0/0/0	0/0/0/0
28	DMS	U	903[A]	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DMS	U	903[B]	-	-	0/0/0/0	0/0/0/0
28	DMS	U	904	-	-	0/0/0/0	0/0/0/0
37	HEM	V	201	16	-	0/6/54/54	0/0/8/8
32	HTG	V	202	-	-	0/3/24/30	0/1/1/1
28	DMS	V	204	-	-	0/0/0/0	0/0/0/0
28	DMS	V	205	-	-	0/0/0/0	0/0/0/0
28	DMS	V	206	-	-	0/0/0/0	0/0/0/0
28	DMS	V	207	-	-	0/0/0/0	0/0/0/0
28	DMS	V	208	-	-	0/0/0/0	0/0/0/0
28	DMS	V	209	-	-	0/0/0/0	0/0/0/0
34	LMT	Z	101	-	-	0/21/61/61	0/2/2/2
23	SQD	a	401	-	-	0/49/69/69	0/1/1/1
20	CLA	a	403	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	a	404	40	2/2/19/25	0/31/129/135	0/0/9/9
21	PHO	a	405	-	-	0/53/103/103	0/1/6/6
21	PHO	a	406	-	-	0/53/103/103	0/1/6/6
20	CLA	a	407	-	1/1/16/25	0/16/114/135	0/0/9/9
22	BCR	a	408	-	-	0/29/63/63	0/2/2/2
23	SQD	a	409	-	-	0/49/69/69	0/1/1/1
24	LMG	a	410	-	-	0/46/66/70	0/1/1/1
31	BCT	a	413	29	-	0/0/0/0	0/0/0/0
27	PL9	a	415	-	-	0/53/73/73	0/1/1/1
34	LMT	a	418	-	-	0/21/61/61	0/2/2/2
30	OEX	a	419	1,3,40	-	0/0/68/68	0/0/6/6
32	HTG	b	601	-	-	0/10/30/30	0/1/1/1
32	HTG	b	602	-	-	0/10/30/30	0/1/1/1
20	CLA	b	603	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	609	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	610	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	b	611	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	b	612	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	613	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	BCR	b	619	-	-	0/29/63/63	0/2/2/2
22	BCR	b	620	-	-	0/29/63/63	0/2/2/2
22	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	SQD	b	622	-	-	0/49/69/69	0/1/1/1
24	LMG	b	623	-	-	0/44/64/70	0/1/1/1
32	HTG	b	624	-	-	0/10/30/30	0/1/1/1
32	HTG	b	625	-	-	0/10/30/30	0/1/1/1
34	LMT	b	627	-	-	0/18/58/61	0/2/2/2
34	LMT	b	628	-	-	0/17/37/61	0/1/1/2
28	DMS	b	631	-	-	0/0/0/0	0/0/0/0
28	DMS	b	632	-	-	0/0/0/0	0/0/0/0
28	DMS	b	633	-	-	0/0/0/0	0/0/0/0
28	DMS	b	634	-	-	0/0/0/0	0/0/0/0
28	DMS	b	635	-	-	0/0/0/0	0/0/0/0
28	DMS	b	636	-	-	0/0/0/0	0/0/0/0
28	DMS	b	637	-	-	0/0/0/0	0/0/0/0
28	DMS	b	638	-	-	0/0/0/0	0/0/0/0
28	DMS	b	639	-	-	0/0/0/0	0/0/0/0
28	DMS	b	640	-	-	0/0/0/0	0/0/0/0
28	DMS	b	641	-	-	0/0/0/0	0/0/0/0
20	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	502	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	c	503	-	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	c	504	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	505	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	c	506	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	c	507	40	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	508	-	2/2/19/25	0/31/129/135	0/0/9/9
20	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
20	CLA	c	513	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	c	514	-	-	0/29/63/63	0/2/2/2
35	DGD	c	515	-	-	0/51/91/95	0/2/2/2
35	DGD	c	516	-	-	0/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	c	517	-	-	0/51/91/95	0/2/2/2
24	LMG	c	518	-	-	0/46/66/70	0/1/1/1
24	LMG	c	519	-	-	0/46/66/70	0/1/1/1
32	HTG	c	520	-	-	0/10/30/30	0/1/1/1
32	HTG	c	521	-	-	0/10/30/30	0/1/1/1
34	LMT	c	523	-	-	0/21/61/61	0/2/2/2
28	DMS	c	527	-	-	0/0/0/0	0/0/0/0
28	DMS	c	528	-	-	0/0/0/0	0/0/0/0
28	DMS	c	529	-	-	0/0/0/0	0/0/0/0
28	DMS	c	530	-	-	0/0/0/0	0/0/0/0
28	DMS	c	531	-	-	0/0/0/0	0/0/0/0
28	DMS	c	532	-	-	0/0/0/0	0/0/0/0
28	DMS	c	533	-	-	0/0/0/0	0/0/0/0
28	DMS	c	534	-	-	0/0/0/0	0/0/0/0
28	DMS	c	535	-	-	0/0/0/0	0/0/0/0
28	DMS	c	536	-	-	0/0/0/0	0/0/0/0
32	HTG	d	401	-	-	1/10/30/30	0/1/1/1
20	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
20	CLA	d	403	40	1/1/20/25	0/37/135/135	0/0/9/9
20	CLA	d	404	-	1/1/20/25	0/37/135/135	0/0/9/9
22	BCR	d	405	-	-	0/29/63/63	0/2/2/2
36	LHG	d	406	-	-	0/53/53/53	0/0/0/0
36	LHG	d	407	-	-	0/53/53/53	0/0/0/0
36	LHG	d	408	-	-	0/53/53/53	0/0/0/0
27	PL9	d	412	-	-	0/53/73/73	0/1/1/1
28	DMS	d	413	-	-	0/0/0/0	0/0/0/0
28	DMS	d	414	-	-	0/0/0/0	0/0/0/0
28	DMS	d	415	-	-	0/0/0/0	0/0/0/0
35	DGD	d	416	-	-	0/46/66/95	0/1/1/2
37	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
23	SQD	f	101	-	-	0/34/54/69	0/1/1/1
34	LMT	f	102	-	-	0/15/35/61	0/1/1/2
35	DGD	h	101	-	-	0/51/91/95	0/2/2/2
28	DMS	h	102	-	-	0/0/0/0	0/0/0/0
28	DMS	i	104	-	-	0/0/0/0	0/0/0/0
24	LMG	j	101	39	-	0/40/60/70	0/1/1/1
22	BCR	j	102	-	-	0/29/63/63	0/2/2/2
28	DMS	j	105	-	-	0/0/0/0	0/0/0/0
22	BCR	k	101	-	-	0/29/63/63	0/2/2/2
22	BCR	k	102	-	-	0/29/63/63	0/2/2/2
23	SQD	l	101	-	-	0/49/69/69	0/1/1/1
36	LHG	l	102	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	m	101	-	-	0/21/61/61	0/2/2/2
34	LMT	m	102	-	-	0/21/61/61	0/2/2/2
28	DMS	o	302	-	-	0/0/0/0	0/0/0/0
28	DMS	o	303	-	-	0/0/0/0	0/0/0/0
28	DMS	o	304	-	-	0/0/0/0	0/0/0/0
28	DMS	o	305	-	-	0/0/0/0	0/0/0/0
28	DMS	o	306	-	-	0/0/0/0	0/0/0/0
28	DMS	o	307	-	-	0/0/0/0	0/0/0/0
28	DMS	o	308	-	-	0/0/0/0	0/0/0/0
22	BCR	t	101	-	-	0/29/63/63	0/2/2/2
32	HTG	u	201	-	-	0/5/5/30	0/0/0/1
28	DMS	u	202	-	-	0/0/0/0	0/0/0/0
28	DMS	u	203	-	-	0/0/0/0	0/0/0/0
28	DMS	u	204	-	-	0/0/0/0	0/0/0/0
37	HEM	v	201	16	-	0/6/54/54	0/0/8/8
28	DMS	v	202	-	-	0/0/0/0	0/0/0/0
28	DMS	v	203	-	-	0/0/0/0	0/0/0/0
28	DMS	v	204	-	-	0/0/0/0	0/0/0/0
28	DMS	v	205	-	-	0/0/0/0	0/0/0/0
28	DMS	v	206	-	-	0/0/0/0	0/0/0/0
28	DMS	v	207	-	-	0/0/0/0	0/0/0/0
28	DMS	v	208	-	-	0/0/0/0	0/0/0/0
28	DMS	v	209	-	-	0/0/0/0	0/0/0/0
32	HTG	v	210	-	-	0/5/25/30	0/1/1/1
38	RRX	x	101	-	-	0/29/65/65	0/2/2/2
34	LMT	z	102	-	-	0/21/61/61	0/2/2/2

All (1152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	SQD	C6-S	-9.84	1.65	1.77
23	A	412	SQD	C6-S	-8.74	1.67	1.77
23	a	401	SQD	C6-S	-8.68	1.67	1.77
23	A	406	SQD	C6-S	-8.28	1.67	1.77
23	b	622	SQD	C6-S	-7.92	1.68	1.77
23	f	101	SQD	C6-S	-7.50	1.68	1.77
23	F	101	SQD	C6-S	-7.33	1.68	1.77
23	l	101	SQD	C6-S	-6.55	1.69	1.77
32	B	621	HTG	C1'-S1	-4.77	1.74	1.81
20	c	510	CLA	C4C-NC	-4.05	1.31	1.37
37	E	104	HEM	C3B-C2B	-3.96	1.35	1.40
21	a	406	PHO	C1A-NA	-3.92	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	v	201	HEM	C3C-C2C	-3.80	1.35	1.40
20	a	404	CLA	C4C-NC	-3.66	1.32	1.37
32	B	622	HTG	C1'-S1	-3.58	1.76	1.81
32	D	417	HTG	C1'-S1	-3.54	1.76	1.81
32	b	624	HTG	C1'-S1	-3.50	1.76	1.81
32	O	302	HTG	C1'-S1	-3.49	1.76	1.81
32	C	534	HTG	C1'-S1	-3.43	1.76	1.81
32	d	401	HTG	C1'-S1	-3.42	1.76	1.81
20	c	508	CLA	C1C-NC	-3.40	1.32	1.37
37	v	201	HEM	C3B-C2B	-3.39	1.36	1.40
21	D	403	PHO	C1A-NA	-3.34	1.30	1.37
37	V	201	HEM	C3C-C2C	-3.32	1.36	1.40
37	e	102	HEM	C3C-C2C	-3.32	1.36	1.40
32	C	522	HTG	C1'-S1	-3.28	1.76	1.81
21	A	403	PHO	C1A-NA	-3.25	1.30	1.37
32	B	632	HTG	C1'-S1	-3.24	1.77	1.81
37	e	102	HEM	C3B-C2B	-3.15	1.36	1.40
32	B	631	HTG	C1'-S1	-3.12	1.77	1.81
20	B	615	CLA	C1C-NC	-3.10	1.32	1.37
32	b	601	HTG	C1'-S1	-3.08	1.77	1.81
21	D	403	PHO	C3D-C4D	-3.00	1.33	1.43
32	b	602	HTG	C1'-S1	-2.94	1.77	1.81
20	b	603	CLA	C4C-NC	-2.90	1.33	1.37
32	B	623	HTG	C1'-S1	-2.88	1.77	1.81
32	c	521	HTG	C1'-S1	-2.84	1.77	1.81
21	a	405	PHO	C1A-NA	-2.81	1.31	1.37
32	b	624	HTG	C1-S1	-2.76	1.76	1.80
32	C	520	HTG	C1'-S1	-2.76	1.77	1.81
32	C	521	HTG	C1'-S1	-2.74	1.77	1.81
37	E	104	HEM	C3C-C2C	-2.70	1.36	1.40
20	A	402	CLA	C1C-NC	-2.69	1.33	1.37
20	C	510	CLA	C1C-NC	-2.69	1.33	1.37
37	V	201	HEM	C3B-C2B	-2.67	1.37	1.40
20	a	403	CLA	O2A-C1	-2.62	1.38	1.46
20	b	615	CLA	C1C-NC	-2.62	1.33	1.37
20	b	607	CLA	C1D-ND	-2.60	1.31	1.37
20	B	616	CLA	C4C-NC	-2.58	1.33	1.37
20	D	402	CLA	C1C-NC	-2.51	1.33	1.37
32	c	520	HTG	C1'-S1	-2.50	1.78	1.81
20	b	603	CLA	C1C-NC	-2.49	1.33	1.37
21	a	405	PHO	C1C-NC	-2.46	1.33	1.38
32	b	601	HTG	C1-S1	-2.44	1.76	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	504	CLA	C1C-NC	-2.42	1.34	1.37
21	a	406	PHO	C3D-C4D	-2.40	1.35	1.43
20	B	604	CLA	C1C-NC	-2.39	1.34	1.37
20	a	407	CLA	C1D-ND	-2.37	1.32	1.37
20	c	502	CLA	C4C-NC	-2.35	1.34	1.37
20	c	506	CLA	C1C-NC	-2.33	1.34	1.37
20	D	404	CLA	C1C-NC	-2.31	1.34	1.37
21	A	403	PHO	C3D-C4D	-2.29	1.36	1.43
20	C	511	CLA	C1C-NC	-2.26	1.34	1.37
32	C	522	HTG	C1-S1	-2.26	1.77	1.80
20	c	509	CLA	C1C-NC	-2.22	1.34	1.37
20	b	610	CLA	C1D-ND	-2.21	1.32	1.37
20	B	603	CLA	C4C-NC	-2.20	1.34	1.37
20	b	604	CLA	C1D-ND	-2.19	1.32	1.37
20	B	601	CLA	C1D-ND	-2.17	1.32	1.37
20	C	511	CLA	C4C-NC	-2.17	1.34	1.37
20	C	505	CLA	C1D-ND	-2.16	1.32	1.37
20	D	404	CLA	C4C-NC	-2.16	1.34	1.37
20	c	511	CLA	C4C-NC	-2.14	1.34	1.37
32	c	520	HTG	C1-S1	-2.13	1.77	1.80
36	L	101	LHG	O7-C5	-2.13	1.40	1.46
32	b	602	HTG	C1-S1	-2.11	1.77	1.80
20	C	508	CLA	C1C-NC	-2.11	1.34	1.37
20	B	611	CLA	C1C-NC	-2.10	1.34	1.37
35	c	517	DGD	O2G-C2G	-2.10	1.41	1.46
20	a	403	CLA	CMD-C2D	-2.09	1.47	1.51
20	B	602	CLA	C1C-NC	-2.09	1.34	1.37
20	A	404	CLA	C1C-NC	-2.09	1.34	1.37
20	c	503	CLA	C1C-NC	-2.05	1.34	1.37
20	b	609	CLA	C1C-NC	-2.03	1.34	1.37
20	A	402	CLA	C4C-NC	-2.03	1.34	1.37
21	D	403	PHO	CHB-C4A	-2.03	1.34	1.40
20	C	508	CLA	C4C-NC	-2.02	1.34	1.37
20	b	612	CLA	CHB-C4A	2.00	1.36	1.33
20	a	403	CLA	C4C-C3C	2.01	1.48	1.45
22	a	408	BCR	C20-C21	2.01	1.49	1.43
20	B	604	CLA	CHB-C4A	2.01	1.36	1.33
36	d	408	LHG	C4-C5	2.01	1.56	1.50
20	c	511	CLA	C3D-CAD	2.01	1.51	1.45
20	b	609	CLA	CHB-C4A	2.01	1.36	1.33
20	C	502	CLA	CAA-C2A	2.01	1.58	1.54
20	A	404	CLA	CHD-C4C	2.02	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	617	CLA	C4B-CHC	2.02	1.45	1.40
37	e	102	HEM	CMA-C3A	2.02	1.55	1.51
20	C	505	CLA	C1C-C2C	2.02	1.48	1.44
20	C	501	CLA	C4C-C3C	2.02	1.48	1.45
37	v	201	HEM	CMD-C2D	2.03	1.55	1.51
20	b	615	CLA	CHB-C4A	2.03	1.36	1.33
20	B	603	CLA	O2A-CGA	2.03	1.39	1.33
20	a	403	CLA	OBD-CAD	2.03	1.25	1.22
20	B	614	CLA	C1-C2	2.04	1.55	1.49
20	D	401	CLA	C4C-C3C	2.04	1.48	1.45
20	D	404	CLA	C1C-C2C	2.04	1.48	1.44
32	B	621	HTG	O5-C1	2.04	1.45	1.42
22	t	101	BCR	C23-C22	2.04	1.50	1.45
22	A	405	BCR	C8-C9	2.05	1.50	1.45
34	I	101	LMT	O1'-C1'	2.05	1.43	1.40
22	K	101	BCR	C12-C13	2.05	1.50	1.45
20	d	402	CLA	O2D-CGD	2.05	1.38	1.33
20	B	612	CLA	CHD-C4C	2.06	1.46	1.41
20	c	509	CLA	CHB-C4A	2.06	1.36	1.33
20	B	614	CLA	C3B-CAB	2.08	1.52	1.47
36	E	103	LHG	P-O6	2.08	1.61	1.54
20	b	614	CLA	C4C-C3C	2.08	1.48	1.45
20	B	602	CLA	C4C-C3C	2.09	1.48	1.45
20	C	502	CLA	C1C-C2C	2.09	1.48	1.44
37	e	102	HEM	CMC-C2C	2.10	1.56	1.51
22	A	405	BCR	C15-C14	2.10	1.49	1.43
22	B	618	BCR	C37-C22	2.12	1.54	1.50
20	c	503	CLA	C1C-C2C	2.12	1.48	1.44
20	b	603	CLA	C1C-C2C	2.12	1.48	1.44
22	B	619	BCR	C20-C21	2.12	1.49	1.43
37	V	201	HEM	CMB-C2B	2.13	1.56	1.51
20	D	402	CLA	OBD-CAD	2.13	1.25	1.22
20	b	615	CLA	C4B-CHC	2.13	1.45	1.40
22	D	405	BCR	C20-C21	2.14	1.49	1.43
34	J	103	LMT	O1'-C1'	2.14	1.44	1.40
22	t	101	BCR	C20-C21	2.15	1.49	1.43
20	D	402	CLA	C3D-C2D	2.15	1.44	1.40
32	B	622	HTG	C1-S1	2.15	1.84	1.80
20	C	507	CLA	C1A-CHA	2.15	1.52	1.43
20	A	401	CLA	C1B-CHB	2.15	1.45	1.40
20	b	604	CLA	C4B-CHC	2.15	1.45	1.40
20	b	603	CLA	C4C-C3C	2.15	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	605	CLA	C4C-C3C	2.15	1.48	1.45
22	b	621	BCR	C26-C25	2.15	1.38	1.34
20	B	601	CLA	C4C-C3C	2.16	1.48	1.45
20	b	610	CLA	C4B-CHC	2.16	1.45	1.40
20	c	506	CLA	C1C-C2C	2.17	1.48	1.44
22	A	405	BCR	C19-C18	2.17	1.50	1.45
20	c	502	CLA	C4B-CHC	2.17	1.46	1.40
37	e	102	HEM	C4D-ND	2.17	1.39	1.36
20	d	402	CLA	C4B-CHC	2.17	1.46	1.40
35	c	517	DGD	O5D-C1E	2.17	1.44	1.40
22	D	405	BCR	C21-C22	2.17	1.38	1.35
20	D	402	CLA	C1B-CHB	2.18	1.46	1.40
20	B	613	CLA	C4B-CHC	2.18	1.46	1.40
34	a	418	LMT	O5B-C1B	2.18	1.47	1.41
37	V	201	HEM	CMC-C2C	2.18	1.56	1.51
21	a	406	PHO	C3B-C4B	2.19	1.47	1.43
20	C	507	CLA	C1C-C2C	2.19	1.48	1.44
32	B	621	HTG	C1-C2	2.19	1.57	1.53
20	B	614	CLA	CHB-C4A	2.20	1.36	1.33
36	d	407	LHG	O7-C7	2.20	1.40	1.34
37	E	104	HEM	CMD-C2D	2.21	1.56	1.51
37	v	201	HEM	CMC-C2C	2.21	1.56	1.51
20	c	501	CLA	C1C-C2C	2.22	1.48	1.44
27	d	412	PL9	C43-C44	2.22	1.38	1.32
20	d	404	CLA	CHD-C4C	2.22	1.46	1.41
20	a	407	CLA	CHB-C4A	2.22	1.36	1.33
32	b	625	HTG	O5-C1	2.22	1.46	1.42
20	c	502	CLA	C4C-C3C	2.23	1.49	1.45
20	b	606	CLA	C4C-C3C	2.23	1.49	1.45
20	C	504	CLA	CHB-C4A	2.23	1.36	1.33
20	C	513	CLA	C1C-C2C	2.23	1.48	1.44
20	b	611	CLA	C4C-C3C	2.23	1.49	1.45
20	b	614	CLA	C1B-CHB	2.24	1.46	1.40
20	A	402	CLA	O2A-CGA	2.24	1.40	1.33
21	D	403	PHO	CHD-C4C	2.24	1.46	1.40
20	a	404	CLA	CHB-C4A	2.25	1.36	1.33
20	b	607	CLA	C1B-CHB	2.25	1.46	1.40
20	B	605	CLA	C4C-C3C	2.25	1.49	1.45
37	V	201	HEM	C4C-NC	2.25	1.39	1.36
34	E	101	LMT	O1'-C1'	2.26	1.44	1.40
37	E	104	HEM	CAD-C3D	2.26	1.55	1.52
20	B	614	CLA	C1C-C2C	2.26	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	509	CLA	CHD-C4C	2.27	1.46	1.41
20	b	611	CLA	C1C-C2C	2.27	1.49	1.44
20	c	501	CLA	C4C-C3C	2.27	1.49	1.45
37	V	201	HEM	CMA-C3A	2.28	1.56	1.51
35	d	416	DGD	O3G-C1D	2.28	1.44	1.40
27	d	412	PL9	C6-C5	2.28	1.48	1.35
20	d	402	CLA	CHD-C4C	2.29	1.46	1.41
20	b	618	CLA	CHD-C4C	2.29	1.46	1.41
37	e	102	HEM	C1C-NC	2.29	1.39	1.36
20	B	601	CLA	CHD-C4C	2.29	1.46	1.41
20	d	403	CLA	O2D-CGD	2.29	1.39	1.33
20	b	612	CLA	C1B-CHB	2.29	1.46	1.40
24	C	524	LMG	O1-C1	2.29	1.44	1.40
20	c	508	CLA	CHD-C4C	2.29	1.46	1.41
20	c	504	CLA	C1B-CHB	2.30	1.46	1.40
24	c	518	LMG	O1-C1	2.31	1.44	1.40
20	B	616	CLA	C4B-CHC	2.31	1.46	1.40
22	a	408	BCR	C40-C30	2.31	1.58	1.53
20	b	606	CLA	CHB-C4A	2.32	1.36	1.33
20	C	506	CLA	CHB-C4A	2.32	1.36	1.33
23	l	101	SQD	O6-C1	2.33	1.44	1.40
20	D	401	CLA	C3D-C2D	2.33	1.45	1.40
20	B	612	CLA	O2A-CGA	2.33	1.40	1.33
20	B	605	CLA	C4B-CHC	2.33	1.46	1.40
20	c	512	CLA	C1C-C2C	2.34	1.49	1.44
20	C	509	CLA	C4C-C3C	2.34	1.49	1.45
20	b	613	CLA	C4B-CHC	2.34	1.46	1.40
20	B	604	CLA	C4C-C3C	2.35	1.49	1.45
20	a	407	CLA	CHD-C4C	2.35	1.46	1.41
35	c	515	DGD	O5D-C1E	2.35	1.44	1.40
37	v	201	HEM	C4D-ND	2.36	1.39	1.36
27	A	411	PL9	C6-C5	2.36	1.48	1.35
20	d	404	CLA	C1C-C2C	2.36	1.49	1.44
20	b	617	CLA	C4C-C3C	2.36	1.49	1.45
20	d	402	CLA	C4C-C3C	2.37	1.49	1.45
20	B	608	CLA	C4C-C3C	2.37	1.49	1.45
20	b	609	CLA	C4B-CHC	2.37	1.46	1.40
20	b	614	CLA	C4B-CHC	2.37	1.46	1.40
20	D	401	CLA	C1B-CHB	2.37	1.46	1.40
32	O	302	HTG	O5-C1	2.37	1.46	1.42
27	a	415	PL9	C6-C5	2.37	1.48	1.35
20	c	505	CLA	C4C-C3C	2.37	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	401	CLA	OBD-CAD	2.38	1.25	1.22
20	C	503	CLA	C1B-CHB	2.39	1.46	1.40
34	z	102	LMT	O1'-C1'	2.39	1.44	1.40
20	A	402	CLA	C1B-CHB	2.39	1.46	1.40
20	d	403	CLA	O2A-CGA	2.40	1.40	1.33
20	d	402	CLA	C3D-C2D	2.40	1.45	1.40
20	b	608	CLA	C4C-C3C	2.40	1.49	1.45
34	f	102	LMT	O1'-C1'	2.41	1.44	1.40
20	C	502	CLA	CHD-C4C	2.41	1.46	1.41
20	c	501	CLA	CHD-C4C	2.41	1.46	1.41
21	A	403	PHO	C1D-C2D	2.41	1.51	1.45
20	b	608	CLA	C1C-C2C	2.41	1.49	1.44
24	c	519	LMG	O1-C1	2.41	1.44	1.40
20	C	506	CLA	C1C-C2C	2.42	1.49	1.44
20	c	506	CLA	C1B-CHB	2.42	1.46	1.40
20	B	607	CLA	CHD-C4C	2.42	1.46	1.41
20	b	607	CLA	C3D-C2D	2.42	1.45	1.40
27	D	412	PL9	C2-C3	2.42	1.41	1.34
20	B	613	CLA	CHB-C4A	2.43	1.36	1.33
22	D	405	BCR	C12-C13	2.43	1.51	1.45
27	A	411	PL9	C2-C3	2.43	1.41	1.34
20	C	510	CLA	C4B-CHC	2.44	1.46	1.40
20	b	604	CLA	C3B-CAB	2.44	1.53	1.47
20	C	512	CLA	C1C-C2C	2.44	1.49	1.44
20	b	615	CLA	C1B-CHB	2.44	1.46	1.40
20	c	510	CLA	C4B-CHC	2.44	1.46	1.40
20	b	608	CLA	CHD-C4C	2.45	1.46	1.41
20	C	508	CLA	CHD-C4C	2.45	1.46	1.41
36	d	407	LHG	O8-C23	2.45	1.40	1.33
20	B	602	CLA	C1C-C2C	2.45	1.49	1.44
20	A	404	CLA	C4C-C3C	2.46	1.49	1.45
20	c	511	CLA	C1C-C2C	2.46	1.49	1.44
20	B	616	CLA	C4C-C3C	2.46	1.49	1.45
20	c	503	CLA	C4C-C3C	2.47	1.49	1.45
20	c	510	CLA	CHD-C4C	2.47	1.47	1.41
20	b	606	CLA	CHD-C4C	2.47	1.47	1.41
20	C	502	CLA	C4B-CHC	2.47	1.46	1.40
20	B	612	CLA	C1B-CHB	2.47	1.46	1.40
20	c	507	CLA	C1C-C2C	2.48	1.49	1.44
27	D	412	PL9	C6-C5	2.48	1.49	1.35
20	A	401	CLA	O2A-CGA	2.48	1.40	1.33
20	c	504	CLA	C4B-CHC	2.48	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	406	PHO	CHD-C4C	2.49	1.46	1.40
20	B	603	CLA	C4B-CHC	2.49	1.46	1.40
20	D	402	CLA	C4C-C3C	2.49	1.49	1.45
20	b	615	CLA	C3D-C2D	2.49	1.45	1.40
20	B	613	CLA	CHD-C4C	2.49	1.47	1.41
21	a	405	PHO	O2A-CGA	2.49	1.40	1.33
20	B	606	CLA	C3D-C2D	2.50	1.45	1.40
37	e	102	HEM	CAD-C3D	2.50	1.55	1.52
20	C	510	CLA	CHD-C4C	2.50	1.47	1.41
20	C	509	CLA	C4B-CHC	2.50	1.46	1.40
32	B	622	HTG	O5-C1	2.50	1.46	1.42
20	c	509	CLA	C4B-CHC	2.50	1.46	1.40
20	b	605	CLA	O2A-CGA	2.51	1.40	1.33
20	B	614	CLA	C3D-C2D	2.51	1.45	1.40
20	A	401	CLA	C3B-C2B	2.52	1.43	1.40
36	l	102	LHG	O7-C7	2.52	1.41	1.34
20	b	616	CLA	CHD-C4C	2.52	1.47	1.41
20	B	601	CLA	C1B-CHB	2.52	1.46	1.40
20	B	610	CLA	CHB-C4A	2.52	1.36	1.33
20	C	506	CLA	C4C-C3C	2.52	1.49	1.45
20	c	510	CLA	C3D-C2D	2.53	1.45	1.40
20	c	505	CLA	C4B-CHC	2.53	1.46	1.40
20	C	503	CLA	C1C-C2C	2.54	1.49	1.44
37	v	201	HEM	C1B-NB	2.54	1.40	1.36
20	c	507	CLA	CHD-C4C	2.54	1.47	1.41
20	A	402	CLA	O2D-CGD	2.55	1.39	1.33
35	c	515	DGD	O2G-C1B	2.56	1.41	1.34
20	B	611	CLA	C1C-C2C	2.56	1.49	1.44
21	a	406	PHO	OBD-CAD	2.56	1.26	1.22
20	B	607	CLA	C1B-CHB	2.56	1.47	1.40
37	E	104	HEM	C4D-ND	2.56	1.40	1.36
20	b	612	CLA	CHD-C4C	2.57	1.47	1.41
20	c	509	CLA	C4C-C3C	2.57	1.49	1.45
20	a	403	CLA	CHB-C4A	2.57	1.37	1.33
20	C	504	CLA	C1B-CHB	2.57	1.47	1.40
20	B	614	CLA	CHD-C4C	2.57	1.47	1.41
20	b	609	CLA	C1B-CHB	2.58	1.47	1.40
20	B	607	CLA	C4C-C3C	2.58	1.49	1.45
20	b	603	CLA	CHD-C4C	2.58	1.47	1.41
20	C	511	CLA	CHD-C4C	2.59	1.47	1.41
20	b	618	CLA	C1C-C2C	2.59	1.49	1.44
20	B	605	CLA	C3D-C2D	2.60	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	406	PHO	CHC-C4B	2.60	1.46	1.40
20	B	609	CLA	C4B-CHC	2.60	1.47	1.40
20	B	610	CLA	C4B-CHC	2.60	1.47	1.40
27	a	415	PL9	C2-C3	2.60	1.41	1.34
20	d	403	CLA	C3D-C2D	2.60	1.45	1.40
20	C	510	CLA	C4C-C3C	2.60	1.49	1.45
20	D	402	CLA	O2A-CGA	2.61	1.41	1.33
20	c	506	CLA	C4B-CHC	2.61	1.47	1.40
20	b	610	CLA	O2A-CGA	2.61	1.41	1.33
20	c	503	CLA	OBD-CAD	2.62	1.26	1.22
20	b	614	CLA	CHD-C4C	2.62	1.47	1.41
20	c	513	CLA	C1C-C2C	2.62	1.49	1.44
20	C	507	CLA	C4B-CHC	2.62	1.47	1.40
20	C	511	CLA	C4B-CHC	2.62	1.47	1.40
20	b	612	CLA	C3D-C2D	2.63	1.45	1.40
20	b	616	CLA	C1B-CHB	2.63	1.47	1.40
20	B	615	CLA	C3D-C2D	2.63	1.45	1.40
20	C	509	CLA	C1B-CHB	2.64	1.47	1.40
20	B	615	CLA	C4B-CHC	2.64	1.47	1.40
20	B	603	CLA	CHD-C4C	2.64	1.47	1.41
20	D	404	CLA	CHD-C4C	2.65	1.47	1.41
20	c	502	CLA	CHD-C4C	2.66	1.47	1.41
20	d	403	CLA	CHD-C4C	2.67	1.47	1.41
20	b	607	CLA	O2A-CGA	2.67	1.41	1.33
20	c	511	CLA	CHD-C4C	2.67	1.47	1.41
20	B	611	CLA	CHD-C4C	2.68	1.47	1.41
20	c	509	CLA	CHD-C4C	2.68	1.47	1.41
20	C	505	CLA	C1B-CHB	2.68	1.47	1.40
20	b	605	CLA	C1B-CHB	2.69	1.47	1.40
20	b	616	CLA	C4C-C3C	2.69	1.49	1.45
20	c	503	CLA	C4B-CHC	2.69	1.47	1.40
20	B	608	CLA	CHD-C4C	2.69	1.47	1.41
20	b	609	CLA	CHD-C4C	2.70	1.47	1.41
20	b	609	CLA	OBD-CAD	2.70	1.26	1.22
20	B	608	CLA	O2A-CGA	2.70	1.41	1.33
20	b	618	CLA	C4B-CHC	2.70	1.47	1.40
20	b	611	CLA	CHD-C4C	2.70	1.47	1.41
20	c	506	CLA	CHD-C4C	2.70	1.47	1.41
20	b	612	CLA	O2A-CGA	2.71	1.41	1.33
20	C	507	CLA	C4C-C3C	2.71	1.49	1.45
20	c	505	CLA	O2D-CGD	2.71	1.40	1.33
20	D	404	CLA	C4C-C3C	2.71	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	503	CLA	CHD-C4C	2.72	1.47	1.41
20	C	505	CLA	C4C-C3C	2.72	1.50	1.45
20	b	604	CLA	C3D-C2D	2.72	1.46	1.40
34	Z	101	LMT	O1'-C1'	2.73	1.45	1.40
20	a	403	CLA	C3D-C2D	2.73	1.46	1.40
21	A	403	PHO	CHD-C4C	2.73	1.47	1.40
20	b	612	CLA	OBD-CAD	2.73	1.26	1.22
20	c	513	CLA	C4B-CHC	2.73	1.47	1.40
20	A	404	CLA	C3D-C2D	2.74	1.46	1.40
20	b	606	CLA	O2A-CGA	2.74	1.41	1.33
20	B	605	CLA	CHD-C4C	2.74	1.47	1.41
20	A	401	CLA	C3D-C2D	2.75	1.46	1.40
20	B	616	CLA	C1B-CHB	2.75	1.47	1.40
20	b	617	CLA	O2A-CGA	2.75	1.41	1.33
37	V	201	HEM	CMD-C2D	2.75	1.57	1.51
20	c	504	CLA	C4C-C3C	2.75	1.50	1.45
20	B	611	CLA	C1B-CHB	2.75	1.47	1.40
20	B	614	CLA	OBD-CAD	2.76	1.26	1.22
20	b	609	CLA	O2A-CGA	2.77	1.41	1.33
20	B	609	CLA	C1B-CHB	2.78	1.47	1.40
20	b	617	CLA	CHB-C4A	2.78	1.37	1.33
20	B	602	CLA	CHD-C4C	2.78	1.47	1.41
20	b	605	CLA	CHD-C4C	2.79	1.47	1.41
20	b	604	CLA	C1B-CHB	2.79	1.47	1.40
20	b	606	CLA	C1B-CHB	2.79	1.47	1.40
20	C	512	CLA	C4B-CHC	2.80	1.47	1.40
20	B	605	CLA	C1B-CHB	2.80	1.47	1.40
20	c	511	CLA	C4C-C3C	2.80	1.50	1.45
20	C	501	CLA	C1B-CHB	2.80	1.47	1.40
20	B	608	CLA	OBD-CAD	2.80	1.26	1.22
20	B	616	CLA	CHD-C4C	2.80	1.47	1.41
20	c	501	CLA	C1B-CHB	2.81	1.47	1.40
20	B	615	CLA	C4C-C3C	2.82	1.50	1.45
20	c	508	CLA	C1B-CHB	2.83	1.47	1.40
20	C	508	CLA	C4C-C3C	2.83	1.50	1.45
20	B	608	CLA	CHB-C4A	2.83	1.37	1.33
20	D	404	CLA	C4B-CHC	2.83	1.47	1.40
20	b	617	CLA	C3D-C2D	2.84	1.46	1.40
20	B	604	CLA	C3B-C2B	2.84	1.44	1.40
20	c	508	CLA	C4B-CHC	2.85	1.47	1.40
20	B	602	CLA	C3D-C2D	2.85	1.46	1.40
20	b	616	CLA	C4B-CHC	2.85	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	CLA	CHD-C4C	2.85	1.47	1.41
20	c	512	CLA	C1B-CHB	2.86	1.47	1.40
20	b	608	CLA	OBD-CAD	2.86	1.26	1.22
20	a	403	CLA	CHD-C4C	2.86	1.47	1.41
20	a	404	CLA	C1B-CHB	2.87	1.47	1.40
20	B	601	CLA	C4B-CHC	2.87	1.47	1.40
20	c	511	CLA	C4B-CHC	2.88	1.47	1.40
20	B	605	CLA	CHB-C4A	2.88	1.37	1.33
20	C	506	CLA	CHD-C4C	2.88	1.48	1.41
20	B	604	CLA	C3D-C2D	2.88	1.46	1.40
20	C	511	CLA	C4C-C3C	2.89	1.50	1.45
20	B	614	CLA	O2D-CGD	2.89	1.40	1.33
20	B	613	CLA	C3D-C2D	2.89	1.46	1.40
20	b	604	CLA	O2D-CGD	2.90	1.40	1.33
36	d	408	LHG	O7-C7	2.90	1.42	1.34
20	B	616	CLA	C3D-C2D	2.90	1.46	1.40
20	b	612	CLA	C4B-CHC	2.91	1.48	1.40
20	A	402	CLA	OBD-CAD	2.92	1.26	1.22
20	B	605	CLA	OBD-CAD	2.92	1.26	1.22
20	B	614	CLA	C1B-CHB	2.92	1.48	1.40
20	C	513	CLA	C4B-CHC	2.92	1.48	1.40
20	a	403	CLA	O2A-CGA	2.92	1.42	1.33
20	D	401	CLA	CHD-C4C	2.93	1.48	1.41
20	b	618	CLA	OBD-CAD	2.93	1.26	1.22
20	B	611	CLA	C4B-CHC	2.94	1.48	1.40
20	B	604	CLA	CHD-C4C	2.94	1.48	1.41
20	C	508	CLA	C4B-CHC	2.94	1.48	1.40
35	c	516	DGD	O2G-C1B	2.94	1.42	1.34
20	d	404	CLA	O2D-CGD	2.94	1.40	1.33
20	b	608	CLA	O2A-CGA	2.94	1.42	1.33
20	b	615	CLA	CHD-C4C	2.95	1.48	1.41
20	b	603	CLA	C1B-CHB	2.95	1.48	1.40
20	c	513	CLA	CHD-C4C	2.95	1.48	1.41
20	b	607	CLA	C3B-C2B	2.95	1.44	1.40
36	D	409	LHG	O7-C7	2.95	1.43	1.34
20	B	609	CLA	C3D-C2D	2.95	1.46	1.40
35	h	101	DGD	O1G-C1A	2.96	1.42	1.33
22	a	408	BCR	C26-C25	2.96	1.39	1.34
20	c	502	CLA	C1B-CHB	2.96	1.48	1.40
20	B	612	CLA	C3D-C2D	2.96	1.46	1.40
20	A	401	CLA	C3C-C2C	2.96	1.43	1.36
20	B	606	CLA	C1B-CHB	2.97	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	C4B-CHC	2.97	1.48	1.40
20	c	507	CLA	C4B-CHC	2.97	1.48	1.40
20	C	513	CLA	C4C-C3C	2.98	1.50	1.45
20	A	402	CLA	C3D-C2D	2.98	1.46	1.40
20	B	613	CLA	O2A-CGA	2.98	1.42	1.33
20	b	611	CLA	C1B-CHB	2.99	1.48	1.40
20	B	602	CLA	C1B-CHB	2.99	1.48	1.40
20	B	606	CLA	CHD-C4C	2.99	1.48	1.41
20	D	402	CLA	C4B-CHC	3.00	1.48	1.40
28	B	634	DMS	O-S	3.01	1.70	1.50
20	B	609	CLA	CHD-C4C	3.02	1.48	1.41
20	b	614	CLA	O2A-CGA	3.02	1.42	1.33
20	B	613	CLA	OBD-CAD	3.02	1.26	1.22
20	D	401	CLA	O2D-CGD	3.02	1.41	1.33
20	c	508	CLA	C4C-C3C	3.03	1.50	1.45
32	b	625	HTG	C1-S1	3.03	1.85	1.80
20	a	403	CLA	C1B-CHB	3.03	1.48	1.40
20	B	612	CLA	C4B-CHC	3.04	1.48	1.40
20	B	602	CLA	C4B-CHC	3.04	1.48	1.40
20	B	605	CLA	O2A-CGA	3.04	1.42	1.33
36	d	406	LHG	O7-C7	3.04	1.43	1.34
20	a	404	CLA	C3D-C2D	3.05	1.46	1.40
20	b	604	CLA	OBD-CAD	3.05	1.26	1.22
20	B	610	CLA	C1B-CHB	3.05	1.48	1.40
36	D	408	LHG	O7-C7	3.05	1.43	1.34
21	a	405	PHO	OBD-CAD	3.05	1.27	1.22
20	C	512	CLA	CHD-C4C	3.05	1.48	1.41
20	c	510	CLA	C1B-CHB	3.06	1.48	1.40
20	B	606	CLA	O2A-CGA	3.06	1.42	1.33
20	c	505	CLA	CHD-C4C	3.06	1.48	1.41
20	C	508	CLA	C1B-CHB	3.08	1.48	1.40
20	d	404	CLA	C1B-CHB	3.08	1.48	1.40
20	C	501	CLA	C4B-CHC	3.10	1.48	1.40
20	C	503	CLA	C4B-CHC	3.10	1.48	1.40
20	b	604	CLA	C4C-C3C	3.10	1.50	1.45
20	c	506	CLA	C3D-C2D	3.10	1.46	1.40
21	a	405	PHO	C3D-C2D	3.10	1.47	1.38
20	C	505	CLA	C4B-CHC	3.10	1.48	1.40
35	C	517	DGD	O2G-C1B	3.10	1.43	1.34
20	b	603	CLA	C4B-CHC	3.11	1.48	1.40
21	D	403	PHO	OBD-CAD	3.11	1.27	1.22
20	b	617	CLA	CHD-C4C	3.11	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	618	CLA	C1B-CHB	3.11	1.48	1.40
20	b	614	CLA	C3D-C2D	3.11	1.46	1.40
20	c	501	CLA	C3D-C2D	3.11	1.46	1.40
20	B	604	CLA	OBD-CAD	3.12	1.27	1.22
21	A	403	PHO	O2D-CGD	3.12	1.41	1.33
20	D	401	CLA	CHB-C4A	3.12	1.37	1.33
34	b	627	LMT	O1'-C1'	3.12	1.45	1.40
20	c	507	CLA	C1B-CHB	3.12	1.48	1.40
20	C	512	CLA	C4C-C3C	3.13	1.50	1.45
20	b	610	CLA	CHD-C4C	3.13	1.48	1.41
21	A	403	PHO	CHD-C1D	3.13	1.44	1.38
20	b	616	CLA	C3D-C2D	3.13	1.46	1.40
20	C	513	CLA	CHD-C4C	3.13	1.48	1.41
20	a	404	CLA	O2D-CGD	3.14	1.41	1.33
20	c	507	CLA	C3D-C2D	3.14	1.46	1.40
20	B	604	CLA	O2A-CGA	3.14	1.42	1.33
20	B	608	CLA	C4B-CHC	3.15	1.48	1.40
20	C	510	CLA	C1B-CHB	3.15	1.48	1.40
20	C	502	CLA	OBD-CAD	3.16	1.27	1.22
20	b	610	CLA	C3D-C2D	3.16	1.47	1.40
20	B	607	CLA	C3D-C2D	3.16	1.47	1.40
20	d	404	CLA	C4B-CHC	3.16	1.48	1.40
20	C	507	CLA	C1B-CHB	3.16	1.48	1.40
21	a	406	PHO	C3D-C2D	3.17	1.47	1.38
20	c	512	CLA	CHD-C4C	3.17	1.48	1.41
20	b	615	CLA	OBD-CAD	3.18	1.27	1.22
20	c	512	CLA	C4B-CHC	3.18	1.48	1.40
20	b	607	CLA	OBD-CAD	3.18	1.27	1.22
20	D	401	CLA	CHC-C1C	3.18	1.44	1.35
20	B	609	CLA	O2A-CGA	3.19	1.42	1.33
20	b	614	CLA	C3B-C2B	3.19	1.44	1.40
21	a	405	PHO	CHD-C1D	3.19	1.45	1.38
20	b	610	CLA	C1B-CHB	3.19	1.48	1.40
20	A	404	CLA	C4B-CHC	3.19	1.48	1.40
20	c	503	CLA	O2A-CGA	3.20	1.42	1.33
20	B	615	CLA	O2D-CGD	3.20	1.41	1.33
20	C	504	CLA	CHD-C4C	3.20	1.48	1.41
36	l	102	LHG	O8-C23	3.20	1.42	1.33
20	A	401	CLA	C4B-CHC	3.21	1.48	1.40
20	D	404	CLA	C1B-CHB	3.21	1.48	1.40
20	b	604	CLA	CHD-C4C	3.21	1.48	1.41
20	B	603	CLA	C1B-CHB	3.21	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	101	LHG	O7-C7	3.22	1.43	1.34
20	B	613	CLA	C1B-CHB	3.22	1.48	1.40
20	b	605	CLA	C3D-C2D	3.22	1.47	1.40
20	c	513	CLA	C1B-CHB	3.22	1.48	1.40
20	b	617	CLA	C1B-CHB	3.23	1.48	1.40
20	B	601	CLA	OBD-CAD	3.23	1.27	1.22
20	d	404	CLA	C3D-C2D	3.23	1.47	1.40
28	A	414	DMS	O-S	3.24	1.72	1.50
20	B	614	CLA	C4C-C3C	3.25	1.50	1.45
20	b	612	CLA	C4C-C3C	3.25	1.50	1.45
20	B	608	CLA	C1B-CHB	3.25	1.48	1.40
20	A	404	CLA	O2D-CGD	3.25	1.41	1.33
20	C	511	CLA	O2A-CGA	3.25	1.43	1.33
20	d	402	CLA	O2A-CGA	3.26	1.43	1.33
20	B	611	CLA	OBD-CAD	3.26	1.27	1.22
20	B	611	CLA	O2A-CGA	3.26	1.43	1.33
20	b	613	CLA	C1B-CHB	3.26	1.48	1.40
20	C	506	CLA	C3D-C2D	3.27	1.47	1.40
20	D	402	CLA	O2D-CGD	3.27	1.41	1.33
35	H	102	DGD	O5D-C1E	3.27	1.46	1.40
20	C	503	CLA	OBD-CAD	3.27	1.27	1.22
36	L	101	LHG	O8-C23	3.28	1.43	1.33
20	b	613	CLA	C3D-C2D	3.29	1.47	1.40
20	A	402	CLA	C3B-C2B	3.30	1.44	1.40
36	D	408	LHG	O8-C23	3.30	1.43	1.33
20	C	507	CLA	CHD-C4C	3.30	1.49	1.41
20	C	506	CLA	C4B-CHC	3.31	1.49	1.40
20	c	513	CLA	C3D-C2D	3.31	1.47	1.40
21	D	403	PHO	C3D-C2D	3.31	1.47	1.38
20	c	502	CLA	O2A-CGA	3.32	1.43	1.33
20	a	404	CLA	O2A-CGA	3.33	1.43	1.33
22	b	620	BCR	C5-C6	3.33	1.40	1.34
20	c	501	CLA	C4B-CHC	3.33	1.49	1.40
20	d	403	CLA	OBD-CAD	3.33	1.27	1.22
20	c	511	CLA	O2A-CGA	3.34	1.43	1.33
34	c	523	LMT	O1'-C1'	3.34	1.46	1.40
20	b	608	CLA	C1B-CHB	3.34	1.49	1.40
35	C	516	DGD	O1G-C1A	3.34	1.43	1.33
20	c	505	CLA	C1B-CHB	3.34	1.49	1.40
20	c	509	CLA	C1B-CHB	3.34	1.49	1.40
20	A	401	CLA	CHD-C4C	3.34	1.49	1.41
20	c	512	CLA	C4C-C3C	3.35	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	404	CLA	CHD-C4C	3.35	1.49	1.41
20	B	610	CLA	O2A-CGA	3.35	1.43	1.33
20	C	510	CLA	O2A-CGA	3.36	1.43	1.33
20	a	407	CLA	C1B-CHB	3.36	1.49	1.40
20	c	504	CLA	C3D-C2D	3.36	1.47	1.40
20	b	614	CLA	OBD-CAD	3.36	1.27	1.22
24	B	620	LMG	O7-C10	3.37	1.44	1.34
20	D	404	CLA	C3D-C2D	3.37	1.47	1.40
20	c	508	CLA	O2A-CGA	3.37	1.43	1.33
20	B	610	CLA	O2D-CGD	3.38	1.41	1.33
21	D	403	PHO	CHC-C1C	3.38	1.45	1.38
36	d	408	LHG	O8-C23	3.38	1.43	1.33
20	D	401	CLA	O2A-CGA	3.39	1.43	1.33
20	c	503	CLA	C3D-C2D	3.39	1.47	1.40
20	D	404	CLA	OBD-CAD	3.39	1.27	1.22
20	c	503	CLA	C1B-CHB	3.39	1.49	1.40
20	C	501	CLA	OBD-CAD	3.39	1.27	1.22
20	B	609	CLA	OBD-CAD	3.40	1.27	1.22
20	b	606	CLA	C3D-C2D	3.40	1.47	1.40
20	A	402	CLA	C3C-C2C	3.40	1.44	1.36
20	c	502	CLA	C3C-C2C	3.41	1.44	1.36
35	C	518	DGD	O2G-C1B	3.41	1.44	1.34
20	C	501	CLA	O2A-CGA	3.41	1.43	1.33
20	b	604	CLA	O2A-CGA	3.42	1.43	1.33
20	a	404	CLA	C3B-C2B	3.42	1.44	1.40
37	V	201	HEM	C3D-C2D	3.42	1.47	1.37
20	B	609	CLA	CHC-C1C	3.42	1.45	1.35
20	C	512	CLA	OBD-CAD	3.43	1.27	1.22
20	C	511	CLA	C1B-CHB	3.44	1.49	1.40
21	a	406	PHO	O2A-CGA	3.44	1.43	1.33
20	c	505	CLA	C3D-C2D	3.44	1.47	1.40
20	C	507	CLA	O2A-CGA	3.44	1.43	1.33
20	B	612	CLA	C3B-C2B	3.44	1.44	1.40
20	C	513	CLA	C1B-CHB	3.45	1.49	1.40
20	b	608	CLA	C4B-CHC	3.45	1.49	1.40
35	H	102	DGD	O1G-C1A	3.45	1.43	1.33
35	h	101	DGD	O5D-C1E	3.45	1.46	1.40
20	a	404	CLA	C3C-C2C	3.46	1.44	1.36
20	D	402	CLA	CHC-C1C	3.47	1.45	1.35
20	c	509	CLA	C3D-C2D	3.47	1.47	1.40
20	B	604	CLA	C1B-CHB	3.47	1.49	1.40
20	B	612	CLA	O2D-CGD	3.48	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	615	CLA	O2A-CGA	3.48	1.43	1.33
20	c	509	CLA	O2A-CGA	3.49	1.43	1.33
20	B	601	CLA	C3D-C2D	3.49	1.47	1.40
20	C	505	CLA	CHD-C4C	3.49	1.49	1.41
20	c	512	CLA	C3D-C2D	3.49	1.47	1.40
20	B	603	CLA	C3D-C2D	3.50	1.47	1.40
20	b	616	CLA	O2A-CGA	3.51	1.43	1.33
20	b	603	CLA	C3D-C2D	3.51	1.47	1.40
20	C	513	CLA	OBD-CAD	3.51	1.27	1.22
20	A	404	CLA	O2A-CGA	3.51	1.43	1.33
35	c	515	DGD	O1G-C1A	3.51	1.43	1.33
20	D	404	CLA	O2A-CGA	3.52	1.43	1.33
20	C	504	CLA	O2A-CGA	3.52	1.43	1.33
20	c	505	CLA	O2A-CGA	3.53	1.43	1.33
20	a	407	CLA	C3D-C2D	3.53	1.47	1.40
20	B	615	CLA	C1B-CHB	3.53	1.49	1.40
20	B	616	CLA	O2A-CGA	3.53	1.43	1.33
20	C	503	CLA	C3D-C2D	3.53	1.47	1.40
20	D	404	CLA	O2D-CGD	3.53	1.42	1.33
20	B	601	CLA	O2A-CGA	3.54	1.43	1.33
20	B	603	CLA	C4C-C3C	3.54	1.51	1.45
20	C	506	CLA	C1B-CHB	3.55	1.49	1.40
20	C	512	CLA	C3D-C2D	3.55	1.47	1.40
23	A	406	SQD	O48-C23	3.55	1.43	1.33
20	b	616	CLA	O2D-CGD	3.55	1.42	1.33
20	c	502	CLA	C3D-C2D	3.55	1.47	1.40
20	D	402	CLA	CHD-C4C	3.56	1.49	1.41
20	C	505	CLA	C3D-C2D	3.56	1.47	1.40
37	e	102	HEM	C3B-CAB	3.56	1.55	1.47
20	A	401	CLA	C4C-C3C	3.56	1.51	1.45
20	C	506	CLA	OBD-CAD	3.57	1.27	1.22
20	B	607	CLA	C1C-C2C	3.58	1.51	1.44
20	C	502	CLA	C3D-C2D	3.58	1.47	1.40
20	B	607	CLA	O2A-CGA	3.58	1.44	1.33
20	A	404	CLA	C1B-CHB	3.58	1.49	1.40
24	j	101	LMG	O7-C10	3.59	1.44	1.34
20	c	506	CLA	OBD-CAD	3.59	1.27	1.22
20	b	614	CLA	O2D-CGD	3.59	1.42	1.33
21	A	403	PHO	O2A-CGA	3.59	1.44	1.33
23	a	409	SQD	O47-C7	3.59	1.44	1.34
20	B	610	CLA	C3D-C2D	3.59	1.47	1.40
20	C	503	CLA	CHD-C4C	3.60	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	501	CLA	O2A-CGA	3.61	1.44	1.33
20	C	512	CLA	C1B-CHB	3.61	1.49	1.40
20	C	509	CLA	C3B-C2B	3.61	1.44	1.40
21	A	403	PHO	CHC-C1C	3.62	1.45	1.38
20	c	511	CLA	C1B-CHB	3.62	1.49	1.40
20	B	605	CLA	O2D-CGD	3.62	1.42	1.33
20	b	615	CLA	O2A-CGA	3.62	1.44	1.33
35	c	516	DGD	O1G-C1A	3.62	1.44	1.33
37	e	102	HEM	C3C-CAC	3.62	1.55	1.47
20	c	510	CLA	O2A-CGA	3.63	1.44	1.33
21	D	403	PHO	CHC-C4B	3.63	1.49	1.40
20	C	507	CLA	C3D-C2D	3.64	1.48	1.40
20	c	504	CLA	O2A-CGA	3.64	1.44	1.33
20	c	510	CLA	C3B-C2B	3.64	1.45	1.40
21	D	403	PHO	O2A-CGA	3.66	1.44	1.33
20	b	609	CLA	O2D-CGD	3.66	1.42	1.33
20	B	611	CLA	C3D-C2D	3.66	1.48	1.40
20	d	404	CLA	C4C-C3C	3.66	1.51	1.45
24	J	101	LMG	O8-C28	3.66	1.44	1.33
20	C	511	CLA	C3D-C2D	3.67	1.48	1.40
20	C	505	CLA	OBD-CAD	3.67	1.27	1.22
20	C	502	CLA	C1B-CHB	3.67	1.50	1.40
20	a	403	CLA	O2D-CGD	3.68	1.42	1.33
20	c	508	CLA	OBD-CAD	3.70	1.27	1.22
20	b	610	CLA	O2D-CGD	3.70	1.42	1.33
20	B	610	CLA	OBD-CAD	3.70	1.27	1.22
20	B	608	CLA	C3D-C2D	3.71	1.48	1.40
20	B	612	CLA	C3C-C2C	3.71	1.44	1.36
20	C	502	CLA	O2A-CGA	3.71	1.44	1.33
35	c	517	DGD	O2G-C1B	3.72	1.45	1.34
20	b	613	CLA	O2A-CGA	3.73	1.44	1.33
37	E	104	HEM	C3B-CAB	3.73	1.55	1.47
21	a	405	PHO	CHD-C4C	3.73	1.49	1.40
20	b	609	CLA	C3B-C2B	3.73	1.45	1.40
20	c	510	CLA	OBD-CAD	3.74	1.28	1.22
20	c	501	CLA	O2D-CGD	3.74	1.42	1.33
20	B	607	CLA	C4B-CHC	3.75	1.50	1.40
20	A	401	CLA	O2D-CGD	3.76	1.42	1.33
20	C	501	CLA	O2D-CGD	3.76	1.42	1.33
20	b	608	CLA	CHC-C1C	3.76	1.46	1.35
35	C	516	DGD	O2G-C1B	3.76	1.45	1.34
20	d	402	CLA	C1B-CHB	3.76	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	518	DGD	O1G-C1A	3.76	1.44	1.33
37	E	104	HEM	C3C-CAC	3.77	1.55	1.47
20	c	503	CLA	O2D-CGD	3.78	1.42	1.33
20	C	507	CLA	O2D-CGD	3.78	1.42	1.33
20	C	501	CLA	C3D-C2D	3.78	1.48	1.40
20	d	404	CLA	O2A-CGA	3.78	1.44	1.33
20	b	607	CLA	O2D-CGD	3.78	1.42	1.33
20	B	605	CLA	C3C-C2C	3.79	1.44	1.36
28	C	528	DMS	O-S	3.79	1.75	1.50
20	b	618	CLA	C3D-C2D	3.79	1.48	1.40
20	C	508	CLA	C3D-C2D	3.80	1.48	1.40
21	D	403	PHO	CHD-C1D	3.80	1.46	1.38
20	C	503	CLA	O2A-CGA	3.80	1.44	1.33
20	D	401	CLA	C3B-C2B	3.80	1.45	1.40
20	B	615	CLA	OBD-CAD	3.81	1.28	1.22
35	C	517	DGD	O1G-C1A	3.81	1.44	1.33
20	c	504	CLA	CHC-C1C	3.82	1.46	1.35
37	V	201	HEM	C3C-CAC	3.83	1.55	1.47
20	C	511	CLA	CHC-C1C	3.84	1.46	1.35
20	b	616	CLA	C3B-C2B	3.84	1.45	1.40
20	c	512	CLA	O2A-CGA	3.84	1.44	1.33
24	C	519	LMG	O7-C10	3.84	1.45	1.34
20	c	505	CLA	OBD-CAD	3.85	1.28	1.22
20	b	609	CLA	CHC-C1C	3.85	1.46	1.35
20	a	404	CLA	OBD-CAD	3.85	1.28	1.22
20	B	609	CLA	C3C-C2C	3.86	1.45	1.36
20	B	611	CLA	C4C-C3C	3.86	1.52	1.45
35	H	102	DGD	O2G-C1B	3.86	1.45	1.34
20	C	508	CLA	O2A-CGA	3.87	1.44	1.33
35	h	101	DGD	O2G-C1B	3.87	1.45	1.34
20	C	504	CLA	C3D-C2D	3.87	1.48	1.40
20	B	616	CLA	OBD-CAD	3.87	1.28	1.22
20	B	614	CLA	O2A-CGA	3.87	1.44	1.33
20	B	601	CLA	O2D-CGD	3.87	1.43	1.33
20	B	608	CLA	CHC-C1C	3.88	1.46	1.35
20	c	513	CLA	OBD-CAD	3.88	1.28	1.22
20	b	615	CLA	C3B-C2B	3.88	1.45	1.40
28	c	527	DMS	O-S	3.89	1.76	1.50
20	b	605	CLA	OBD-CAD	3.89	1.28	1.22
20	C	513	CLA	O2A-CGA	3.90	1.44	1.33
20	B	610	CLA	C3B-C2B	3.90	1.45	1.40
23	a	409	SQD	O48-C23	3.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	507	CLA	O2A-CGA	3.92	1.45	1.33
20	d	404	CLA	OBD-CAD	3.92	1.28	1.22
20	B	613	CLA	O2D-CGD	3.92	1.43	1.33
20	D	404	CLA	CHC-C1C	3.92	1.46	1.35
36	d	406	LHG	O8-C23	3.92	1.45	1.33
20	b	617	CLA	O2D-CGD	3.92	1.43	1.33
20	d	404	CLA	CHC-C1C	3.92	1.46	1.35
20	A	401	CLA	CHC-C1C	3.92	1.46	1.35
20	C	505	CLA	O2A-CGA	3.92	1.45	1.33
23	A	412	SQD	O47-C7	3.92	1.45	1.34
20	B	616	CLA	CHC-C1C	3.94	1.46	1.35
20	c	507	CLA	O2D-CGD	3.94	1.43	1.33
20	b	614	CLA	CHC-C1C	3.95	1.47	1.35
24	c	519	LMG	O7-C10	3.95	1.45	1.34
20	C	510	CLA	C3D-C2D	3.95	1.48	1.40
20	C	507	CLA	OBD-CAD	3.95	1.28	1.22
20	c	510	CLA	CHC-C1C	3.95	1.47	1.35
24	a	410	LMG	O7-C10	3.96	1.45	1.34
20	b	618	CLA	O2A-CGA	3.96	1.45	1.33
24	b	623	LMG	O7-C10	3.96	1.45	1.34
20	d	403	CLA	CHB-C4A	3.96	1.38	1.33
20	B	615	CLA	C3B-C2B	3.96	1.45	1.40
20	c	501	CLA	CHC-C1C	3.96	1.47	1.35
20	d	402	CLA	C3C-C2C	3.97	1.45	1.36
20	b	611	CLA	O2A-CGA	3.97	1.45	1.33
20	c	502	CLA	OBD-CAD	3.97	1.28	1.22
24	a	410	LMG	O8-C28	3.98	1.45	1.33
20	B	603	CLA	CHC-C1C	3.98	1.47	1.35
20	D	402	CLA	C3C-C2C	3.98	1.45	1.36
37	V	201	HEM	C3B-CAB	3.98	1.56	1.47
20	b	604	CLA	C3B-C2B	3.98	1.45	1.40
20	c	507	CLA	CHC-C1C	3.99	1.47	1.35
20	d	403	CLA	CHC-C1C	3.99	1.47	1.35
21	A	403	PHO	C3C-C2C	3.99	1.45	1.36
20	c	513	CLA	O2A-CGA	3.99	1.45	1.33
21	D	403	PHO	O2D-CGD	4.01	1.43	1.33
20	B	605	CLA	CHC-C1C	4.01	1.47	1.35
20	c	506	CLA	O2A-CGA	4.02	1.45	1.33
20	b	615	CLA	C3C-C2C	4.02	1.45	1.36
20	c	513	CLA	CHC-C1C	4.03	1.47	1.35
35	c	517	DGD	O1G-C1A	4.05	1.45	1.33
36	D	409	LHG	O8-C23	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	605	CLA	O2D-CGD	4.05	1.43	1.33
23	A	406	SQD	O47-C7	4.05	1.46	1.34
20	D	402	CLA	CHB-C4A	4.07	1.39	1.33
24	j	101	LMG	O8-C28	4.07	1.45	1.33
20	B	614	CLA	C3B-C2B	4.08	1.45	1.40
20	C	510	CLA	CHC-C1C	4.08	1.47	1.35
20	C	509	CLA	CHC-C1C	4.08	1.47	1.35
20	C	511	CLA	OBD-CAD	4.09	1.28	1.22
20	B	608	CLA	C3C-C2C	4.09	1.45	1.36
20	b	612	CLA	C3B-C2B	4.10	1.45	1.40
20	b	605	CLA	C3B-C2B	4.10	1.45	1.40
28	B	640	DMS	O-S	4.10	1.77	1.50
24	A	407	LMG	O8-C28	4.10	1.45	1.33
20	C	509	CLA	O2A-CGA	4.10	1.45	1.33
20	C	507	CLA	CHC-C1C	4.11	1.47	1.35
37	v	201	HEM	C3B-CAB	4.11	1.56	1.47
20	b	611	CLA	C3D-C2D	4.12	1.49	1.40
20	b	609	CLA	C3D-C2D	4.12	1.49	1.40
20	c	507	CLA	OBD-CAD	4.12	1.28	1.22
20	c	508	CLA	CHC-C1C	4.12	1.47	1.35
20	b	606	CLA	C3B-C2B	4.12	1.45	1.40
20	c	511	CLA	C3D-C2D	4.13	1.49	1.40
20	b	610	CLA	C3B-C2B	4.13	1.45	1.40
20	d	402	CLA	OBD-CAD	4.13	1.28	1.22
28	U	903[B]	DMS	O-S	4.13	1.78	1.50
20	C	513	CLA	CHC-C1C	4.13	1.47	1.35
20	B	612	CLA	CHC-C1C	4.14	1.47	1.35
20	b	604	CLA	CHC-C1C	4.14	1.47	1.35
20	C	503	CLA	O2D-CGD	4.14	1.43	1.33
20	C	504	CLA	CHC-C1C	4.14	1.47	1.35
20	B	604	CLA	CHC-C1C	4.14	1.47	1.35
20	C	512	CLA	O2A-CGA	4.15	1.45	1.33
20	B	606	CLA	O2D-CGD	4.16	1.43	1.33
20	B	607	CLA	OBD-CAD	4.16	1.28	1.22
20	a	407	CLA	O2D-CGD	4.16	1.43	1.33
20	b	608	CLA	C3D-C2D	4.17	1.49	1.40
20	B	606	CLA	C3B-C2B	4.17	1.45	1.40
24	A	407	LMG	O7-C10	4.17	1.46	1.34
28	v	202	DMS	O-S	4.18	1.78	1.50
20	b	617	CLA	CHC-C1C	4.18	1.47	1.35
24	b	623	LMG	O8-C28	4.18	1.45	1.33
24	c	519	LMG	O8-C28	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	505	CLA	C3B-C2B	4.19	1.45	1.40
21	a	406	PHO	O2D-CGD	4.19	1.44	1.33
20	a	407	CLA	O2A-CGA	4.20	1.45	1.33
20	B	606	CLA	OBD-CAD	4.20	1.28	1.22
20	c	509	CLA	O2D-CGD	4.20	1.44	1.33
20	b	616	CLA	OBD-CAD	4.20	1.28	1.22
36	D	407	LHG	O8-C23	4.20	1.45	1.33
20	c	508	CLA	C3D-C2D	4.21	1.49	1.40
28	O	306	DMS	O-S	4.21	1.78	1.50
20	B	603	CLA	O2D-CGD	4.21	1.44	1.33
20	c	510	CLA	O2D-CGD	4.21	1.44	1.33
20	B	605	CLA	C3B-C2B	4.21	1.45	1.40
20	b	613	CLA	O2D-CGD	4.22	1.44	1.33
20	B	608	CLA	C3B-C2B	4.22	1.45	1.40
20	B	602	CLA	CHC-C1C	4.22	1.47	1.35
20	c	502	CLA	O2D-CGD	4.22	1.44	1.33
20	B	611	CLA	O2D-CGD	4.22	1.44	1.33
23	a	401	SQD	O47-C7	4.23	1.46	1.34
24	C	524	LMG	O7-C10	4.23	1.46	1.34
28	u	203	DMS	O-S	4.23	1.78	1.50
20	C	505	CLA	O2D-CGD	4.23	1.44	1.33
23	l	101	SQD	O48-C23	4.24	1.45	1.33
21	a	406	PHO	CHD-C1D	4.24	1.47	1.38
23	A	412	SQD	O48-C23	4.24	1.45	1.33
20	b	606	CLA	O2D-CGD	4.24	1.44	1.33
20	b	613	CLA	CHC-C1C	4.26	1.47	1.35
28	d	414	DMS	O-S	4.26	1.78	1.50
28	B	637	DMS	O-S	4.26	1.78	1.50
20	C	509	CLA	C3D-C2D	4.26	1.49	1.40
23	f	101	SQD	O48-C23	4.27	1.46	1.33
28	C	530	DMS	O-S	4.27	1.79	1.50
20	b	606	CLA	CHC-C1C	4.27	1.47	1.35
28	d	413	DMS	O-S	4.28	1.79	1.50
20	A	404	CLA	CHC-C1C	4.28	1.47	1.35
28	U	902	DMS	O-S	4.28	1.79	1.50
28	b	633	DMS	O-S	4.28	1.79	1.50
20	C	506	CLA	O2A-CGA	4.28	1.46	1.33
20	C	513	CLA	C3D-C2D	4.29	1.49	1.40
20	B	615	CLA	CHC-C1C	4.30	1.48	1.35
23	l	101	SQD	O47-C7	4.30	1.47	1.34
28	D	414	DMS	O-S	4.30	1.79	1.50
28	C	527	DMS	O-S	4.31	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	526	DMS	O-S	4.31	1.79	1.50
28	U	903[A]	DMS	O-S	4.31	1.79	1.50
20	C	510	CLA	OBD-CAD	4.32	1.28	1.22
20	c	506	CLA	CHC-C1C	4.32	1.48	1.35
20	A	404	CLA	OBD-CAD	4.33	1.28	1.22
20	c	508	CLA	O2D-CGD	4.33	1.44	1.33
20	c	504	CLA	OBD-CAD	4.33	1.28	1.22
28	c	528	DMS	O-S	4.33	1.79	1.50
20	C	502	CLA	CHC-C1C	4.33	1.48	1.35
23	F	101	SQD	O48-C23	4.33	1.46	1.33
21	a	405	PHO	CHC-C1C	4.34	1.47	1.38
28	u	202	DMS	O-S	4.34	1.79	1.50
20	c	509	CLA	CHC-C1C	4.34	1.48	1.35
28	v	203	DMS	O-S	4.34	1.79	1.50
20	b	611	CLA	OBD-CAD	4.34	1.28	1.22
20	a	404	CLA	CHC-C1C	4.34	1.48	1.35
28	V	207	DMS	O-S	4.34	1.79	1.50
28	O	304	DMS	O-S	4.35	1.79	1.50
28	C	525[B]	DMS	O-S	4.35	1.79	1.50
28	V	209	DMS	O-S	4.35	1.79	1.50
28	O	303	DMS	O-S	4.35	1.79	1.50
21	a	405	PHO	O2D-CGD	4.35	1.44	1.33
20	B	611	CLA	CHC-C1C	4.36	1.48	1.35
28	c	532	DMS	O-S	4.36	1.79	1.50
20	b	616	CLA	CHC-C1C	4.36	1.48	1.35
20	c	512	CLA	OBD-CAD	4.36	1.28	1.22
23	b	622	SQD	O48-C23	4.37	1.46	1.33
20	C	512	CLA	CHC-C1C	4.37	1.48	1.35
20	B	613	CLA	CHC-C1C	4.39	1.48	1.35
20	C	508	CLA	CHC-C1C	4.39	1.48	1.35
28	v	209	DMS	O-S	4.39	1.79	1.50
21	a	405	PHO	C3B-C2B	4.39	1.45	1.37
20	c	506	CLA	C3C-C2C	4.39	1.46	1.36
36	E	103	LHG	O7-C7	4.40	1.46	1.33
20	b	617	CLA	OBD-CAD	4.40	1.29	1.22
28	o	304	DMS	O-S	4.40	1.79	1.50
20	c	509	CLA	C3C-C2C	4.41	1.46	1.36
20	B	602	CLA	OBD-CAD	4.41	1.29	1.22
28	v	208	DMS	O-S	4.41	1.79	1.50
20	b	603	CLA	OBD-CAD	4.41	1.29	1.22
28	C	533	DMS	O-S	4.42	1.80	1.50
36	E	103	LHG	O8-C23	4.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	609	CLA	O2D-CGD	4.42	1.44	1.33
20	C	505	CLA	CHC-C1C	4.42	1.48	1.35
20	b	607	CLA	CHC-C1C	4.42	1.48	1.35
20	a	407	CLA	C3C-C2C	4.42	1.46	1.36
28	A	417	DMS	O-S	4.42	1.80	1.50
28	O	309	DMS	O-S	4.43	1.80	1.50
28	B	635	DMS	O-S	4.43	1.80	1.50
20	B	612	CLA	OBD-CAD	4.43	1.29	1.22
28	v	205	DMS	O-S	4.43	1.80	1.50
28	V	204	DMS	O-S	4.44	1.80	1.50
28	O	305	DMS	O-S	4.44	1.80	1.50
23	b	622	SQD	O47-C7	4.44	1.47	1.34
24	c	518	LMG	O7-C10	4.44	1.47	1.34
20	a	403	CLA	CHC-C1C	4.44	1.48	1.35
28	V	208	DMS	O-S	4.44	1.80	1.50
20	b	608	CLA	O2D-CGD	4.45	1.44	1.33
28	u	204	DMS	O-S	4.45	1.80	1.50
28	i	104	DMS	O-S	4.45	1.80	1.50
28	b	634	DMS	O-S	4.45	1.80	1.50
20	b	618	CLA	O2D-CGD	4.45	1.44	1.33
28	F	102	DMS	O-S	4.46	1.80	1.50
28	C	531	DMS	O-S	4.46	1.80	1.50
20	C	509	CLA	O2D-CGD	4.46	1.44	1.33
20	C	508	CLA	OBD-CAD	4.46	1.29	1.22
28	v	204	DMS	O-S	4.47	1.80	1.50
28	o	307	DMS	O-S	4.48	1.80	1.50
20	c	511	CLA	CHC-C1C	4.48	1.48	1.35
20	c	501	CLA	C3C-C2C	4.48	1.46	1.36
28	c	534	DMS	O-S	4.48	1.80	1.50
20	C	510	CLA	C3B-C2B	4.48	1.46	1.40
20	B	616	CLA	C3C-C2C	4.48	1.46	1.36
28	c	529	DMS	O-S	4.48	1.80	1.50
28	b	637	DMS	O-S	4.48	1.80	1.50
20	C	501	CLA	C3B-C2B	4.49	1.46	1.40
28	c	531	DMS	O-S	4.49	1.80	1.50
28	B	641	DMS	O-S	4.49	1.80	1.50
28	v	206	DMS	O-S	4.49	1.80	1.50
20	d	404	CLA	C3C-C2C	4.49	1.46	1.36
28	V	206	DMS	O-S	4.50	1.80	1.50
28	D	416	DMS	O-S	4.50	1.80	1.50
28	C	529	DMS	O-S	4.50	1.80	1.50
20	B	607	CLA	O2D-CGD	4.50	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	601	CLA	C3B-C2B	4.50	1.46	1.40
20	C	510	CLA	C3C-C2C	4.50	1.46	1.36
20	B	613	CLA	C3C-C2C	4.51	1.46	1.36
24	J	101	LMG	O7-C10	4.51	1.47	1.34
20	B	614	CLA	C3C-C2C	4.51	1.46	1.36
20	d	403	CLA	C3B-C2B	4.52	1.46	1.40
21	a	406	PHO	C3C-C2C	4.53	1.46	1.36
28	b	635	DMS	O-S	4.53	1.80	1.50
28	o	303	DMS	O-S	4.53	1.80	1.50
28	O	307	DMS	O-S	4.53	1.80	1.50
20	B	615	CLA	C3C-C2C	4.53	1.46	1.36
21	a	405	PHO	C3C-C2C	4.53	1.46	1.36
21	a	406	PHO	CHC-C1C	4.54	1.47	1.38
28	A	416	DMS	O-S	4.54	1.80	1.50
20	c	511	CLA	C3C-C2C	4.54	1.46	1.36
20	a	403	CLA	C3B-C2B	4.54	1.46	1.40
28	b	632	DMS	O-S	4.54	1.80	1.50
20	c	510	CLA	C3C-C2C	4.55	1.46	1.36
20	b	615	CLA	O2D-CGD	4.55	1.44	1.33
28	d	415	DMS	O-S	4.55	1.80	1.50
20	b	611	CLA	O2D-CGD	4.55	1.44	1.33
28	b	636	DMS	O-S	4.55	1.80	1.50
28	O	310	DMS	O-S	4.56	1.80	1.50
20	B	606	CLA	CHC-C1C	4.56	1.48	1.35
28	V	205	DMS	O-S	4.56	1.81	1.50
28	B	639	DMS	O-S	4.56	1.81	1.50
20	B	616	CLA	O2D-CGD	4.57	1.45	1.33
28	B	645	DMS	O-S	4.57	1.81	1.50
20	B	611	CLA	C3B-C2B	4.57	1.46	1.40
28	o	305	DMS	O-S	4.58	1.81	1.50
20	a	407	CLA	OBD-CAD	4.58	1.29	1.22
20	c	503	CLA	CHC-C1C	4.58	1.48	1.35
20	C	501	CLA	CHC-C1C	4.59	1.48	1.35
28	c	533	DMS	O-S	4.59	1.81	1.50
28	D	413	DMS	O-S	4.59	1.81	1.50
20	b	613	CLA	C3C-C2C	4.59	1.46	1.36
28	H	103	DMS	O-S	4.60	1.81	1.50
20	b	608	CLA	C3C-C2C	4.60	1.46	1.36
20	B	602	CLA	O2D-CGD	4.60	1.45	1.33
35	D	406	DGD	O2G-C1B	4.60	1.47	1.34
28	h	102	DMS	O-S	4.60	1.81	1.50
28	b	640	DMS	O-S	4.61	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	535	DMS	O-S	4.61	1.81	1.50
20	b	603	CLA	CHC-C1C	4.61	1.48	1.35
23	a	401	SQD	O48-C23	4.61	1.47	1.33
28	v	207	DMS	O-S	4.61	1.81	1.50
28	B	636	DMS	O-S	4.62	1.81	1.50
37	v	201	HEM	C3C-CAC	4.62	1.57	1.47
20	c	502	CLA	CHC-C1C	4.63	1.49	1.35
28	B	638	DMS	O-S	4.63	1.81	1.50
28	b	641	DMS	O-S	4.63	1.81	1.50
35	d	416	DGD	O1G-C1A	4.63	1.47	1.33
24	C	524	LMG	O8-C28	4.63	1.47	1.33
28	O	308	DMS	O-S	4.63	1.81	1.50
20	D	401	CLA	C3C-C2C	4.64	1.46	1.36
24	C	519	LMG	O8-C28	4.64	1.47	1.33
20	C	502	CLA	C3C-C2C	4.64	1.46	1.36
35	d	416	DGD	O2G-C1B	4.64	1.48	1.34
24	c	518	LMG	O8-C28	4.65	1.47	1.33
28	A	415	DMS	O-S	4.65	1.81	1.50
20	c	505	CLA	CHC-C1C	4.65	1.49	1.35
28	o	306	DMS	O-S	4.66	1.81	1.50
20	c	512	CLA	CHC-C1C	4.66	1.49	1.35
20	b	613	CLA	C3B-C2B	4.66	1.46	1.40
28	b	638	DMS	O-S	4.67	1.81	1.50
28	j	105	DMS	O-S	4.68	1.81	1.50
20	b	618	CLA	CHC-C1C	4.69	1.49	1.35
20	c	512	CLA	O2D-CGD	4.69	1.45	1.33
28	A	418	DMS	O-S	4.69	1.81	1.50
20	B	604	CLA	O2D-CGD	4.69	1.45	1.33
20	b	612	CLA	CHC-C1C	4.69	1.49	1.35
28	B	643	DMS	O-S	4.69	1.81	1.50
28	B	642	DMS	O-S	4.69	1.81	1.50
20	B	610	CLA	CHC-C1C	4.69	1.49	1.35
28	o	302	DMS	O-S	4.69	1.81	1.50
20	B	603	CLA	C3C-C2C	4.70	1.46	1.36
20	c	507	CLA	C3B-C2B	4.70	1.46	1.40
20	c	504	CLA	C3B-C2B	4.70	1.46	1.40
35	D	406	DGD	O1G-C1A	4.70	1.47	1.33
28	C	525[A]	DMS	O-S	4.70	1.81	1.50
20	C	504	CLA	O2D-CGD	4.71	1.45	1.33
20	B	614	CLA	CHC-C1C	4.72	1.49	1.35
20	B	613	CLA	C3B-C2B	4.72	1.46	1.40
20	C	506	CLA	O2D-CGD	4.72	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	617	CLA	C3C-C2C	4.72	1.47	1.36
20	A	404	CLA	C3C-C2C	4.73	1.47	1.36
28	c	530	DMS	O-S	4.73	1.82	1.50
20	b	612	CLA	C3C-C2C	4.73	1.47	1.36
20	C	511	CLA	O2D-CGD	4.73	1.45	1.33
20	b	616	CLA	C3C-C2C	4.75	1.47	1.36
20	C	506	CLA	CHC-C1C	4.75	1.49	1.35
20	d	404	CLA	C3B-C2B	4.75	1.46	1.40
20	B	610	CLA	C3C-C2C	4.75	1.47	1.36
20	b	618	CLA	C3C-C2C	4.75	1.47	1.36
20	A	402	CLA	CHC-C1C	4.76	1.49	1.35
20	b	611	CLA	CHC-C1C	4.76	1.49	1.35
28	U	904	DMS	O-S	4.76	1.82	1.50
20	c	513	CLA	O2D-CGD	4.76	1.45	1.33
20	C	502	CLA	O2D-CGD	4.76	1.45	1.33
37	v	201	HEM	C3D-C2D	4.76	1.51	1.37
20	B	606	CLA	C3C-C2C	4.77	1.47	1.36
20	c	506	CLA	O2D-CGD	4.77	1.45	1.33
20	C	513	CLA	O2D-CGD	4.78	1.45	1.33
28	o	308	DMS	O-S	4.78	1.82	1.50
28	b	639	DMS	O-S	4.78	1.82	1.50
20	C	511	CLA	C3C-C2C	4.79	1.47	1.36
28	O	311	DMS	O-S	4.80	1.82	1.50
20	A	401	CLA	OBD-CAD	4.81	1.29	1.22
28	B	644	DMS	O-S	4.81	1.82	1.50
20	c	506	CLA	C3B-C2B	4.81	1.46	1.40
20	c	504	CLA	O2D-CGD	4.82	1.45	1.33
28	c	536	DMS	O-S	4.82	1.82	1.50
21	D	403	PHO	C3C-C2C	4.83	1.47	1.36
20	B	611	CLA	C3C-C2C	4.84	1.47	1.36
20	C	508	CLA	O2D-CGD	4.84	1.45	1.33
20	B	601	CLA	CHC-C1C	4.84	1.49	1.35
20	C	505	CLA	C3B-C2B	4.85	1.46	1.40
20	b	610	CLA	OBD-CAD	4.85	1.29	1.22
21	D	403	PHO	CHB-C1B	4.85	1.48	1.38
20	b	615	CLA	CHC-C1C	4.86	1.49	1.35
20	b	618	CLA	C3B-C2B	4.87	1.46	1.40
20	b	614	CLA	C3C-C2C	4.89	1.47	1.36
20	C	506	CLA	C3C-C2C	4.89	1.47	1.36
20	c	505	CLA	C3C-C2C	4.89	1.47	1.36
20	a	403	CLA	C3C-C2C	4.90	1.47	1.36
20	B	604	CLA	C3C-C2C	4.90	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	503	CLA	CHC-C1C	4.90	1.49	1.35
28	D	415	DMS	O-S	4.91	1.83	1.50
20	C	507	CLA	C3C-C2C	4.91	1.47	1.36
20	b	603	CLA	O2D-CGD	4.92	1.45	1.33
20	C	510	CLA	O2D-CGD	4.92	1.45	1.33
28	b	631	DMS	O-S	4.94	1.83	1.50
20	c	513	CLA	C3C-C2C	4.94	1.47	1.36
21	a	405	PHO	CHB-C1B	4.94	1.48	1.38
20	B	602	CLA	C3B-C2B	4.94	1.46	1.40
20	b	605	CLA	CHC-C1C	4.94	1.49	1.35
20	D	404	CLA	C3C-C2C	4.95	1.47	1.36
20	c	502	CLA	C3B-C2B	4.97	1.46	1.40
20	a	407	CLA	CHC-C1C	4.98	1.50	1.35
20	c	508	CLA	C3C-C2C	4.98	1.47	1.36
24	B	620	LMG	O8-C28	4.98	1.48	1.33
20	b	607	CLA	C3C-C2C	5.00	1.47	1.36
20	B	602	CLA	O2A-CGA	5.01	1.48	1.33
20	b	609	CLA	C3C-C2C	5.01	1.47	1.36
20	b	610	CLA	CHC-C1C	5.03	1.50	1.35
20	b	603	CLA	C3C-C2C	5.03	1.47	1.36
20	d	402	CLA	CHC-C1C	5.03	1.50	1.35
20	B	607	CLA	CHC-C1C	5.05	1.50	1.35
20	C	508	CLA	C3C-C2C	5.06	1.47	1.36
20	c	513	CLA	C3B-C2B	5.08	1.46	1.40
20	C	512	CLA	O2D-CGD	5.10	1.46	1.33
20	b	605	CLA	C3C-C2C	5.10	1.47	1.36
20	c	511	CLA	OBD-CAD	5.10	1.30	1.22
20	b	603	CLA	O2A-CGA	5.12	1.48	1.33
20	d	403	CLA	C3C-C2C	5.13	1.47	1.36
21	a	406	PHO	C3B-C2B	5.14	1.46	1.37
21	A	403	PHO	CHB-C1B	5.14	1.48	1.38
20	B	602	CLA	C3C-C2C	5.15	1.47	1.36
20	c	507	CLA	C3C-C2C	5.16	1.48	1.36
20	C	502	CLA	C3B-C2B	5.17	1.46	1.40
20	c	511	CLA	O2D-CGD	5.17	1.46	1.33
20	D	402	CLA	C3B-C2B	5.17	1.46	1.40
20	C	501	CLA	C3C-C2C	5.18	1.48	1.36
20	B	616	CLA	C3B-C2B	5.19	1.46	1.40
20	B	601	CLA	C3C-C2C	5.19	1.48	1.36
20	c	508	CLA	C3B-C2B	5.20	1.47	1.40
20	b	604	CLA	C3C-C2C	5.20	1.48	1.36
20	b	612	CLA	O2D-CGD	5.20	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	104	HEM	C3D-C2D	5.20	1.53	1.37
20	B	603	CLA	OBD-CAD	5.21	1.30	1.22
20	C	504	CLA	C3C-C2C	5.22	1.48	1.36
20	B	609	CLA	C3B-C2B	5.25	1.47	1.40
20	C	511	CLA	C3B-C2B	5.26	1.47	1.40
20	C	504	CLA	C3B-C2B	5.26	1.47	1.40
20	b	611	CLA	C3C-C2C	5.29	1.48	1.36
20	c	504	CLA	C3C-C2C	5.30	1.48	1.36
21	A	403	PHO	C3B-C2B	5.30	1.47	1.37
20	C	503	CLA	C3C-C2C	5.31	1.48	1.36
20	D	404	CLA	C3B-C2B	5.34	1.47	1.40
20	c	512	CLA	C3C-C2C	5.34	1.48	1.36
20	C	509	CLA	C3C-C2C	5.35	1.48	1.36
23	f	101	SQD	O47-C7	5.35	1.47	1.35
20	B	607	CLA	C3B-C2B	5.39	1.47	1.40
20	C	505	CLA	C3C-C2C	5.40	1.48	1.36
37	e	102	HEM	C3D-C2D	5.42	1.53	1.37
20	A	404	CLA	C3B-C2B	5.48	1.47	1.40
20	a	407	CLA	C3B-C2B	5.48	1.47	1.40
20	b	606	CLA	C3C-C2C	5.48	1.48	1.36
20	B	603	CLA	C3B-C2B	5.50	1.47	1.40
21	a	406	PHO	CHB-C1B	5.54	1.49	1.38
20	C	513	CLA	C3C-C2C	5.56	1.48	1.36
28	C	532	DMS	O-S	5.58	1.87	1.50
20	c	509	CLA	OBD-CAD	5.59	1.30	1.22
20	C	509	CLA	OBD-CAD	5.60	1.30	1.22
20	c	503	CLA	C3C-C2C	5.62	1.49	1.36
20	b	610	CLA	C3C-C2C	5.64	1.49	1.36
20	c	511	CLA	C3B-C2B	5.68	1.47	1.40
20	C	512	CLA	C3C-C2C	5.69	1.49	1.36
20	c	501	CLA	OBD-CAD	5.77	1.31	1.22
20	C	503	CLA	C3B-C2B	5.79	1.47	1.40
20	C	506	CLA	C3B-C2B	5.80	1.47	1.40
20	B	607	CLA	C3C-C2C	5.87	1.49	1.36
20	c	503	CLA	C3B-C2B	5.91	1.47	1.40
20	b	603	CLA	C3B-C2B	5.93	1.47	1.40
20	c	501	CLA	C3B-C2B	5.94	1.47	1.40
20	b	611	CLA	C3B-C2B	5.94	1.47	1.40
20	C	508	CLA	C3B-C2B	6.05	1.48	1.40
20	d	402	CLA	C3B-C2B	6.07	1.48	1.40
20	c	509	CLA	C3B-C2B	6.11	1.48	1.40
21	D	403	PHO	C3B-C2B	6.16	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	617	CLA	C3B-C2B	6.43	1.48	1.40
20	C	513	CLA	C3B-C2B	6.49	1.48	1.40
20	C	512	CLA	C3B-C2B	6.49	1.48	1.40
20	c	512	CLA	C3B-C2B	6.53	1.48	1.40
20	C	507	CLA	C3B-C2B	6.81	1.49	1.40
20	b	608	CLA	C3B-C2B	6.92	1.49	1.40

All (1894) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	f	101	SQD	O9-S-C6	-23.68	90.24	106.92
23	f	101	SQD	O9-S-O7	-11.63	81.11	113.96
23	f	101	SQD	O8-S-O9	-11.61	85.57	111.26
37	E	104	HEM	CBD-CAD-C3D	-7.33	99.61	112.47
22	d	405	BCR	C24-C23-C22	-6.78	115.96	126.21
20	b	604	CLA	C3B-CAB-CBB	-6.56	113.20	126.40
37	e	102	HEM	CBA-CAA-C2A	-6.51	101.04	112.49
20	B	612	CLA	CHD-C4C-C3C	-6.49	114.89	124.91
20	B	606	CLA	CHD-C4C-C3C	-6.41	115.02	124.91
20	B	615	CLA	O2D-CGD-O1D	-5.89	111.37	123.77
37	e	102	HEM	CBD-CAD-C3D	-5.82	102.25	112.47
22	b	619	BCR	C7-C8-C9	-5.76	117.50	126.21
20	B	607	CLA	CHD-C4C-C3C	-5.76	116.02	124.91
20	C	510	CLA	CHD-C4C-C3C	-5.66	116.17	124.91
20	b	618	CLA	CHD-C4C-C3C	-5.58	116.30	124.91
20	c	510	CLA	CHD-C4C-C3C	-5.56	116.33	124.91
32	V	202	HTG	O5-C1-C2	-5.55	102.65	110.22
23	a	409	SQD	C1-O5-C5	-5.54	102.88	113.74
20	c	501	CLA	CHD-C4C-C3C	-5.53	116.38	124.91
38	H	101	RRX	C24-C23-C22	-5.48	117.93	126.21
20	B	602	CLA	CHD-C4C-C3C	-5.45	116.50	124.91
37	V	201	HEM	CBD-CAD-C3D	-5.44	102.93	112.47
20	b	605	CLA	C1C-C2C-C3C	-5.42	100.92	106.93
20	a	404	CLA	C1C-C2C-C3C	-5.41	100.93	106.93
20	B	604	CLA	C1C-C2C-C3C	-5.37	100.97	106.93
20	c	513	CLA	CHD-C4C-C3C	-5.35	116.66	124.91
20	b	614	CLA	CHD-C4C-C3C	-5.33	116.69	124.91
20	B	611	CLA	CHD-C4C-C3C	-5.24	116.82	124.91
20	B	604	CLA	CHD-C4C-C3C	-5.21	116.87	124.91
22	D	405	BCR	C24-C23-C22	-5.20	118.35	126.21
20	B	609	CLA	C3B-CAB-CBB	-5.17	116.00	126.40
20	b	605	CLA	O2D-CGD-O1D	-5.15	112.93	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	504	CLA	C1C-C2C-C3C	-5.15	101.22	106.93
22	B	617	BCR	C7-C8-C9	-5.14	118.44	126.21
22	D	405	BCR	C7-C8-C9	-5.14	118.44	126.21
20	C	502	CLA	CHD-C4C-C3C	-5.10	117.05	124.91
37	v	201	HEM	CBD-CAD-C3D	-5.09	103.54	112.47
23	A	406	SQD	C1-C2-C3	-5.08	99.91	109.98
20	B	613	CLA	C4B-CHC-C1C	-5.07	119.27	129.34
21	A	403	PHO	C3D-C2D-C1D	-5.02	97.52	105.76
20	B	609	CLA	CHD-C4C-C3C	-5.02	117.16	124.91
20	c	505	CLA	CHD-C4C-C3C	-4.99	117.20	124.91
20	C	510	CLA	C4B-CHC-C1C	-4.98	119.43	129.34
20	b	606	CLA	CHD-C4C-C3C	-4.98	117.22	124.91
20	c	507	CLA	CHD-C4C-C3C	-4.98	117.23	124.91
20	C	505	CLA	CHD-C4C-C3C	-4.95	117.28	124.91
20	a	403	CLA	CHD-C4C-C3C	-4.94	117.28	124.91
20	B	610	CLA	CHD-C4C-C3C	-4.93	117.29	124.91
20	d	404	CLA	CHD-C4C-C3C	-4.92	117.32	124.91
20	c	513	CLA	C3B-CAB-CBB	-4.91	116.53	126.40
20	B	616	CLA	C3B-CAB-CBB	-4.89	116.57	126.40
34	a	418	LMT	C3'-C4'-C5'	-4.87	99.72	110.85
20	c	506	CLA	CHD-C4C-C3C	-4.85	117.42	124.91
20	a	403	CLA	C4B-CHC-C1C	-4.85	119.70	129.34
22	B	619	BCR	C38-C26-C25	-4.83	119.48	124.62
20	C	501	CLA	O2D-CGD-O1D	-4.80	113.66	123.77
20	b	607	CLA	CHD-C4C-C3C	-4.79	117.51	124.91
20	B	602	CLA	O1D-CGD-CBD	-4.79	117.19	124.64
23	a	409	SQD	C1-C2-C3	-4.77	100.52	109.98
20	D	402	CLA	CHD-C4C-C3C	-4.77	117.55	124.91
21	a	405	PHO	C4C-C3C-C2C	-4.75	101.63	106.80
20	b	607	CLA	C1C-C2C-C3C	-4.73	101.69	106.93
20	a	407	CLA	CHD-C4C-C3C	-4.73	117.61	124.91
22	b	619	BCR	C24-C23-C22	-4.72	119.07	126.21
20	B	614	CLA	CHD-C4C-C3C	-4.72	117.63	124.91
20	c	507	CLA	C1C-C2C-C3C	-4.69	101.72	106.93
20	C	509	CLA	C1C-C2C-C3C	-4.69	101.73	106.93
21	a	405	PHO	C3D-C2D-C1D	-4.68	98.08	105.76
20	b	608	CLA	CHD-C4C-C3C	-4.68	117.69	124.91
22	c	514	BCR	C24-C23-C22	-4.68	119.14	126.21
37	v	201	HEM	C3B-CAB-CBB	-4.67	117.01	126.40
20	B	613	CLA	C3B-CAB-CBB	-4.64	117.07	126.40
20	d	403	CLA	CHD-C4C-C3C	-4.64	117.75	124.91
20	b	610	CLA	CHD-C4C-C3C	-4.63	117.76	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	101	BCR	C33-C5-C6	-4.63	119.69	124.62
20	b	605	CLA	CHD-C4C-C3C	-4.63	117.77	124.91
20	C	503	CLA	C3B-CAB-CBB	-4.61	117.12	126.40
20	C	506	CLA	CHD-C4C-C3C	-4.59	117.83	124.91
20	c	512	CLA	CHD-C4C-C3C	-4.55	117.88	124.91
20	C	501	CLA	CHD-C4C-C3C	-4.54	117.90	124.91
20	b	615	CLA	C1C-C2C-C3C	-4.54	101.90	106.93
21	D	403	PHO	C3D-C2D-C1D	-4.54	98.32	105.76
20	B	607	CLA	O2D-CGD-O1D	-4.54	114.22	123.77
32	v	210	HTG	O5-C1-C2	-4.53	104.03	110.22
20	b	613	CLA	CHD-C4C-C3C	-4.53	117.93	124.91
20	c	503	CLA	CHD-C4C-C3C	-4.51	117.95	124.91
22	b	621	BCR	C24-C23-C22	-4.51	119.40	126.21
20	c	501	CLA	C3B-CAB-CBB	-4.50	117.35	126.40
20	b	615	CLA	CHD-C4C-C3C	-4.50	117.96	124.91
36	D	407	LHG	O8-C23-O10	-4.50	111.72	123.51
20	D	402	CLA	C1C-C2C-C3C	-4.49	101.95	106.93
20	B	608	CLA	C1C-C2C-C3C	-4.48	101.96	106.93
20	A	402	CLA	C4B-CHC-C1C	-4.48	120.44	129.34
20	B	607	CLA	C4B-CHC-C1C	-4.47	120.45	129.34
20	C	503	CLA	C1C-C2C-C3C	-4.47	101.97	106.93
20	B	614	CLA	C3B-CAB-CBB	-4.45	117.44	126.40
20	c	502	CLA	C3B-CAB-CBB	-4.44	117.47	126.40
20	b	610	CLA	C1C-C2C-C3C	-4.44	102.01	106.93
20	C	507	CLA	C1C-C2C-C3C	-4.43	102.01	106.93
20	c	511	CLA	CHD-C4C-C3C	-4.41	118.11	124.91
23	A	412	SQD	C1-O5-C5	-4.40	105.10	113.74
20	b	617	CLA	CHD-C4C-C3C	-4.40	118.12	124.91
20	C	504	CLA	CHD-C4C-C3C	-4.37	118.17	124.91
20	c	501	CLA	C1C-C2C-C3C	-4.36	102.10	106.93
20	B	601	CLA	C4B-CHC-C1C	-4.34	120.71	129.34
20	c	509	CLA	CHD-C4C-C3C	-4.34	118.21	124.91
20	c	507	CLA	C4B-CHC-C1C	-4.34	120.72	129.34
20	c	512	CLA	C3B-CAB-CBB	-4.32	117.72	126.40
20	B	613	CLA	CHD-C4C-C3C	-4.31	118.25	124.91
20	b	603	CLA	CHD-C4C-C3C	-4.31	118.26	124.91
20	C	513	CLA	C1C-C2C-C3C	-4.31	102.15	106.93
20	d	404	CLA	C3B-CAB-CBB	-4.31	117.74	126.40
20	c	501	CLA	O2D-CGD-O1D	-4.29	114.73	123.77
20	c	503	CLA	C1C-C2C-C3C	-4.29	102.17	106.93
20	a	407	CLA	C3B-CAB-CBB	-4.28	117.79	126.40
20	D	401	CLA	C1C-C2C-C3C	-4.28	102.19	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	516	DGD	O3G-C3G-C2G	-4.28	100.82	110.99
20	C	504	CLA	C3B-CAB-CBB	-4.27	117.81	126.40
21	A	403	PHO	C4D-ND-C1D	-4.26	99.19	106.99
20	d	403	CLA	C1C-C2C-C3C	-4.26	102.21	106.93
20	b	614	CLA	C3B-CAB-CBB	-4.25	117.85	126.40
20	c	504	CLA	CHD-C4C-C3C	-4.25	118.35	124.91
20	D	401	CLA	C3B-CAB-CBB	-4.25	117.86	126.40
20	A	402	CLA	CHD-C4C-C3C	-4.24	118.36	124.91
20	C	503	CLA	CHD-C4C-C3C	-4.24	118.37	124.91
20	b	609	CLA	CHD-C4C-C3C	-4.23	118.39	124.91
20	b	603	CLA	C1C-C2C-C3C	-4.22	102.25	106.93
20	C	502	CLA	C4B-CHC-C1C	-4.21	120.98	129.34
20	b	606	CLA	C1C-C2C-C3C	-4.20	102.28	106.93
22	B	617	BCR	C15-C14-C13	-4.20	121.12	127.22
20	B	608	CLA	CHD-C4C-C3C	-4.19	118.44	124.91
20	C	505	CLA	C1C-C2C-C3C	-4.19	102.29	106.93
20	D	404	CLA	C1C-C2C-C3C	-4.18	102.30	106.93
20	c	511	CLA	C1C-C2C-C3C	-4.17	102.31	106.93
20	d	404	CLA	C1C-C2C-C3C	-4.16	102.32	106.93
20	D	401	CLA	CHD-C4C-C3C	-4.15	118.50	124.91
20	B	614	CLA	C1C-C2C-C3C	-4.15	102.33	106.93
20	d	402	CLA	C3B-CAB-CBB	-4.15	118.06	126.40
20	B	616	CLA	C1C-C2C-C3C	-4.14	102.34	106.93
20	B	601	CLA	CHD-C4C-C3C	-4.14	118.52	124.91
22	K	102	BCR	C7-C8-C9	-4.14	119.96	126.21
20	b	618	CLA	O1D-CGD-CBD	-4.14	118.20	124.64
24	b	623	LMG	C9-C8-C7	-4.13	102.45	112.08
20	B	602	CLA	C1C-C2C-C3C	-4.12	102.36	106.93
32	V	202	HTG	C1-O5-C5	-4.12	104.78	112.73
20	c	510	CLA	C1C-C2C-C3C	-4.11	102.38	106.93
20	C	511	CLA	C1C-C2C-C3C	-4.10	102.39	106.93
22	B	619	BCR	C24-C23-C22	-4.09	120.03	126.21
20	b	604	CLA	C1C-C2C-C3C	-4.06	102.43	106.93
20	B	603	CLA	C1C-C2C-C3C	-4.06	102.43	106.93
20	b	614	CLA	C4B-CHC-C1C	-4.06	121.28	129.34
20	c	508	CLA	CHD-C4C-C3C	-4.05	118.66	124.91
20	b	612	CLA	CHD-C4C-C3C	-4.05	118.66	124.91
20	C	501	CLA	C1C-C2C-C3C	-4.04	102.45	106.93
20	c	506	CLA	C1C-C2C-C3C	-4.03	102.46	106.93
34	B	627	LMT	O5'-C1'-O1'	-4.03	108.91	113.00
20	B	605	CLA	CHD-C4C-C3C	-4.03	118.69	124.91
20	C	512	CLA	CHD-C4C-C3C	-4.02	118.70	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	406	PHO	C3D-C2D-C1D	-4.01	99.18	105.76
23	a	401	SQD	C1-O5-C5	-4.01	105.89	113.74
20	b	608	CLA	C4B-CHC-C1C	-4.00	121.38	129.34
21	a	406	PHO	C4C-C3C-C2C	-4.00	102.44	106.80
20	B	605	CLA	C1C-C2C-C3C	-4.00	102.50	106.93
22	d	405	BCR	C11-C10-C9	-4.00	121.41	127.22
20	b	609	CLA	C4B-CHC-C1C	-4.00	121.39	129.34
20	b	609	CLA	C3B-CAB-CBB	-3.98	118.40	126.40
20	B	612	CLA	C4B-CHC-C1C	-3.97	121.45	129.34
35	H	102	DGD	O1G-C1A-O1A	-3.95	113.15	123.51
21	A	403	PHO	C4C-C3C-C2C	-3.95	102.50	106.80
20	b	608	CLA	C1C-C2C-C3C	-3.94	102.56	106.93
22	t	101	BCR	C33-C5-C6	-3.93	120.43	124.62
35	c	515	DGD	O5D-C6D-C5D	-3.91	102.18	109.14
20	b	617	CLA	C1C-C2C-C3C	-3.91	102.60	106.93
20	c	513	CLA	C1C-C2C-C3C	-3.90	102.60	106.93
22	d	405	BCR	C39-C30-C25	-3.90	104.38	110.33
20	a	404	CLA	CHD-C4C-C3C	-3.90	118.90	124.91
20	b	611	CLA	C1C-C2C-C3C	-3.89	102.61	106.93
20	d	402	CLA	C2A-C1A-CHA	-3.88	117.54	123.80
20	A	402	CLA	C1C-C2C-C3C	-3.88	102.63	106.93
22	b	619	BCR	C33-C5-C6	-3.87	120.50	124.62
20	C	507	CLA	CHD-C4C-C3C	-3.87	118.94	124.91
20	c	501	CLA	C4B-CHC-C1C	-3.86	121.66	129.34
20	B	616	CLA	CHD-C4C-C3C	-3.84	118.98	124.91
23	A	406	SQD	C1-O5-C5	-3.83	106.23	113.74
20	C	513	CLA	CHD-C4C-C3C	-3.81	119.03	124.91
20	b	614	CLA	C1C-C2C-C3C	-3.81	102.70	106.93
20	C	512	CLA	C3B-CAB-CBB	-3.81	118.74	126.40
20	C	508	CLA	C1C-C2C-C3C	-3.81	102.71	106.93
20	C	509	CLA	CHD-C4C-C3C	-3.81	119.03	124.91
22	C	514	BCR	C38-C26-C25	-3.79	120.59	124.62
20	A	404	CLA	CHD-C4C-C3C	-3.78	119.07	124.91
22	t	101	BCR	C29-C28-C27	-3.78	101.86	111.42
20	B	609	CLA	C1C-C2C-C3C	-3.76	102.77	106.93
32	V	202	HTG	C1-C2-C3	-3.75	102.19	110.58
27	d	412	PL9	C36-C37-C38	-3.75	101.77	111.61
20	b	616	CLA	CHD-C4C-C3C	-3.75	119.12	124.91
20	b	610	CLA	O2A-CGA-O1A	-3.75	113.69	123.51
21	D	403	PHO	C4C-C3C-C2C	-3.74	102.73	106.80
27	D	412	PL9	C40-C39-C38	-3.74	116.34	123.58
20	b	616	CLA	C1C-C2C-C3C	-3.74	102.79	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	509	CLA	C4B-CHC-C1C	-3.73	121.92	129.34
20	B	608	CLA	O2D-CGD-O1D	-3.73	115.92	123.77
20	c	511	CLA	O2D-CGD-O1D	-3.72	115.95	123.77
20	c	504	CLA	C1C-C2C-C3C	-3.71	102.81	106.93
20	A	402	CLA	O2D-CGD-O1D	-3.71	115.95	123.77
22	b	620	BCR	C38-C26-C25	-3.71	120.67	124.62
20	A	401	CLA	C1D-CHD-C4C	-3.71	115.75	125.40
20	B	615	CLA	C2A-C1A-CHA	-3.71	117.82	123.80
20	B	608	CLA	C2A-C1A-CHA	-3.70	117.83	123.80
20	a	403	CLA	C3B-CAB-CBB	-3.70	118.96	126.40
20	b	616	CLA	C4B-CHC-C1C	-3.69	122.01	129.34
20	b	611	CLA	CHD-C4C-C3C	-3.69	119.22	124.91
20	B	602	CLA	C3B-CAB-CBB	-3.69	118.98	126.40
20	C	510	CLA	C1C-C2C-C3C	-3.68	102.85	106.93
20	c	505	CLA	C3B-CAB-CBB	-3.68	118.99	126.40
20	B	615	CLA	CHD-C4C-C3C	-3.67	119.24	124.91
20	B	610	CLA	OBD-CAD-C3D	-3.67	121.61	128.09
20	B	603	CLA	CHD-C4C-C3C	-3.66	119.26	124.91
20	b	606	CLA	O2D-CGD-O1D	-3.63	116.13	123.77
21	A	403	PHO	C1C-C2C-C3C	-3.63	102.24	106.43
20	c	512	CLA	C1C-C2C-C3C	-3.62	102.92	106.93
20	B	606	CLA	C3B-CAB-CBB	-3.61	119.13	126.40
21	D	403	PHO	C4D-ND-C1D	-3.61	100.38	106.99
22	B	617	BCR	C24-C23-C22	-3.61	120.76	126.21
22	b	621	BCR	C38-C26-C25	-3.60	120.78	124.62
20	C	512	CLA	C1C-C2C-C3C	-3.59	102.95	106.93
22	K	102	BCR	C38-C26-C25	-3.57	120.82	124.62
20	B	606	CLA	C4B-CHC-C1C	-3.57	122.25	129.34
20	c	503	CLA	C3B-CAB-CBB	-3.56	119.23	126.40
20	C	513	CLA	O2D-CGD-O1D	-3.56	116.28	123.77
20	D	402	CLA	C3B-CAB-CBB	-3.56	119.24	126.40
23	F	101	SQD	C1-C2-C3	-3.56	102.93	109.98
20	d	404	CLA	C4B-CHC-C1C	-3.55	122.28	129.34
20	A	401	CLA	CHD-C4C-C3C	-3.55	119.44	124.91
20	b	617	CLA	C3B-CAB-CBB	-3.55	119.26	126.40
20	B	604	CLA	C2A-C1A-CHA	-3.54	118.09	123.80
20	b	604	CLA	OBD-CAD-C3D	-3.54	121.83	128.09
20	D	401	CLA	O2D-CGD-O1D	-3.54	116.32	123.77
20	B	605	CLA	C6-C5-C3	-3.53	106.42	112.76
20	B	614	CLA	C2A-C1A-CHA	-3.51	118.14	123.80
20	a	403	CLA	C1C-C2C-C3C	-3.51	103.04	106.93
20	a	404	CLA	C4B-CHC-C1C	-3.51	122.37	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	T	101	BCR	C38-C26-C25	-3.51	120.89	124.62
22	c	514	BCR	C32-C1-C6	-3.50	104.98	110.33
20	C	506	CLA	C1C-C2C-C3C	-3.50	103.05	106.93
20	C	502	CLA	C1C-C2C-C3C	-3.50	103.05	106.93
20	B	601	CLA	O2D-CGD-O1D	-3.50	116.41	123.77
20	a	403	CLA	C1D-CHD-C4C	-3.49	116.31	125.40
20	B	605	CLA	C3B-CAB-CBB	-3.48	119.40	126.40
20	B	602	CLA	C4-C3-C2	-3.48	116.85	123.58
20	b	616	CLA	C4-C3-C2	-3.47	116.87	123.58
23	b	622	SQD	O5-C1-C2	-3.47	103.07	110.28
22	k	101	BCR	C7-C8-C9	-3.47	120.97	126.21
20	b	609	CLA	C1C-C2C-C3C	-3.47	103.09	106.93
20	A	404	CLA	C1C-C2C-C3C	-3.47	103.09	106.93
34	J	103	LMT	C3'-C4'-C5'	-3.46	104.05	110.23
20	D	401	CLA	C2A-C1A-CHA	-3.46	118.22	123.80
38	H	101	RRX	C7-C8-C9	-3.46	120.98	126.21
20	C	511	CLA	CHD-C4C-C3C	-3.46	119.57	124.91
23	l	101	SQD	C1-O5-C5	-3.46	106.96	113.74
20	b	606	CLA	C6-C5-C3	-3.45	106.57	112.76
22	B	617	BCR	C33-C5-C6	-3.45	120.95	124.62
20	b	613	CLA	C1C-C2C-C3C	-3.44	103.12	106.93
22	D	405	BCR	C38-C26-C25	-3.43	120.97	124.62
20	C	501	CLA	C2A-C1A-CHA	-3.41	118.31	123.80
37	V	201	HEM	C3B-CAB-CBB	-3.40	119.55	126.40
35	c	517	DGD	O1G-C1A-O1A	-3.40	114.60	123.51
20	C	507	CLA	O2D-CGD-O1D	-3.40	116.62	123.77
20	D	402	CLA	C4B-CHC-C1C	-3.39	122.60	129.34
22	B	619	BCR	C33-C5-C6	-3.39	121.01	124.62
20	C	510	CLA	O1D-CGD-CBD	-3.38	119.38	124.64
20	a	404	CLA	C3B-CAB-CBB	-3.37	119.62	126.40
23	A	412	SQD	C1-C2-C3	-3.37	103.31	109.98
20	a	407	CLA	O2D-CGD-O1D	-3.36	116.70	123.77
20	A	401	CLA	C3B-CAB-CBB	-3.36	119.65	126.40
20	d	403	CLA	C4B-CHC-C1C	-3.35	122.67	129.34
21	a	405	PHO	O2D-CGD-O1D	-3.35	116.72	123.77
20	A	401	CLA	C7-C6-C5	-3.35	103.28	113.16
24	j	101	LMG	O2-C2-C1	-3.34	102.60	110.01
20	b	613	CLA	C4B-CHC-C1C	-3.34	122.71	129.34
27	D	412	PL9	C36-C37-C38	-3.34	102.85	111.61
20	B	612	CLA	C1D-CHD-C4C	-3.34	116.72	125.40
36	d	406	LHG	O8-C23-O10	-3.34	114.77	123.51
20	B	608	CLA	C3B-CAB-CBB	-3.33	119.69	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	502	CLA	CHD-C4C-C3C	-3.33	119.77	124.91
20	d	402	CLA	C1C-C2C-C3C	-3.32	103.25	106.93
20	c	508	CLA	C1C-C2C-C3C	-3.32	103.25	106.93
22	b	621	BCR	C33-C5-C6	-3.32	121.08	124.62
20	B	606	CLA	C1C-C2C-C3C	-3.31	103.26	106.93
24	C	519	LMG	O1-C7-C8	-3.31	103.12	110.99
22	d	405	BCR	C38-C26-C25	-3.30	121.10	124.62
20	B	613	CLA	C2A-C1A-CHA	-3.30	118.48	123.80
20	B	610	CLA	C1C-C2C-C3C	-3.29	103.28	106.93
20	B	614	CLA	C4B-CHC-C1C	-3.29	122.80	129.34
22	b	619	BCR	C23-C22-C21	-3.29	113.66	118.95
21	A	403	PHO	O2D-CGD-O1D	-3.28	116.86	123.77
22	K	102	BCR	C24-C23-C22	-3.28	121.26	126.21
20	b	604	CLA	C2A-C1A-CHA	-3.28	118.52	123.80
22	C	515	BCR	C7-C8-C9	-3.26	121.28	126.21
20	b	610	CLA	C6-C5-C3	-3.26	106.91	112.76
20	B	607	CLA	C1C-C2C-C3C	-3.26	103.32	106.93
20	B	609	CLA	C2A-C3A-C4A	-3.26	98.49	101.84
20	c	509	CLA	C3B-CAB-CBB	-3.26	119.85	126.40
20	B	608	CLA	CBC-CAC-C3C	-3.26	102.49	112.38
21	a	406	PHO	C4D-ND-C1D	-3.25	101.03	106.99
22	A	405	BCR	C38-C26-C25	-3.25	121.16	124.62
27	D	412	PL9	C22-C23-C24	-3.25	120.59	127.75
20	B	605	CLA	O2D-CGD-O1D	-3.24	116.95	123.77
20	C	509	CLA	C3B-CAB-CBB	-3.24	119.88	126.40
22	K	101	BCR	C38-C26-C25	-3.23	121.18	124.62
20	C	501	CLA	C3B-CAB-CBB	-3.23	119.90	126.40
24	B	620	LMG	C9-C8-C7	-3.22	104.57	112.08
37	E	104	HEM	C3B-CAB-CBB	-3.22	119.92	126.40
38	H	101	RRX	C10-C11-C12	-3.22	113.16	123.11
21	a	405	PHO	C1C-C2C-C3C	-3.21	102.72	106.43
20	B	602	CLA	C2A-C1A-CHA	-3.21	118.62	123.80
20	d	402	CLA	O2D-CGD-O1D	-3.21	117.02	123.77
20	B	613	CLA	O2D-CGD-O1D	-3.21	117.02	123.77
20	c	502	CLA	C1C-C2C-C3C	-3.20	103.38	106.93
20	b	618	CLA	C4-C3-C2	-3.20	117.39	123.58
20	b	605	CLA	C3B-CAB-CBB	-3.20	119.96	126.40
20	B	611	CLA	C4C-C3C-C2C	-3.20	101.83	106.94
20	B	606	CLA	C1D-CHD-C4C	-3.19	117.10	125.40
20	b	617	CLA	O2D-CGD-O1D	-3.19	117.06	123.77
20	b	617	CLA	C1D-CHD-C4C	-3.19	117.11	125.40
20	b	613	CLA	OBD-CAD-CBD	-3.19	121.13	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	605	CLA	C2A-C3A-C4A	-3.19	98.57	101.84
20	c	510	CLA	C2A-C1A-CHA	-3.19	118.66	123.80
20	c	509	CLA	C1C-C2C-C3C	-3.18	103.41	106.93
20	b	610	CLA	O2D-CGD-O1D	-3.17	117.09	123.77
27	a	415	PL9	O1-C4-C3	-3.17	116.73	120.71
20	C	508	CLA	CHD-C4C-C3C	-3.17	120.02	124.91
20	b	618	CLA	CBC-CAC-C3C	-3.16	102.79	112.38
20	c	508	CLA	C2A-C1A-CHA	-3.16	118.71	123.80
20	b	608	CLA	O2D-CGD-O1D	-3.15	117.13	123.77
37	e	102	HEM	C3C-CAC-CBC	-3.15	120.06	126.40
27	A	411	PL9	C17-C18-C19	-3.15	120.81	127.75
20	c	512	CLA	CBA-CAA-C2A	-3.14	105.87	113.96
20	b	618	CLA	C4B-CHC-C1C	-3.13	123.11	129.34
21	A	403	PHO	C1C-NC-C4C	-3.13	100.54	106.50
20	b	610	CLA	C3B-CAB-CBB	-3.13	120.11	126.40
38	x	101	RRX	C33-C5-C6	-3.12	121.30	124.62
20	B	612	CLA	C3B-CAB-CBB	-3.12	120.12	126.40
23	A	412	SQD	O6-C44-C45	-3.12	103.56	110.99
20	B	616	CLA	C1D-CHD-C4C	-3.12	117.28	125.40
22	k	102	BCR	C33-C5-C6	-3.11	121.30	124.62
20	c	505	CLA	O2D-CGD-O1D	-3.11	117.22	123.77
20	c	505	CLA	C1C-C2C-C3C	-3.10	103.49	106.93
20	C	507	CLA	C3B-CAB-CBB	-3.10	120.16	126.40
20	a	407	CLA	C1C-C2C-C3C	-3.10	103.50	106.93
20	C	508	CLA	C5-C3-C2	-3.09	115.22	120.98
20	C	506	CLA	O1D-CGD-CBD	-3.09	119.83	124.64
22	B	619	BCR	C32-C1-C6	-3.08	105.62	110.33
27	d	412	PL9	C36-C34-C33	-3.08	115.24	120.98
20	B	609	CLA	C6-C5-C3	-3.08	107.23	112.76
20	d	403	CLA	CBC-CAC-C3C	-3.08	103.03	112.38
20	a	403	CLA	C5-C3-C2	-3.08	115.25	120.98
20	B	608	CLA	C4B-CHC-C1C	-3.07	123.23	129.34
20	A	401	CLA	OBD-CAD-C3D	-3.07	122.66	128.09
27	d	412	PL9	C7-C8-C9	-3.07	121.47	126.70
20	b	603	CLA	O2D-CGD-O1D	-3.07	117.31	123.77
22	B	619	BCR	C23-C24-C25	-3.06	118.36	127.24
22	T	101	BCR	C23-C24-C25	-3.06	118.36	127.24
27	a	415	PL9	C42-C43-C44	-3.06	121.00	127.75
20	a	404	CLA	O2D-CGD-O1D	-3.06	117.33	123.77
20	d	403	CLA	C1D-CHD-C4C	-3.06	117.45	125.40
22	T	101	BCR	C7-C8-C9	-3.06	121.59	126.21
20	B	613	CLA	C1C-C2C-C3C	-3.05	103.55	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	506	CLA	C3B-CAB-CBB	-3.05	120.26	126.40
20	B	611	CLA	CAA-CBA-CGA	-3.05	104.47	113.28
22	b	620	BCR	C8-C7-C6	-3.05	118.39	127.24
34	B	625	LMT	C1-O1'-C1'	-3.04	108.68	114.00
20	b	612	CLA	C1C-C2C-C3C	-3.04	103.56	106.93
38	H	101	RRX	C16-C15-C14	-3.04	116.67	123.23
24	B	620	LMG	O7-C10-O9	-3.03	115.43	123.67
20	c	512	CLA	O2D-CGD-O1D	-3.03	117.40	123.77
32	b	624	HTG	O5-C1-C2	-3.02	106.11	110.22
20	B	603	CLA	O2A-CGA-O1A	-3.01	115.61	123.51
20	b	603	CLA	O1D-CGD-CBD	-3.01	119.95	124.64
20	c	507	CLA	O2D-CGD-O1D	-3.00	117.44	123.77
20	C	511	CLA	C3B-CAB-CBB	-3.00	120.37	126.40
38	x	101	RRX	C38-C26-C25	-3.00	121.43	124.62
22	t	101	BCR	C12-C13-C14	-2.99	114.13	118.95
20	b	613	CLA	C2A-C1A-CHA	-2.99	118.97	123.80
35	c	515	DGD	O3G-C3G-C2G	-2.99	103.88	110.99
20	A	404	CLA	C2A-C1A-CHA	-2.99	118.98	123.80
34	b	627	LMT	O2'-C2'-C3'	-2.99	103.62	110.36
27	d	412	PL9	C31-C32-C33	-2.99	103.77	111.61
22	t	101	BCR	C28-C27-C26	-2.98	108.92	113.87
27	d	412	PL9	C21-C19-C18	-2.98	115.44	120.98
20	b	616	CLA	O2A-CGA-O1A	-2.98	115.71	123.51
22	a	408	BCR	C7-C8-C9	-2.98	121.71	126.21
20	b	617	CLA	C6-C5-C3	-2.97	107.43	112.76
22	C	514	BCR	C15-C14-C13	-2.97	122.90	127.22
20	C	503	CLA	C5-C3-C2	-2.97	115.46	120.98
20	B	611	CLA	O2D-CGD-O1D	-2.96	117.53	123.77
20	b	604	CLA	C16-C17-C18	-2.96	101.28	115.92
38	x	101	RRX	C16-C17-C18	-2.96	122.91	127.22
35	c	517	DGD	O3G-C3G-C2G	-2.96	103.94	110.99
22	a	408	BCR	C15-C16-C17	-2.96	116.85	123.23
22	b	621	BCR	C7-C8-C9	-2.96	121.74	126.21
22	B	617	BCR	C20-C21-C22	-2.96	122.92	127.22
22	c	514	BCR	C38-C26-C25	-2.96	121.47	124.62
20	B	606	CLA	C2A-C1A-CHA	-2.95	119.04	123.80
34	T	102	LMT	O1'-C1'-C2'	-2.94	104.38	108.00
20	C	504	CLA	C4B-CHC-C1C	-2.94	123.49	129.34
22	C	515	BCR	C23-C24-C25	-2.94	118.71	127.24
20	c	510	CLA	C4-C3-C2	-2.93	117.91	123.58
34	m	102	LMT	C3'-C4'-C5'	-2.92	104.18	110.85
23	A	406	SQD	O9-S-O7	-2.91	105.73	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	502	CLA	O2D-CGD-O1D	-2.91	117.64	123.77
20	c	502	CLA	OBD-CAD-C3D	-2.91	122.94	128.09
22	k	101	BCR	C3-C4-C5	-2.91	109.05	113.87
20	C	505	CLA	C3B-CAB-CBB	-2.91	120.55	126.40
27	a	415	PL9	C37-C38-C39	-2.90	121.36	127.75
20	c	509	CLA	C4B-CHC-C1C	-2.90	123.58	129.34
20	C	507	CLA	CBC-CAC-C3C	-2.89	103.59	112.38
22	b	619	BCR	C11-C10-C9	-2.89	123.01	127.22
22	t	101	BCR	C38-C26-C25	-2.89	121.54	124.62
27	D	412	PL9	C36-C34-C33	-2.89	115.60	120.98
20	c	504	CLA	C4B-CHC-C1C	-2.88	123.62	129.34
20	D	404	CLA	C6-C7-C8	-2.88	106.56	115.46
20	a	403	CLA	CHC-C1C-C2C	-2.88	118.34	126.31
20	b	618	CLA	O2D-CGD-O1D	-2.88	117.72	123.77
20	d	404	CLA	C2A-C1A-CHA	-2.87	119.17	123.80
20	b	617	CLA	C2A-C1A-CHA	-2.87	119.17	123.80
20	C	508	CLA	C4B-CHC-C1C	-2.87	123.63	129.34
20	b	615	CLA	C3B-CAB-CBB	-2.86	120.64	126.40
23	a	409	SQD	O9-S-O7	-2.86	105.89	113.96
20	B	615	CLA	C3B-CAB-CBB	-2.86	120.65	126.40
27	a	415	PL9	C7-C8-C9	-2.86	121.84	126.70
23	A	406	SQD	C44-O6-C1	-2.86	107.85	113.81
20	C	502	CLA	C3B-CAB-CBB	-2.85	120.66	126.40
20	b	614	CLA	C2A-C1A-CHA	-2.85	119.20	123.80
20	b	610	CLA	C1D-CHD-C4C	-2.84	118.00	125.40
21	a	406	PHO	O2D-CGD-O1D	-2.84	117.79	123.77
24	b	623	LMG	O8-C28-O10	-2.84	116.06	123.51
20	D	402	CLA	O2D-CGD-O1D	-2.84	117.79	123.77
37	V	201	HEM	C3C-CAC-CBC	-2.84	120.69	126.40
20	b	616	CLA	O2D-CGD-O1D	-2.83	117.80	123.77
20	B	603	CLA	C3B-CAB-CBB	-2.83	120.70	126.40
20	b	603	CLA	C1D-CHD-C4C	-2.83	118.05	125.40
21	D	403	PHO	O2D-CGD-O1D	-2.82	117.83	123.77
20	B	606	CLA	OBD-CAD-C3D	-2.82	123.10	128.09
22	j	102	BCR	C33-C5-C6	-2.82	121.62	124.62
20	b	609	CLA	C2A-C1A-CHA	-2.82	119.26	123.80
20	D	404	CLA	O2D-CGD-O1D	-2.81	117.84	123.77
20	D	404	CLA	C6-C5-C3	-2.81	107.72	112.76
20	a	403	CLA	C2A-C1A-CHA	-2.81	119.27	123.80
20	B	615	CLA	C1C-C2C-C3C	-2.81	103.81	106.93
34	z	102	LMT	O5'-C1'-C2'	-2.81	104.44	110.28
20	b	615	CLA	C2A-C1A-CHA	-2.81	119.27	123.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	510	CLA	C1D-CHD-C4C	-2.80	118.10	125.40
22	c	514	BCR	C21-C20-C19	-2.80	114.47	123.11
21	A	403	PHO	CHC-C1C-C2C	-2.79	119.05	125.52
20	c	502	CLA	C6-C5-C3	-2.79	107.75	112.76
20	a	404	CLA	C2A-C1A-CHA	-2.79	119.30	123.80
21	A	403	PHO	C3B-C2B-C1B	-2.79	100.16	106.36
22	B	619	BCR	C21-C20-C19	-2.79	114.49	123.11
20	C	512	CLA	OBD-CAD-C3D	-2.79	123.16	128.09
20	D	404	CLA	CHD-C4C-C3C	-2.79	120.61	124.91
21	a	405	PHO	C1C-NC-C4C	-2.78	101.20	106.50
20	B	603	CLA	O2D-CGD-O1D	-2.78	117.91	123.77
20	c	512	CLA	CBC-CAC-C3C	-2.78	103.93	112.38
20	d	403	CLA	C3B-CAB-CBB	-2.78	120.80	126.40
20	B	601	CLA	C4C-C3C-C2C	-2.78	102.49	106.94
22	t	101	BCR	C15-C16-C17	-2.78	117.24	123.23
20	b	604	CLA	CMB-C2B-C1B	-2.78	123.58	128.31
32	v	210	HTG	C1-C2-C3	-2.78	104.37	110.58
20	D	402	CLA	CBC-CAC-C3C	-2.78	103.95	112.38
20	B	604	CLA	O2D-CGD-O1D	-2.78	117.93	123.77
20	B	601	CLA	C4-C3-C2	-2.78	118.21	123.58
22	C	515	BCR	C33-C5-C6	-2.77	121.67	124.62
20	b	614	CLA	O2D-CGD-O1D	-2.77	117.94	123.77
20	C	512	CLA	O2D-CGD-O1D	-2.77	117.94	123.77
20	C	510	CLA	O2A-CGA-O1A	-2.77	116.25	123.51
22	B	618	BCR	C11-C10-C9	-2.76	123.21	127.22
20	c	506	CLA	C2A-C1A-CHA	-2.76	119.35	123.80
20	b	603	CLA	C2A-C1A-CHA	-2.76	119.35	123.80
20	B	601	CLA	C1C-C2C-C3C	-2.76	103.87	106.93
20	c	503	CLA	OBD-CAD-C3D	-2.76	123.22	128.09
35	C	516	DGD	C3D-C4D-C5D	-2.76	105.31	110.23
20	C	505	CLA	C4B-CHC-C1C	-2.76	123.87	129.34
20	c	507	CLA	O2A-CGA-O1A	-2.75	116.29	123.51
20	B	604	CLA	C3B-CAB-CBB	-2.75	120.86	126.40
35	H	102	DGD	O3G-C3G-C2G	-2.75	104.44	110.99
27	d	412	PL9	O1-C4-C3	-2.75	117.26	120.71
20	b	604	CLA	C2A-C3A-C4A	-2.75	99.02	101.84
22	t	101	BCR	C21-C20-C19	-2.75	114.62	123.11
22	j	102	BCR	C38-C26-C25	-2.75	121.70	124.62
20	C	508	CLA	O2D-CGD-O1D	-2.74	118.00	123.77
22	K	101	BCR	C7-C8-C9	-2.74	122.07	126.21
20	b	607	CLA	C2A-C1A-CHA	-2.74	119.38	123.80
20	B	611	CLA	C1C-C2C-C3C	-2.74	103.89	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	517	DGD	O6D-C1D-O3G	-2.74	103.43	109.99
24	C	519	LMG	C8-O7-C10	-2.73	111.17	117.91
23	a	409	SQD	C44-O6-C1	-2.72	108.12	113.81
20	c	509	CLA	O2D-CGD-O1D	-2.72	118.04	123.77
38	x	101	RRX	C24-C23-C22	-2.72	122.10	126.21
22	t	101	BCR	C11-C10-C9	-2.72	123.27	127.22
20	c	507	CLA	O1D-CGD-CBD	-2.72	120.41	124.64
23	a	409	SQD	O5-C1-C2	-2.72	104.63	110.28
32	B	622	HTG	O2-C2-C3	-2.72	104.24	110.36
37	V	201	HEM	CBA-CAA-C2A	-2.72	107.72	112.49
20	c	513	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
20	B	607	CLA	O2A-CGA-O1A	-2.71	116.41	123.51
22	B	617	BCR	C21-C20-C19	-2.71	114.75	123.11
20	B	604	CLA	O1D-CGD-CBD	-2.70	120.44	124.64
22	T	101	BCR	C33-C5-C6	-2.70	121.75	124.62
20	c	508	CLA	C4C-C3C-C2C	-2.70	102.63	106.94
20	b	613	CLA	CBC-CAC-C3C	-2.69	104.20	112.38
20	b	618	CLA	C1C-C2C-C3C	-2.69	103.95	106.93
20	C	512	CLA	O1D-CGD-CBD	-2.69	120.46	124.64
20	B	610	CLA	C4B-CHC-C1C	-2.69	124.00	129.34
20	b	612	CLA	O1D-CGD-CBD	-2.68	120.46	124.64
20	B	610	CLA	C4C-C3C-C2C	-2.68	102.65	106.94
20	c	501	CLA	C2A-C1A-CHA	-2.68	119.48	123.80
20	B	611	CLA	C1D-CHD-C4C	-2.68	118.43	125.40
20	b	605	CLA	O2A-CGA-O1A	-2.68	116.49	123.51
27	A	411	PL9	C32-C33-C34	-2.67	121.85	127.75
20	B	603	CLA	C2A-C3A-C4A	-2.67	99.10	101.84
24	C	519	LMG	O8-C28-O10	-2.67	116.51	123.51
36	d	408	LHG	O7-C7-O9	-2.67	116.41	123.67
20	A	401	CLA	C4B-CHC-C1C	-2.66	124.05	129.34
22	k	101	BCR	C38-C26-C25	-2.66	121.78	124.62
23	A	406	SQD	O48-C23-O10	-2.66	116.53	123.51
20	A	402	CLA	CAC-C3C-C2C	-2.66	122.94	127.51
20	b	605	CLA	C5-C3-C2	-2.66	116.02	120.98
35	c	516	DGD	O1G-C1A-O1A	-2.66	116.53	123.51
38	H	101	RRX	C16-C17-C18	-2.66	123.35	127.22
20	C	502	CLA	C16-C17-C18	-2.66	102.78	115.92
24	c	519	LMG	O5-C6-C5	-2.66	102.42	111.30
21	a	406	PHO	CHD-C4C-C3C	-2.66	119.28	124.57
20	b	604	CLA	CHD-C4C-C3C	-2.66	120.81	124.91
22	C	515	BCR	C38-C26-C25	-2.66	121.79	124.62
22	B	618	BCR	C24-C23-C22	-2.65	122.20	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	E	104	HEM	CMA-C3A-C4A	-2.65	123.80	128.31
20	b	612	CLA	C1D-CHD-C4C	-2.65	118.51	125.40
22	T	101	BCR	C15-C16-C17	-2.65	117.52	123.23
20	b	604	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
20	B	601	CLA	CBC-CAC-C3C	-2.64	104.36	112.38
36	D	407	LHG	C11-C10-C9	-2.64	100.83	114.54
38	H	101	RRX	C38-C26-C25	-2.64	121.81	124.62
20	C	508	CLA	C2A-C1A-CHA	-2.64	119.55	123.80
35	H	102	DGD	C2G-O2G-C1B	-2.63	111.40	117.91
22	k	102	BCR	C11-C10-C9	-2.63	123.40	127.22
20	c	502	CLA	O2D-CGD-O1D	-2.63	118.24	123.77
20	b	611	CLA	CBC-CAC-C3C	-2.63	104.40	112.38
20	D	401	CLA	CAA-CBA-CGA	-2.62	105.69	113.28
20	b	606	CLA	C4B-CHC-C1C	-2.62	124.14	129.34
20	b	615	CLA	C4B-CHC-C1C	-2.62	124.14	129.34
22	t	101	BCR	C7-C6-C5	-2.62	115.29	121.36
20	c	504	CLA	O2A-CGA-O1A	-2.62	116.65	123.51
21	D	403	PHO	C1C-C2C-C3C	-2.61	103.42	106.43
22	b	619	BCR	C15-C16-C17	-2.61	117.60	123.23
20	b	616	CLA	OBD-CAD-C3D	-2.61	123.47	128.09
21	a	406	PHO	CMA-C3A-C4A	-2.61	104.24	112.30
20	C	506	CLA	C2A-C3A-C4A	-2.61	99.16	101.84
21	D	403	PHO	C3B-C2B-C1B	-2.61	100.58	106.36
20	b	613	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
20	B	612	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
22	t	101	BCR	C23-C24-C25	-2.60	119.69	127.24
20	B	602	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
35	c	515	DGD	O2G-C1B-O1B	-2.60	116.60	123.67
20	A	404	CLA	C4B-CHC-C1C	-2.60	124.18	129.34
20	B	611	CLA	O2A-CGA-O1A	-2.59	116.71	123.51
20	B	604	CLA	O2A-CGA-O1A	-2.59	116.72	123.51
36	D	408	LHG	C13-C12-C11	-2.59	101.10	114.54
20	B	613	CLA	CAC-C3C-C2C	-2.59	123.06	127.51
20	c	502	CLA	C1D-CHD-C4C	-2.58	118.68	125.40
20	c	502	CLA	C2A-C1A-CHA	-2.58	119.64	123.80
20	C	510	CLA	C4-C3-C2	-2.58	118.59	123.58
20	D	404	CLA	O2A-CGA-O1A	-2.58	116.75	123.51
20	B	604	CLA	CHC-C1C-NC	-2.58	119.15	123.92
20	B	609	CLA	C4B-CHC-C1C	-2.58	124.22	129.34
22	K	102	BCR	C20-C21-C22	-2.57	123.48	127.22
20	C	504	CLA	OBD-CAD-C3D	-2.57	123.54	128.09
20	B	606	CLA	O2A-CGA-O1A	-2.57	116.77	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	405	BCR	C24-C23-C22	-2.57	122.33	126.21
20	c	507	CLA	CBC-CAC-C3C	-2.57	104.58	112.38
27	D	412	PL9	C27-C28-C29	-2.57	122.09	127.75
22	B	618	BCR	C33-C5-C6	-2.56	121.90	124.62
24	j	101	LMG	C9-C8-C7	-2.56	106.13	112.08
20	C	513	CLA	O2A-CGA-O1A	-2.55	116.81	123.51
20	c	511	CLA	CBC-CAC-C3C	-2.55	104.62	112.38
20	C	510	CLA	O2D-CGD-O1D	-2.55	118.39	123.77
20	B	614	CLA	C16-C15-C13	-2.55	107.56	115.46
20	C	513	CLA	C2A-C1A-CHA	-2.55	119.69	123.80
35	c	515	DGD	O1G-C1G-C2G	-2.55	101.83	108.70
22	d	405	BCR	C10-C11-C12	-2.54	115.25	123.11
21	a	405	PHO	C4D-ND-C1D	-2.54	102.34	106.99
20	b	618	CLA	C4C-C3C-C2C	-2.54	102.88	106.94
20	C	506	CLA	C1D-CHD-C4C	-2.54	118.79	125.40
20	c	513	CLA	C2A-C1A-CHA	-2.54	119.71	123.80
21	A	403	PHO	CHD-C4C-NC	-2.54	120.15	124.89
21	a	406	PHO	CHD-C1D-ND	-2.53	120.07	124.67
22	D	405	BCR	C10-C11-C12	-2.53	115.29	123.11
35	C	518	DGD	O3G-C3G-C2G	-2.53	104.98	110.99
27	d	412	PL9	C15-C14-C13	-2.53	118.69	123.58
35	h	101	DGD	O1G-C1A-O1A	-2.53	116.89	123.51
21	a	405	PHO	CHD-C1D-ND	-2.53	120.08	124.67
20	b	605	CLA	C2A-C1A-CHA	-2.52	119.73	123.80
23	a	409	SQD	C45-O47-C7	-2.52	111.67	117.91
23	F	101	SQD	C1-O5-C5	-2.52	108.81	113.74
24	c	518	LMG	C8-O7-C10	-2.52	111.69	117.91
23	b	622	SQD	O9-S-O7	-2.51	106.86	113.96
20	A	401	CLA	C4C-C3C-C2C	-2.51	102.93	106.94
21	A	403	PHO	CBC-CAC-C3C	-2.51	104.76	112.38
34	I	101	LMT	C3'-C4'-C5'	-2.51	105.11	110.85
34	m	102	LMT	C1'-O5'-C5'	-2.51	108.82	113.74
20	C	505	CLA	O2A-CGA-O1A	-2.51	116.93	123.51
20	d	404	CLA	C6-C5-C3	-2.50	108.27	112.76
23	A	406	SQD	C45-O47-C7	-2.50	111.73	117.91
20	b	606	CLA	C3B-CAB-CBB	-2.50	121.37	126.40
21	a	406	PHO	C3B-C2B-C1B	-2.50	100.82	106.36
20	b	613	CLA	C3B-CAB-CBB	-2.49	121.38	126.40
20	A	401	CLA	C2A-C1A-CHA	-2.49	119.78	123.80
22	j	102	BCR	C16-C17-C18	-2.49	123.60	127.22
20	d	402	CLA	O2A-CGA-O1A	-2.49	116.99	123.51
20	a	407	CLA	C4B-CHC-C1C	-2.49	124.40	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	411	PL9	C37-C38-C39	-2.49	122.26	127.75
20	c	506	CLA	C1D-CHD-C4C	-2.49	118.93	125.40
27	d	412	PL9	C11-C9-C8	-2.49	116.35	120.98
27	A	411	PL9	C16-C14-C13	-2.48	116.36	120.98
20	B	607	CLA	C3B-CAB-CBB	-2.48	121.41	126.40
20	C	504	CLA	O2D-CGD-O1D	-2.48	118.54	123.77
20	c	506	CLA	O1D-CGD-CBD	-2.48	120.79	124.64
20	C	501	CLA	C4B-CHC-C1C	-2.47	124.44	129.34
27	D	412	PL9	C31-C32-C33	-2.47	105.13	111.61
20	b	612	CLA	O2D-CGD-O1D	-2.47	118.58	123.77
20	C	503	CLA	C2A-C1A-CHA	-2.47	119.82	123.80
22	k	101	BCR	C20-C21-C22	-2.46	123.64	127.22
20	B	612	CLA	C1C-C2C-C3C	-2.46	104.20	106.93
20	d	403	CLA	C6-C5-C3	-2.46	108.35	112.76
24	c	519	LMG	O3-C3-C4	-2.46	104.81	110.36
35	H	102	DGD	O4D-C4D-C3D	-2.46	104.82	110.36
20	B	605	CLA	O2A-CGA-O1A	-2.46	117.07	123.51
22	B	617	BCR	C34-C9-C10	-2.46	119.32	122.89
22	B	618	BCR	C28-C27-C26	-2.45	109.80	113.87
20	b	603	CLA	OBD-CAD-C3D	-2.45	123.76	128.09
20	A	401	CLA	CHC-C1C-C2C	-2.45	119.53	126.31
20	d	403	CLA	O2D-CGD-O1D	-2.45	118.62	123.77
21	A	403	PHO	CHD-C1D-ND	-2.45	120.23	124.67
20	c	508	CLA	C4B-CHC-C1C	-2.45	124.48	129.34
23	A	412	SQD	O5-C1-C2	-2.45	105.20	110.28
20	c	506	CLA	C4B-CHC-C1C	-2.44	124.48	129.34
20	A	402	CLA	CHC-C1C-C2C	-2.44	119.54	126.31
22	K	101	BCR	C24-C23-C22	-2.44	122.52	126.21
20	B	614	CLA	O2A-CGA-O1A	-2.44	117.12	123.51
20	B	616	CLA	OBD-CAD-C3D	-2.44	123.78	128.09
20	b	604	CLA	C1D-CHD-C4C	-2.44	119.06	125.40
20	A	404	CLA	C5-C3-C2	-2.44	116.44	120.98
22	A	405	BCR	C15-C16-C17	-2.44	117.98	123.23
24	C	519	LMG	C9-C8-C7	-2.43	106.41	112.08
20	D	404	CLA	CBC-CAC-C3C	-2.43	105.00	112.38
20	B	616	CLA	C11-C10-C8	-2.43	107.94	115.46
20	b	617	CLA	C11-C10-C8	-2.43	107.94	115.46
34	M	101	LMT	O1'-C1-C2	-2.43	102.65	109.63
20	B	605	CLA	CGD-CBD-CAD	-2.43	102.48	110.70
22	D	405	BCR	C40-C30-C25	-2.43	106.62	110.33
20	c	506	CLA	C3B-CAB-CBB	-2.43	121.52	126.40
20	B	612	CLA	O2A-CGA-O1A	-2.43	117.15	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	411	PL9	O2-C1-C2	-2.42	116.32	121.78
20	C	507	CLA	OBD-CAD-C3D	-2.42	123.81	128.09
20	b	616	CLA	C2A-C1A-CHA	-2.42	119.90	123.80
20	b	615	CLA	O2A-CGA-O1A	-2.42	117.18	123.51
20	c	504	CLA	C3B-CAB-CBB	-2.41	121.54	126.40
20	c	507	CLA	C3B-CAB-CBB	-2.41	121.55	126.40
20	B	609	CLA	O2D-CGD-O1D	-2.41	118.69	123.77
24	c	519	LMG	O1-C7-C8	-2.41	105.26	110.99
22	c	514	BCR	C11-C10-C9	-2.41	123.72	127.22
20	D	401	CLA	C1D-CHD-C4C	-2.41	119.14	125.40
20	b	609	CLA	O2D-CGD-O1D	-2.40	118.71	123.77
22	D	405	BCR	C28-C27-C26	-2.40	109.89	113.87
20	a	403	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
20	a	404	CLA	O2A-CGA-O1A	-2.39	117.23	123.51
20	b	606	CLA	C4C-C3C-C2C	-2.39	103.12	106.94
20	b	615	CLA	O2D-CGD-O1D	-2.39	118.75	123.77
20	C	509	CLA	O2A-CGA-O1A	-2.38	117.27	123.51
20	b	618	CLA	C3B-CAB-CBB	-2.38	121.61	126.40
20	c	502	CLA	C16-C17-C18	-2.38	104.18	115.92
20	B	615	CLA	OBD-CAD-C3D	-2.38	123.89	128.09
20	c	511	CLA	C3B-CAB-CBB	-2.38	121.62	126.40
20	b	605	CLA	C4B-CHC-C1C	-2.37	124.62	129.34
22	d	405	BCR	C34-C9-C10	-2.37	119.44	122.89
27	d	412	PL9	C40-C39-C38	-2.37	119.00	123.58
20	c	504	CLA	O1D-CGD-CBD	-2.37	120.96	124.64
24	J	101	LMG	O8-C28-O10	-2.36	117.31	123.51
20	b	607	CLA	C3B-CAB-CBB	-2.36	121.64	126.40
27	d	412	PL9	C22-C23-C24	-2.36	122.54	127.75
22	A	405	BCR	C39-C30-C25	-2.36	106.72	110.33
20	B	610	CLA	O2A-CGA-O1A	-2.36	117.32	123.51
20	c	505	CLA	O2A-CGA-O1A	-2.36	117.33	123.51
22	B	617	BCR	C8-C7-C6	-2.36	120.40	127.24
22	d	405	BCR	C7-C8-C9	-2.36	122.65	126.21
37	E	104	HEM	CBA-CAA-C2A	-2.35	108.36	112.49
20	C	505	CLA	C7-C6-C5	-2.35	106.22	113.16
20	b	607	CLA	O2D-CGD-O1D	-2.35	118.83	123.77
20	c	503	CLA	O2D-CGD-O1D	-2.35	118.83	123.77
22	B	618	BCR	C30-C25-C26	-2.35	119.36	122.50
20	c	504	CLA	C2A-C1A-CHA	-2.35	120.02	123.80
20	c	513	CLA	O1D-CGD-CBD	-2.34	120.99	124.64
21	D	403	PHO	CHD-C4C-C3C	-2.34	119.91	124.57
20	A	404	CLA	O2D-CGD-O1D	-2.34	118.84	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	511	CLA	O2A-CGA-O1A	-2.34	117.38	123.51
22	K	101	BCR	C8-C9-C10	-2.34	115.19	118.95
21	a	405	PHO	CHD-C4C-C3C	-2.33	119.92	124.57
27	D	412	PL9	C11-C9-C8	-2.33	116.63	120.98
20	B	605	CLA	C4B-CHC-C1C	-2.33	124.71	129.34
20	B	615	CLA	C4B-CHC-C1C	-2.33	124.71	129.34
36	E	103	LHG	O7-C7-O9	-2.33	117.40	123.51
20	C	511	CLA	O2D-CGD-O1D	-2.33	118.87	123.77
20	B	601	CLA	C2A-C1A-CHA	-2.33	120.05	123.80
20	c	508	CLA	C7-C6-C5	-2.33	106.30	113.16
21	A	403	PHO	CBA-CAA-C2A	-2.33	107.96	113.96
20	b	614	CLA	C4C-C3C-C2C	-2.32	103.23	106.94
27	a	415	PL9	C17-C18-C19	-2.32	122.62	127.75
22	a	408	BCR	C38-C26-C25	-2.32	122.15	124.62
22	a	408	BCR	C33-C5-C6	-2.32	122.15	124.62
20	B	602	CLA	O2A-CGA-O1A	-2.32	117.43	123.51
20	B	606	CLA	O2D-CGD-O1D	-2.32	118.89	123.77
20	C	507	CLA	C7-C6-C5	-2.31	106.33	113.16
20	b	609	CLA	O2A-CGA-O1A	-2.31	117.44	123.51
21	A	403	PHO	CHB-C1B-NB	-2.31	120.47	124.67
21	a	406	PHO	CAA-C2A-C1A	-2.31	106.33	112.36
20	D	404	CLA	C2A-C1A-CHA	-2.31	120.08	123.80
23	b	622	SQD	O47-C7-O49	-2.31	117.39	123.67
22	B	619	BCR	C23-C22-C21	-2.31	115.24	118.95
22	D	405	BCR	C15-C14-C13	-2.30	123.87	127.22
35	C	516	DGD	O1G-C1G-C2G	-2.30	102.48	108.70
20	B	609	CLA	O2A-CGA-O1A	-2.30	117.47	123.51
35	C	517	DGD	O2G-C1B-O1B	-2.30	117.41	123.67
22	B	617	BCR	C40-C30-C25	-2.30	106.83	110.33
20	a	404	CLA	CHC-C1C-C2C	-2.30	119.95	126.31
20	c	505	CLA	C4C-C3C-C2C	-2.29	103.27	106.94
21	D	403	PHO	CHD-C1D-ND	-2.29	120.51	124.67
21	a	406	PHO	CHB-C1B-C2B	-2.29	120.21	125.52
22	a	408	BCR	C8-C7-C6	-2.29	120.60	127.24
20	B	607	CLA	C4C-C3C-C2C	-2.28	103.29	106.94
27	d	412	PL9	C42-C41-C39	-2.28	105.06	112.61
20	b	603	CLA	C3B-CAB-CBB	-2.28	121.81	126.40
20	b	607	CLA	OBD-CAD-C3D	-2.28	124.06	128.09
22	T	101	BCR	C12-C13-C14	-2.28	115.28	118.95
32	B	621	HTG	O4-C4-C3	-2.28	105.22	110.36
20	a	407	CLA	C4C-C3C-C2C	-2.28	103.30	106.94
23	l	101	SQD	O48-C23-O10	-2.27	117.55	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	102	BCR	C37-C22-C21	-2.27	119.58	122.89
20	B	614	CLA	CBC-CAC-C3C	-2.27	105.48	112.38
20	c	504	CLA	CBC-CAC-C3C	-2.27	105.48	112.38
32	B	621	HTG	O3-C3-C4	-2.27	105.24	110.36
20	c	512	CLA	O1D-CGD-CBD	-2.27	121.11	124.64
34	M	101	LMT	C3'-C4'-C5'	-2.27	105.66	110.85
20	A	401	CLA	C2A-C3A-C4A	-2.27	99.51	101.84
21	D	403	PHO	CBA-CAA-C2A	-2.27	108.12	113.96
20	d	404	CLA	C6-C7-C8	-2.27	108.45	115.46
23	A	412	SQD	O48-C23-O10	-2.27	117.57	123.51
20	B	615	CLA	C4C-C3C-C2C	-2.26	103.32	106.94
20	D	404	CLA	C3B-CAB-CBB	-2.26	121.84	126.40
22	K	101	BCR	C7-C6-C5	-2.26	116.11	121.36
20	D	401	CLA	C4B-CHC-C1C	-2.26	124.85	129.34
22	a	408	BCR	C27-C26-C25	-2.26	120.25	122.73
22	C	514	BCR	C23-C24-C25	-2.26	120.69	127.24
21	a	405	PHO	CHB-C1B-NB	-2.26	120.58	124.67
20	b	608	CLA	O2A-CGA-O1A	-2.25	117.60	123.51
24	C	524	LMG	O7-C10-O9	-2.25	117.54	123.67
20	c	505	CLA	C2A-C1A-CHA	-2.25	120.17	123.80
20	c	510	CLA	O2A-CGA-O1A	-2.25	117.61	123.51
22	C	514	BCR	C33-C5-C6	-2.25	122.23	124.62
20	d	402	CLA	C1D-CHD-C4C	-2.25	119.55	125.40
20	b	612	CLA	C4C-C3C-C2C	-2.25	103.35	106.94
20	C	502	CLA	O2A-CGA-O1A	-2.25	117.62	123.51
20	C	503	CLA	O1D-CGD-CBD	-2.24	121.15	124.64
35	c	515	DGD	O2D-C2D-C1D	-2.24	105.03	110.01
20	b	613	CLA	O2A-CGA-O1A	-2.24	117.63	123.51
20	a	407	CLA	C2A-C1A-CHA	-2.24	120.18	123.80
22	t	101	BCR	C7-C8-C9	-2.24	122.83	126.21
27	a	415	PL9	C26-C24-C23	-2.24	116.81	120.98
20	C	513	CLA	C3B-CAB-CBB	-2.24	121.90	126.40
20	c	509	CLA	O1D-CGD-CBD	-2.23	121.16	124.64
20	C	506	CLA	O2D-CGD-O1D	-2.23	119.07	123.77
20	b	617	CLA	OBD-CAD-C3D	-2.23	124.15	128.09
21	D	403	PHO	OBD-CAD-C3D	-2.23	122.11	128.26
22	k	101	BCR	C8-C7-C6	-2.23	120.77	127.24
20	b	609	CLA	C5-C3-C2	-2.23	116.83	120.98
23	a	401	SQD	C1-C2-C3	-2.23	105.57	109.98
22	C	515	BCR	C24-C23-C22	-2.22	122.85	126.21
20	b	612	CLA	O2A-CGA-O1A	-2.22	117.69	123.51
20	d	403	CLA	CHC-C1C-C2C	-2.22	120.16	126.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	d	408	LHG	O8-C23-O10	-2.22	117.69	123.51
20	B	614	CLA	C7-C6-C5	-2.22	106.62	113.16
20	A	402	CLA	C6-C5-C3	-2.22	108.79	112.76
20	D	404	CLA	CBA-CAA-C2A	-2.21	108.25	113.96
20	b	617	CLA	C5-C3-C2	-2.21	116.86	120.98
35	c	517	DGD	C3E-C4E-C5E	-2.21	106.28	110.23
20	B	612	CLA	C4C-C3C-C2C	-2.21	103.41	106.94
20	c	513	CLA	C1D-CHD-C4C	-2.21	119.65	125.40
20	C	511	CLA	C6-C5-C3	-2.21	108.80	112.76
20	c	512	CLA	C2A-C3A-C4A	-2.21	99.57	101.84
22	b	621	BCR	C24-C25-C26	-2.21	116.24	121.36
20	C	503	CLA	C1D-CHD-C4C	-2.20	119.67	125.40
22	c	514	BCR	C34-C9-C10	-2.20	119.68	122.89
20	A	401	CLA	C5-C3-C2	-2.20	116.88	120.98
22	K	101	BCR	C10-C11-C12	-2.20	116.31	123.11
22	t	101	BCR	C40-C30-C25	-2.20	106.97	110.33
20	B	615	CLA	O2A-CGA-O1A	-2.19	117.76	123.51
22	A	405	BCR	C3-C4-C5	-2.19	110.23	113.87
22	b	621	BCR	C16-C15-C14	-2.19	118.50	123.23
20	B	616	CLA	O2D-CGD-O1D	-2.19	119.16	123.77
22	k	102	BCR	C24-C23-C22	-2.19	122.91	126.21
20	b	611	CLA	C4C-C3C-C2C	-2.19	103.44	106.94
20	a	407	CLA	CBC-CAC-C3C	-2.19	105.74	112.38
27	d	412	PL9	C32-C33-C34	-2.18	122.93	127.75
22	K	101	BCR	C21-C20-C19	-2.18	116.37	123.11
32	C	534	HTG	C1-C2-C3	-2.18	105.71	110.58
20	b	609	CLA	CBC-CAC-C3C	-2.18	105.76	112.38
35	C	516	DGD	C4A-C3A-C2A	-2.18	105.23	113.30
20	A	404	CLA	C3B-CAB-CBB	-2.18	122.02	126.40
20	B	609	CLA	OBD-CAD-C3D	-2.18	124.24	128.09
35	H	102	DGD	O5E-C6E-C5E	-2.18	104.03	111.30
20	d	403	CLA	C2A-C1A-CHA	-2.18	120.29	123.80
35	h	101	DGD	O3G-C3G-C2G	-2.17	105.82	110.99
22	B	617	BCR	C16-C15-C14	-2.17	118.56	123.23
20	c	509	CLA	C6-C5-C3	-2.17	108.87	112.76
20	B	602	CLA	C1D-CHD-C4C	-2.17	119.76	125.40
37	e	102	HEM	C3B-CAB-CBB	-2.17	122.04	126.40
32	b	625	HTG	C3-C4-C5	-2.16	106.37	110.23
20	b	615	CLA	C7-C6-C5	-2.16	106.79	113.16
20	c	501	CLA	O2A-CGA-O1A	-2.16	117.85	123.51
22	j	102	BCR	C8-C9-C10	-2.16	115.48	118.95
32	B	622	HTG	C3-C4-C5	-2.16	106.38	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	k	101	BCR	C24-C23-C22	-2.16	122.95	126.21
34	m	102	LMT	O1'-C1-C2	-2.15	103.45	109.63
36	d	407	LHG	O8-C23-O10	-2.15	117.88	123.51
22	T	101	BCR	C7-C6-C5	-2.15	116.38	121.36
22	b	619	BCR	C21-C20-C19	-2.15	116.48	123.11
35	C	518	DGD	C3G-C2G-C1G	-2.14	107.09	112.08
20	d	403	CLA	CGD-CBD-CHA	-2.14	103.53	110.88
20	B	612	CLA	CBC-CAC-C3C	-2.14	105.89	112.38
24	c	519	LMG	O8-C28-O10	-2.14	117.91	123.51
20	D	401	CLA	C4C-C3C-C2C	-2.13	103.53	106.94
35	D	406	DGD	O2G-C1B-O1B	-2.13	117.87	123.67
35	C	516	DGD	O1G-C1A-O1A	-2.13	117.92	123.51
20	a	407	CLA	C2A-C3A-C4A	-2.13	99.65	101.84
24	j	101	LMG	O1-C7-C8	-2.13	105.92	110.99
34	I	101	LMT	C2'-C3'-C4'	-2.13	104.93	109.63
20	b	609	CLA	C4C-C3C-C2C	-2.13	103.54	106.94
23	l	101	SQD	O5-C5-C4	-2.12	105.61	109.67
36	D	409	LHG	O8-C23-O10	-2.12	117.95	123.51
22	T	101	BCR	C20-C21-C22	-2.12	124.14	127.22
20	D	401	CLA	CMB-C2B-C1B	-2.12	124.71	128.31
21	a	406	PHO	CHC-C1C-C2C	-2.12	120.61	125.52
22	k	102	BCR	C20-C21-C22	-2.12	124.15	127.22
20	B	615	CLA	CBC-CAC-C3C	-2.12	105.96	112.38
20	b	606	CLA	C1D-CHD-C4C	-2.11	119.90	125.40
22	b	621	BCR	C23-C24-C25	-2.11	121.10	127.24
20	c	510	CLA	O1D-CGD-CBD	-2.11	121.35	124.64
20	D	402	CLA	CAC-C3C-C2C	-2.11	123.88	127.51
20	b	610	CLA	C5-C3-C2	-2.11	117.05	120.98
20	C	506	CLA	C4C-C3C-C2C	-2.11	103.56	106.94
35	C	517	DGD	O1G-C1A-O1A	-2.11	117.98	123.51
20	a	403	CLA	O2A-CGA-O1A	-2.11	117.98	123.51
21	a	406	PHO	C1C-C2C-C3C	-2.11	104.00	106.43
20	b	612	CLA	OBD-CAD-C3D	-2.11	124.36	128.09
20	c	506	CLA	C2A-C3A-C4A	-2.11	99.67	101.84
21	a	406	PHO	CBA-CAA-C2A	-2.11	108.53	113.96
22	a	408	BCR	C40-C30-C25	-2.11	107.11	110.33
20	c	506	CLA	CBC-CAC-C3C	-2.11	105.99	112.38
20	C	509	CLA	C4-C3-C2	-2.11	119.51	123.58
20	B	610	CLA	C2A-C1A-CHA	-2.10	120.41	123.80
20	b	609	CLA	CGD-CBD-CAD	-2.10	103.59	110.70
20	d	402	CLA	C5-C3-C2	-2.10	117.07	120.98
20	c	503	CLA	CBC-CAC-C3C	-2.10	106.01	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	603	CLA	C4B-CHC-C1C	-2.10	125.17	129.34
20	C	509	CLA	O1D-CGD-CBD	-2.10	121.37	124.64
20	c	502	CLA	O2A-CGA-O1A	-2.10	118.01	123.51
20	B	606	CLA	C4C-C3C-C2C	-2.10	103.59	106.94
20	b	616	CLA	CBC-CAC-C3C	-2.09	106.02	112.38
34	B	626	LMT	O3'-C3'-C4'	-2.09	105.64	110.36
20	C	501	CLA	O2A-CGA-O1A	-2.09	118.03	123.51
27	A	411	PL9	C21-C19-C18	-2.09	117.09	120.98
22	T	101	BCR	C21-C20-C19	-2.09	116.65	123.11
24	c	519	LMG	O7-C10-O9	-2.09	117.99	123.67
20	B	603	CLA	CMB-C2B-C1B	-2.08	124.77	128.31
22	j	102	BCR	C10-C11-C12	-2.08	116.67	123.11
23	f	101	SQD	O48-C23-O10	-2.08	118.06	123.51
38	x	101	RRX	C16-C15-C14	-2.08	118.75	123.23
20	C	503	CLA	O2D-CGD-O1D	-2.08	119.40	123.77
22	D	405	BCR	C33-C5-C6	-2.08	122.41	124.62
20	C	509	CLA	O2D-CGD-O1D	-2.08	119.40	123.77
20	B	606	CLA	CGD-CBD-CHA	-2.08	103.76	110.88
22	d	405	BCR	C32-C1-C2	-2.08	101.46	108.75
20	b	605	CLA	C7-C6-C5	-2.07	107.04	113.16
21	a	405	PHO	C3B-C2B-C1B	-2.07	101.77	106.36
20	B	613	CLA	CBC-CAC-C3C	-2.07	106.10	112.38
20	c	506	CLA	O2A-CGA-O1A	-2.07	118.09	123.51
20	C	511	CLA	C4C-C3C-C2C	-2.07	103.64	106.94
20	C	512	CLA	CBA-CAA-C2A	-2.06	108.64	113.96
20	C	510	CLA	CHC-C1C-C2C	-2.06	120.59	126.31
35	c	515	DGD	CDB-CCB-CBB	-2.06	103.82	114.54
20	B	610	CLA	O2D-CGD-O1D	-2.06	119.42	123.77
23	f	101	SQD	O47-C7-O49	-2.06	118.73	122.92
20	B	609	CLA	C11-C10-C8	-2.06	109.09	115.46
20	C	503	CLA	CBC-CAC-C3C	-2.06	106.13	112.38
20	b	606	CLA	CGD-CBD-CAD	-2.06	103.74	110.70
23	a	401	SQD	C46-C45-C44	-2.06	107.29	112.08
20	D	402	CLA	CHC-C1C-C2C	-2.06	120.61	126.31
23	a	401	SQD	C44-O6-C1	-2.05	109.52	113.81
20	C	512	CLA	C4C-C3C-C2C	-2.05	103.66	106.94
22	k	102	BCR	C16-C17-C18	-2.05	124.24	127.22
20	c	510	CLA	C3B-CAB-CBB	-2.05	122.27	126.40
22	K	102	BCR	C33-C5-C6	-2.05	122.44	124.62
27	a	415	PL9	C27-C28-C29	-2.05	123.23	127.75
20	B	611	CLA	C3B-CAB-CBB	-2.05	122.28	126.40
20	A	404	CLA	C1D-CHD-C4C	-2.05	120.08	125.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	502	CLA	O1D-CGD-CBD	-2.05	121.45	124.64
22	t	101	BCR	C3-C4-C5	-2.05	110.48	113.87
20	c	511	CLA	C5-C3-C2	-2.05	117.17	120.98
22	t	101	BCR	C8-C9-C10	-2.04	115.66	118.95
22	C	515	BCR	C3-C4-C5	-2.04	110.49	113.87
20	B	612	CLA	C2A-C1A-CHA	-2.04	120.51	123.80
20	b	604	CLA	CAA-CBA-CGA	-2.03	107.40	113.28
22	B	618	BCR	C8-C7-C6	-2.03	121.34	127.24
23	A	406	SQD	O47-C7-O49	-2.03	118.14	123.67
20	B	602	CLA	CBC-CAC-C3C	-2.03	106.21	112.38
20	C	508	CLA	O2A-CGA-O1A	-2.03	118.19	123.51
20	b	615	CLA	CAA-CBA-CGA	-2.03	107.41	113.28
22	D	405	BCR	C30-C25-C26	-2.03	119.79	122.50
27	A	411	PL9	O1-C4-C3	-2.03	118.16	120.71
35	c	517	DGD	C3D-C4D-C5D	-2.03	106.61	110.23
20	c	505	CLA	C4B-CHC-C1C	-2.03	125.31	129.34
20	b	617	CLA	C4B-CHC-C1C	-2.03	125.31	129.34
20	c	512	CLA	C2A-C1A-CHA	-2.03	120.53	123.80
27	a	415	PL9	C31-C29-C28	-2.03	117.21	120.98
20	d	404	CLA	O2D-CGD-O1D	-2.02	119.51	123.77
23	b	622	SQD	O48-C23-O10	-2.02	118.21	123.51
20	B	604	CLA	C1D-CHD-C4C	-2.02	120.14	125.40
20	C	507	CLA	C1D-CHD-C4C	-2.02	120.15	125.40
35	c	516	DGD	O3D-C3D-C2D	-2.02	105.81	110.36
22	j	102	BCR	C21-C20-C19	-2.02	116.87	123.11
20	C	505	CLA	O2D-CGD-O1D	-2.02	119.53	123.77
20	d	402	CLA	CHC-C1C-C2C	-2.02	120.72	126.31
24	j	101	LMG	O8-C28-O10	-2.02	118.23	123.51
20	C	511	CLA	CBC-CAC-C3C	-2.01	106.27	112.38
20	d	402	CLA	CHD-C4C-C3C	-2.01	121.80	124.91
37	V	201	HEM	C3B-C4B-NB	-2.01	106.61	109.21
20	D	402	CLA	C5-C3-C2	-2.01	117.24	120.98
37	E	104	HEM	C3C-C4C-NC	-2.01	107.15	110.94
20	b	611	CLA	C4B-CHC-C1C	-2.01	125.35	129.34
35	c	515	DGD	C6D-O5D-C1E	-2.01	109.62	113.81
23	A	406	SQD	O5-C1-C2	-2.01	106.11	110.28
27	a	415	PL9	C45-C44-C43	-2.01	119.70	123.58
20	b	607	CLA	C5-C3-C2	-2.00	117.25	120.98
22	C	514	BCR	C32-C1-C6	-2.00	107.27	110.33
20	C	506	CLA	OBD-CAD-C3D	-2.00	124.55	128.09
22	j	102	BCR	C7-C6-C5	-2.00	116.72	121.36
20	C	504	CLA	C2A-C1A-CHA	-2.00	120.57	123.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	k	102	BCR	C7-C8-C9	-2.00	123.19	126.21
20	B	604	CLA	CBA-CAA-C2A	2.00	119.11	113.96
36	d	408	LHG	O4-P-O5	2.01	123.00	112.56
20	B	609	CLA	C4-C3-C5	2.01	118.43	115.37
27	A	411	PL9	C51-C49-C50	2.01	119.49	114.61
34	M	101	LMT	O5B-C5B-C6B	2.01	111.59	106.38
21	a	406	PHO	C3D-C4D-ND	2.01	115.69	109.76
34	m	102	LMT	O5B-C5B-C6B	2.01	111.59	106.38
32	C	521	HTG	O5-C1-C2	2.02	112.97	110.22
20	c	510	CLA	CED-O2D-CGD	2.02	120.76	115.97
37	e	102	HEM	CMB-C2B-C3B	2.02	129.04	125.09
22	b	619	BCR	C37-C22-C21	2.02	125.82	122.89
24	c	519	LMG	O1-C1-C2	2.02	110.49	108.00
22	k	102	BCR	C35-C13-C12	2.02	121.39	118.08
36	l	102	LHG	O4-P-O5	2.03	123.10	112.56
20	c	509	CLA	CMB-C2B-C3B	2.03	129.06	125.09
20	C	501	CLA	CMC-C2C-C1C	2.03	128.01	125.00
20	B	614	CLA	CAC-C3C-C4C	2.03	127.82	124.82
20	b	609	CLA	CMC-C2C-C1C	2.04	128.02	125.00
32	B	623	HTG	O5-C1-C2	2.04	113.00	110.22
34	E	101	LMT	O5'-C5'-C6'	2.04	111.66	106.38
20	D	401	CLA	O1D-CGD-CBD	2.04	127.81	124.64
20	B	603	CLA	C3B-C4B-NB	2.04	111.85	109.21
22	a	408	BCR	C2-C1-C6	2.04	113.52	110.48
20	c	509	CLA	C3C-C4C-NC	2.05	112.28	110.21
36	d	406	LHG	O4-P-O5	2.05	123.22	112.56
20	C	501	CLA	CAC-C3C-C4C	2.05	127.84	124.82
32	V	202	HTG	O2-C2-C1	2.05	114.56	110.50
20	c	507	CLA	CMC-C2C-C3C	2.06	131.83	125.91
20	c	512	CLA	CMB-C2B-C3B	2.06	129.12	125.09
20	C	507	CLA	CED-O2D-CGD	2.07	120.88	115.97
20	c	501	CLA	CMD-C2D-C3D	2.07	129.14	125.09
22	D	405	BCR	C30-C25-C24	2.07	121.88	115.96
20	C	504	CLA	C3C-C4C-NC	2.08	112.32	110.21
20	D	404	CLA	CMC-C2C-C1C	2.08	128.08	125.00
35	d	416	DGD	C4D-C3D-C2D	2.08	114.62	110.79
24	C	524	LMG	O6-C5-C6	2.08	111.78	106.38
20	d	404	CLA	C4A-NA-C1A	2.08	109.02	106.38
20	c	505	CLA	CBA-CAA-C2A	2.08	119.33	113.96
32	B	622	HTG	C1-O5-C5	2.09	116.75	112.73
22	d	405	BCR	C2-C3-C4	2.09	116.70	111.42
20	b	616	CLA	O2A-CGA-CBA	2.09	118.27	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	D	406	DGD	O6D-C5D-C4D	2.09	113.65	109.67
34	Z	101	LMT	O1'-C1-C2	2.09	115.65	109.63
20	B	614	CLA	CMB-C2B-C3B	2.10	129.19	125.09
20	b	611	CLA	CMD-C2D-C3D	2.10	129.19	125.09
34	M	101	LMT	O1'-C1'-C2'	2.10	110.59	108.00
36	d	407	LHG	O7-C7-C8	2.10	115.96	111.53
20	B	615	CLA	O2A-CGA-CBA	2.10	118.33	111.85
32	b	625	HTG	C4-C3-C2	2.11	114.67	110.79
20	c	507	CLA	CMD-C2D-C3D	2.11	129.21	125.09
20	a	403	CLA	CHC-C1C-NC	2.11	127.83	123.92
20	C	507	CLA	CMB-C2B-C3B	2.11	129.22	125.09
23	a	409	SQD	O48-C23-C24	2.11	118.35	111.85
22	K	101	BCR	C1-C6-C7	2.11	122.00	115.96
20	b	603	CLA	CMC-C2C-C1C	2.12	128.14	125.00
20	B	609	CLA	O2A-CGA-CBA	2.12	118.39	111.85
20	c	502	CLA	CMC-C2C-C1C	2.12	128.15	125.00
20	b	615	CLA	CMC-C2C-C1C	2.12	128.15	125.00
22	T	101	BCR	C29-C30-C25	2.13	113.64	110.48
34	z	102	LMT	O2B-C2B-C3B	2.13	115.16	110.36
35	c	516	DGD	C6D-O5D-C1E	2.13	118.26	113.81
20	C	507	CLA	C3B-C4B-NB	2.13	111.97	109.21
20	c	506	CLA	CAC-C3C-C4C	2.13	127.97	124.82
32	d	401	HTG	C1-C2-C3	2.13	115.35	110.58
20	B	608	CLA	CMC-C2C-C3C	2.14	132.05	125.91
20	c	502	CLA	OBD-CAD-CBD	2.14	129.16	125.94
34	c	523	LMT	O5B-C1B-C2B	2.14	114.72	110.28
20	b	604	CLA	CAC-C3C-C4C	2.14	127.98	124.82
20	d	404	CLA	CAC-C3C-C4C	2.14	127.98	124.82
20	B	608	CLA	O2D-CGD-CBD	2.14	114.31	111.22
20	c	510	CLA	CMD-C2D-C3D	2.14	129.28	125.09
24	b	623	LMG	C13-C12-C11	2.14	121.24	113.30
20	A	404	CLA	C3C-C4C-NC	2.14	112.38	110.21
35	C	518	DGD	O1G-C1A-C2A	2.15	118.46	111.85
20	C	513	CLA	C3C-C4C-NC	2.15	112.39	110.21
20	a	407	CLA	C3B-C4B-NB	2.15	111.99	109.21
34	I	101	LMT	O1B-C4'-C5'	2.15	115.05	109.33
24	j	101	LMG	O8-C28-C29	2.15	118.47	111.85
20	a	407	CLA	O2A-CGA-CBA	2.15	118.47	111.85
20	C	505	CLA	CAC-C3C-C4C	2.15	128.00	124.82
20	B	605	CLA	O2A-CGA-CBA	2.15	118.47	111.85
22	D	405	BCR	C32-C1-C6	2.16	113.63	110.33
20	C	513	CLA	C3B-C4B-NB	2.16	112.00	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	D	409	LHG	O8-C23-C24	2.16	118.50	111.85
35	h	101	DGD	O3G-C1D-C2D	2.16	110.66	108.00
20	c	502	CLA	CMB-C2B-C3B	2.16	129.32	125.09
20	D	402	CLA	C4A-NA-C1A	2.17	109.13	106.38
34	B	625	LMT	C3'-C4'-C5'	2.17	114.09	110.23
20	b	615	CLA	C3B-C4B-NB	2.17	112.02	109.21
34	z	102	LMT	C1B-O5B-C5B	2.17	118.00	113.74
20	C	508	CLA	O2A-CGA-CBA	2.17	118.54	111.85
20	B	613	CLA	O2A-CGA-CBA	2.17	118.54	111.85
20	a	403	CLA	C3B-C4B-NB	2.18	112.03	109.21
20	c	506	CLA	C4A-NA-C1A	2.18	109.14	106.38
20	B	601	CLA	CMC-C2C-C3C	2.18	132.18	125.91
20	c	510	CLA	O2A-CGA-CBA	2.18	118.56	111.85
20	C	512	CLA	CAC-C3C-C4C	2.18	128.04	124.82
20	d	403	CLA	CMB-C2B-C3B	2.18	129.36	125.09
20	b	603	CLA	CED-O2D-CGD	2.18	121.16	115.97
36	l	102	LHG	O7-C7-C8	2.18	116.13	111.53
20	B	612	CLA	C4A-NA-C1A	2.19	109.16	106.38
22	k	102	BCR	C37-C22-C23	2.20	121.68	118.08
20	c	512	CLA	CAC-C3C-C4C	2.21	128.08	124.82
20	C	510	CLA	CMC-C2C-C3C	2.21	132.26	125.91
24	C	519	LMG	O6-C5-C6	2.21	112.10	106.38
20	C	505	CLA	C6-C5-C3	2.21	116.73	112.76
22	b	620	BCR	C33-C5-C6	2.21	126.97	124.62
20	c	501	CLA	O2A-CGA-CBA	2.21	118.64	111.85
20	d	403	CLA	C4A-NA-C1A	2.21	109.18	106.38
20	b	605	CLA	CMB-C2B-C3B	2.21	129.42	125.09
32	B	621	HTG	O3-C3-C2	2.21	115.35	110.36
23	l	101	SQD	C46-O48-C23	2.22	123.60	117.00
35	D	406	DGD	C1G-O1G-C1A	2.22	123.60	117.00
20	b	613	CLA	CMB-C2B-C3B	2.22	129.42	125.09
20	d	404	CLA	CMB-C2B-C1B	2.22	132.09	128.31
20	C	509	CLA	CAC-C3C-C4C	2.22	128.10	124.82
20	b	604	CLA	O2A-CGA-CBA	2.22	118.68	111.85
20	A	404	CLA	CAC-C3C-C4C	2.22	128.10	124.82
20	c	501	CLA	C4-C3-C5	2.22	118.76	115.37
32	V	202	HTG	O5-C5-C6	2.22	112.14	106.38
34	b	627	LMT	O1'-C1'-C2'	2.23	110.74	108.00
36	E	103	LHG	O7-C5-C6	2.23	115.12	108.55
34	f	102	LMT	O1'-C1'-C2'	2.23	110.74	108.00
20	A	401	CLA	O2D-CGD-CBD	2.23	114.43	111.22
35	c	517	DGD	C3A-C2A-C1A	2.23	122.27	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	506	CLA	O2A-CGA-CBA	2.23	118.72	111.85
24	C	524	LMG	C9-O8-C28	2.23	123.65	117.00
22	K	101	BCR	C4-C5-C6	2.24	125.19	122.73
35	h	101	DGD	C6D-C5D-C4D	2.24	117.12	112.00
22	c	514	BCR	C29-C30-C25	2.24	113.82	110.48
20	c	503	CLA	O2D-CGD-CBD	2.25	114.46	111.22
20	B	616	CLA	C3B-C4B-NB	2.25	112.12	109.21
20	b	611	CLA	CED-O2D-CGD	2.25	121.32	115.97
24	j	101	LMG	O7-C10-C11	2.25	116.28	111.53
20	b	607	CLA	CMD-C2D-C3D	2.26	129.50	125.09
22	A	405	BCR	C37-C22-C21	2.26	126.16	122.89
22	t	101	BCR	C2-C1-C6	2.26	113.84	110.48
35	H	102	DGD	C6D-C5D-C4D	2.26	117.16	112.00
20	C	504	CLA	CMB-C2B-C3B	2.27	129.52	125.09
20	B	604	CLA	C6-C5-C3	2.27	116.83	112.76
20	d	403	CLA	CAC-C3C-C4C	2.27	128.17	124.82
20	b	608	CLA	C3B-C4B-NB	2.28	112.15	109.21
20	B	616	CLA	OBD-CAD-CBD	2.28	129.37	125.94
27	d	412	PL9	C35-C34-C36	2.28	118.84	115.37
22	B	619	BCR	C37-C22-C21	2.28	126.20	122.89
23	a	401	SQD	O7-S-C6	2.29	108.53	106.92
20	d	402	CLA	C6-C5-C3	2.29	116.87	112.76
34	a	418	LMT	O3'-C3'-C2'	2.29	115.52	110.36
20	c	506	CLA	C3B-C4B-NB	2.29	112.17	109.21
20	B	613	CLA	CMB-C2B-C3B	2.30	129.58	125.09
20	b	614	CLA	C4A-NA-C1A	2.30	109.30	106.38
20	b	617	CLA	C3B-C4B-NB	2.30	112.18	109.21
22	C	514	BCR	C29-C30-C25	2.30	113.91	110.48
20	D	402	CLA	C3C-C4C-NC	2.30	112.55	110.21
20	B	603	CLA	C3C-C4C-NC	2.30	112.55	110.21
28	b	640	DMS	C2-S-C1	2.31	110.69	98.50
34	J	103	LMT	O1'-C1'-C2'	2.31	110.84	108.00
23	F	101	SQD	O7-S-C6	2.31	108.55	106.92
20	B	611	CLA	O2A-CGA-CBA	2.32	118.97	111.85
20	a	404	CLA	C4-C3-C5	2.32	118.90	115.37
20	b	614	CLA	O2A-CGA-CBA	2.32	118.98	111.85
34	Z	101	LMT	O1'-C1'-C2'	2.32	110.85	108.00
36	D	407	LHG	O4-P-O5	2.32	124.62	112.56
20	b	610	CLA	O2A-CGA-CBA	2.32	118.98	111.85
24	A	407	LMG	O8-C28-C29	2.32	118.99	111.85
20	C	503	CLA	CMB-C2B-C3B	2.32	129.63	125.09
20	C	503	CLA	CAC-C3C-C4C	2.32	128.25	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	601	CLA	O2A-CGA-CBA	2.32	119.00	111.85
20	d	403	CLA	CMD-C2D-C3D	2.33	129.65	125.09
20	b	611	CLA	C4-C3-C5	2.33	118.92	115.37
20	C	504	CLA	C4A-NA-C1A	2.33	109.34	106.38
20	c	501	CLA	CMC-C2C-C1C	2.34	128.46	125.00
36	D	407	LHG	C6-O8-C23	2.34	123.96	117.00
27	A	411	PL9	C10-C9-C11	2.34	118.93	115.37
20	C	506	CLA	CMD-C2D-C3D	2.34	129.67	125.09
20	B	605	CLA	C4-C3-C5	2.35	118.94	115.37
24	J	101	LMG	O7-C10-C11	2.35	116.48	111.53
35	H	102	DGD	O2G-C1B-C2B	2.35	116.48	111.53
20	a	403	CLA	C4A-NA-C1A	2.35	109.37	106.38
24	a	410	LMG	O1-C1-C2	2.36	110.90	108.00
20	b	611	CLA	CMC-C2C-C1C	2.36	128.50	125.00
34	z	102	LMT	O2'-C2'-C3'	2.36	115.68	110.36
36	d	408	LHG	O7-C7-C8	2.36	116.50	111.53
20	a	404	CLA	CMB-C2B-C3B	2.36	129.71	125.09
22	t	101	BCR	C33-C5-C4	2.37	118.06	113.47
20	b	603	CLA	C3C-C4C-NC	2.37	112.61	110.21
20	C	510	CLA	C3C-C4C-NC	2.37	112.62	110.21
21	a	405	PHO	C4A-NA-C1A	2.38	110.01	108.22
20	B	610	CLA	OBD-CAD-CBD	2.38	129.52	125.94
20	A	404	CLA	CMD-C2D-C3D	2.38	129.74	125.09
32	C	534	HTG	C1-O5-C5	2.38	117.32	112.73
32	C	534	HTG	C3-C4-C5	2.38	114.47	110.23
32	O	302	HTG	C1'-S1-C1	2.38	103.66	100.60
20	B	611	CLA	CAC-C3C-C2C	2.39	131.62	127.51
20	d	402	CLA	CMC-C2C-C1C	2.39	128.54	125.00
22	K	101	BCR	C37-C22-C23	2.39	121.99	118.08
22	j	102	BCR	C37-C22-C23	2.39	121.99	118.08
20	D	404	CLA	CED-O2D-CGD	2.39	121.65	115.97
20	c	505	CLA	C4A-NA-C1A	2.39	109.41	106.38
20	B	602	CLA	C5-C3-C2	2.40	125.44	120.98
34	a	418	LMT	O1B-C4'-C5'	2.40	115.71	109.33
20	D	401	CLA	CAC-C3C-C4C	2.40	128.36	124.82
20	C	502	CLA	CED-O2D-CGD	2.40	121.67	115.97
36	d	408	LHG	O8-C23-C24	2.40	119.24	111.85
22	t	101	BCR	C1-C6-C7	2.40	122.82	115.96
20	b	605	CLA	O2A-CGA-CBA	2.40	119.24	111.85
20	D	404	CLA	O2A-CGA-CBA	2.40	119.25	111.85
20	B	607	CLA	C3B-C4B-NB	2.41	112.32	109.21
20	b	612	CLA	C4-C3-C5	2.41	119.04	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	601	CLA	C3B-C4B-NB	2.41	112.32	109.21
20	B	605	CLA	CAC-C3C-C4C	2.41	128.38	124.82
20	C	502	CLA	O2A-CGA-CBA	2.42	119.29	111.85
21	D	403	PHO	C3D-C4D-ND	2.42	116.90	109.76
37	E	104	HEM	CMC-C2C-C3C	2.42	129.82	125.09
20	B	612	CLA	C16-C15-C13	2.42	122.95	115.46
20	b	617	CLA	CMB-C2B-C3B	2.42	129.83	125.09
20	C	510	CLA	C4A-NA-C1A	2.43	109.46	106.38
20	b	605	CLA	CMD-C2D-C3D	2.43	129.84	125.09
20	c	509	CLA	O2A-CGA-CBA	2.43	119.33	111.85
37	v	201	HEM	CMB-C2B-C3B	2.43	129.85	125.09
37	e	102	HEM	CAD-CBD-CGD	2.43	117.52	112.78
35	D	406	DGD	C3D-C4D-C5D	2.43	114.57	110.23
32	v	210	HTG	O5-C1-S1	2.44	116.57	109.89
32	c	520	HTG	C3-C4-C5	2.44	114.58	110.23
20	b	606	CLA	CMC-C2C-C1C	2.44	128.62	125.00
34	m	101	LMT	O1'-C1'-C2'	2.45	111.01	108.00
20	B	603	CLA	C4-C3-C5	2.45	119.10	115.37
20	B	612	CLA	CMC-C2C-C1C	2.45	128.62	125.00
34	b	627	LMT	O2'-C2'-C1'	2.45	115.44	110.01
35	d	416	DGD	O6D-C5D-C4D	2.45	114.34	109.67
34	E	101	LMT	C4'-C3'-C2'	2.45	115.30	110.79
24	B	620	LMG	O6-C5-C6	2.45	112.73	106.38
20	b	609	CLA	O2A-CGA-CBA	2.45	119.39	111.85
20	c	509	CLA	C4-C3-C5	2.45	119.11	115.37
20	C	509	CLA	CMB-C2B-C1B	2.46	132.49	128.31
34	b	627	LMT	C2'-C3'-C4'	2.46	115.06	109.63
20	B	603	CLA	O2A-CGA-CBA	2.46	119.42	111.85
35	c	516	DGD	O1G-C1A-C2A	2.46	119.42	111.85
20	b	608	CLA	CAC-C3C-C4C	2.47	128.46	124.82
20	C	510	CLA	CAC-C3C-C4C	2.47	128.47	124.82
20	c	502	CLA	C3B-C4B-NB	2.47	112.40	109.21
20	b	614	CLA	CMB-C2B-C3B	2.47	129.92	125.09
27	D	412	PL9	C53-C6-C1	2.47	119.92	114.66
20	C	505	CLA	CMC-C2C-C1C	2.47	128.66	125.00
34	Z	101	LMT	O1B-C4'-C5'	2.47	115.91	109.33
20	c	511	CLA	O2A-CGA-CBA	2.48	119.48	111.85
23	A	406	SQD	O48-C23-C24	2.48	119.49	111.85
27	A	411	PL9	C40-C39-C41	2.48	119.15	115.37
21	a	406	PHO	CED-O2D-CGD	2.48	121.87	115.97
20	A	401	CLA	OBD-CAD-CBD	2.48	129.69	125.94
27	a	415	PL9	C35-C34-C36	2.48	119.16	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	V	202	HTG	O5-C1-S1	2.49	117.24	110.55
32	b	625	HTG	C1-C2-C3	2.49	116.15	110.58
20	B	613	CLA	C3B-C4B-NB	2.49	112.43	109.21
20	C	504	CLA	C4-C3-C5	2.49	119.17	115.37
20	C	505	CLA	O2A-CGA-CBA	2.49	119.52	111.85
23	F	101	SQD	C3-C4-C5	2.49	114.67	110.23
20	a	404	CLA	O2A-CGA-CBA	2.49	119.53	111.85
20	b	609	CLA	C3B-C4B-NB	2.50	112.44	109.21
20	C	508	CLA	C3B-C4B-NB	2.50	112.44	109.21
20	c	502	CLA	C3C-C4C-NC	2.50	112.75	110.21
20	B	615	CLA	C4-C3-C5	2.51	119.19	115.37
24	a	410	LMG	O8-C28-C29	2.51	119.59	111.85
20	C	511	CLA	C4-C3-C5	2.52	119.21	115.37
20	b	615	CLA	O2A-CGA-CBA	2.52	119.61	111.85
20	B	610	CLA	C4A-NA-C1A	2.52	109.58	106.38
20	c	507	CLA	C3B-C4B-NB	2.53	112.48	109.21
23	a	409	SQD	O8-S-C6	2.53	110.24	104.99
22	a	408	BCR	C35-C13-C12	2.53	122.22	118.08
20	b	605	CLA	CAC-C3C-C4C	2.53	128.56	124.82
20	C	513	CLA	CMB-C2B-C3B	2.53	130.04	125.09
37	e	102	HEM	CMC-C2C-C3C	2.53	130.04	125.09
20	c	511	CLA	C3C-C4C-NC	2.54	112.78	110.21
21	A	403	PHO	C3D-C4D-ND	2.54	117.25	109.76
20	b	608	CLA	O2A-CGA-CBA	2.54	119.67	111.85
20	C	503	CLA	C4-C3-C5	2.54	119.24	115.37
20	b	616	CLA	CMC-C2C-C1C	2.54	128.77	125.00
32	B	632	HTG	C1-O5-C5	2.54	117.64	112.73
20	B	605	CLA	C3B-C4B-NB	2.55	112.51	109.21
20	b	608	CLA	C4A-NA-C1A	2.55	109.62	106.38
20	B	609	CLA	C4A-NA-C1A	2.55	109.62	106.38
20	C	510	CLA	CMD-C2D-C3D	2.55	130.08	125.09
34	z	102	LMT	O1B-C1B-C2B	2.55	114.47	108.12
20	C	503	CLA	C3C-C4C-NC	2.55	112.80	110.21
20	B	616	CLA	C4A-NA-C1A	2.56	109.62	106.38
20	C	501	CLA	C3C-C4C-NC	2.56	112.80	110.21
34	Z	101	LMT	O1B-C4'-C3'	2.56	113.86	107.18
20	c	503	CLA	C3C-C4C-NC	2.56	112.81	110.21
20	b	610	CLA	C3B-C4B-NB	2.56	112.53	109.21
32	c	521	HTG	O5-C5-C4	2.56	114.56	109.67
27	a	415	PL9	C15-C14-C16	2.57	119.28	115.37
20	C	501	CLA	CMD-C2D-C3D	2.57	130.11	125.09
20	b	613	CLA	C4A-NA-C1A	2.58	109.65	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	415	PL9	C20-C19-C21	2.58	119.29	115.37
20	c	505	CLA	CMD-C2D-C3D	2.58	130.13	125.09
20	d	402	CLA	O2A-CGA-CBA	2.58	119.79	111.85
22	d	405	BCR	C2-C1-C6	2.58	114.32	110.48
20	c	510	CLA	C3B-C4B-NB	2.58	112.55	109.21
20	b	616	CLA	CMB-C2B-C1B	2.59	132.71	128.31
20	b	614	CLA	CMD-C2D-C3D	2.59	130.15	125.09
21	a	405	PHO	CMC-C2C-C1C	2.59	129.20	125.06
23	F	101	SQD	O6-C44-C45	2.59	113.73	108.73
27	d	412	PL9	C20-C19-C21	2.59	119.32	115.37
20	C	512	CLA	C3C-C4C-NC	2.59	112.83	110.21
20	b	616	CLA	CAC-C3C-C4C	2.59	128.64	124.82
20	C	505	CLA	C4A-NA-C1A	2.59	109.67	106.38
22	t	101	BCR	C35-C13-C12	2.60	122.33	118.08
20	a	403	CLA	O2A-CGA-CBA	2.60	119.86	111.85
35	C	518	DGD	O2G-C1B-C2B	2.61	117.02	111.53
20	c	506	CLA	CED-O2D-CGD	2.61	122.17	115.97
20	B	607	CLA	O2A-CGA-CBA	2.61	119.88	111.85
23	b	622	SQD	C4-C3-C2	2.61	115.59	110.79
23	f	101	SQD	O6-C1-C2	2.61	111.22	108.00
21	D	403	PHO	C4A-NA-C1A	2.61	110.19	108.22
27	D	412	PL9	C35-C34-C36	2.61	119.35	115.37
27	A	411	PL9	C3-C4-C5	2.61	122.42	118.64
20	d	402	CLA	CAC-C3C-C4C	2.62	128.69	124.82
20	C	511	CLA	C3C-C4C-NC	2.62	112.87	110.21
32	O	302	HTG	C1-O5-C5	2.63	117.80	112.73
20	D	402	CLA	CMC-C2C-C1C	2.63	128.89	125.00
20	D	404	CLA	CMB-C2B-C3B	2.63	130.23	125.09
23	A	412	SQD	O48-C46-C45	2.63	115.80	108.70
20	C	506	CLA	CMB-C2B-C3B	2.63	130.24	125.09
20	c	508	CLA	C3C-C4C-NC	2.63	112.88	110.21
34	B	626	LMT	O5'-C5'-C6'	2.63	113.20	106.38
20	B	601	CLA	C4-C3-C5	2.64	119.39	115.37
27	d	412	PL9	C25-C24-C26	2.64	119.39	115.37
34	f	102	LMT	O5'-C5'-C6'	2.64	113.22	106.38
38	H	101	RRX	C34-C9-C8	2.64	122.40	118.08
20	b	606	CLA	CAC-C3C-C4C	2.65	128.73	124.82
20	C	512	CLA	CED-O2D-CGD	2.65	122.27	115.97
20	B	613	CLA	C4A-NA-C1A	2.66	109.75	106.38
20	b	618	CLA	O2A-CGA-CBA	2.66	120.04	111.85
27	a	415	PL9	C45-C44-C46	2.66	119.43	115.37
20	b	616	CLA	OBD-CAD-CBD	2.66	129.95	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	510	CLA	CMC-C2C-C1C	2.66	128.95	125.00
24	c	518	LMG	O8-C28-C29	2.67	120.06	111.85
20	C	506	CLA	CAC-C3C-C4C	2.67	128.76	124.82
20	c	503	CLA	CMC-C2C-C1C	2.67	128.96	125.00
20	c	513	CLA	C4-C3-C5	2.67	119.44	115.37
20	c	507	CLA	C4-C3-C5	2.68	119.45	115.37
23	A	406	SQD	O3-C3-C4	2.68	116.40	110.36
20	b	610	CLA	CMB-C2B-C3B	2.68	130.33	125.09
32	B	631	HTG	C1-O5-C5	2.68	117.90	112.73
20	C	505	CLA	CMB-C2B-C3B	2.68	130.33	125.09
22	t	101	BCR	C34-C9-C8	2.68	122.46	118.08
20	b	618	CLA	C4A-NA-C1A	2.68	109.78	106.38
32	C	534	HTG	O5-C5-C4	2.69	114.80	109.67
20	b	612	CLA	C3C-C4C-NC	2.69	112.94	110.21
20	b	612	CLA	CAC-C3C-C4C	2.70	128.80	124.82
23	A	406	SQD	O7-S-C6	2.70	108.82	106.92
35	h	101	DGD	O5D-C1E-C2E	2.70	111.32	108.00
20	c	508	CLA	C4-C3-C5	2.70	119.49	115.37
20	c	505	CLA	CMB-C2B-C3B	2.70	130.38	125.09
21	D	403	PHO	CMB-C2B-C1B	2.71	129.39	125.06
20	d	402	CLA	CMD-C2D-C3D	2.71	130.38	125.09
27	A	411	PL9	C15-C14-C16	2.71	119.50	115.37
20	C	502	CLA	CAC-C3C-C4C	2.71	128.82	124.82
20	c	506	CLA	C3C-C4C-NC	2.72	112.96	110.21
20	b	614	CLA	C3B-C4B-NB	2.72	112.73	109.21
20	B	604	CLA	CMC-C2C-C1C	2.72	129.03	125.00
20	B	604	CLA	C4-C3-C5	2.72	119.52	115.37
20	b	605	CLA	C3B-C4B-NB	2.72	112.73	109.21
20	a	407	CLA	CED-O2D-CGD	2.72	122.44	115.97
20	B	616	CLA	C3C-C4C-NC	2.72	112.97	110.21
22	D	405	BCR	C36-C18-C19	2.73	122.54	118.08
20	C	505	CLA	CMD-C2D-C3D	2.73	130.43	125.09
20	B	608	CLA	CMB-C2B-C3B	2.73	130.43	125.09
20	b	609	CLA	C3C-C4C-NC	2.73	112.98	110.21
20	b	604	CLA	C3C-C4C-NC	2.73	112.98	110.21
20	B	612	CLA	CAC-C3C-C4C	2.74	128.87	124.82
20	A	404	CLA	C4A-NA-C1A	2.74	109.86	106.38
20	c	512	CLA	O2A-CGA-CBA	2.74	120.29	111.85
20	d	402	CLA	C3C-C4C-NC	2.74	112.99	110.21
20	B	609	CLA	CAC-C3C-C4C	2.74	128.87	124.82
20	c	513	CLA	C4A-NA-C1A	2.74	109.86	106.38
20	b	614	CLA	C4-C3-C5	2.75	119.56	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	508	CLA	C3B-C4B-NB	2.75	112.77	109.21
20	b	611	CLA	C6-C5-C3	2.75	117.70	112.76
27	d	412	PL9	C3-C4-C5	2.75	122.62	118.64
34	I	101	LMT	O3'-C3'-C4'	2.75	116.41	109.89
20	C	504	CLA	CMC-C2C-C1C	2.76	129.08	125.00
21	A	403	PHO	CAC-C3C-C4C	2.76	128.39	125.21
20	B	607	CLA	CAC-C3C-C2C	2.76	132.26	127.51
20	b	603	CLA	C4A-NA-C1A	2.77	109.89	106.38
20	b	615	CLA	C3C-C4C-NC	2.77	113.02	110.21
27	a	415	PL9	C3-C4-C5	2.78	122.65	118.64
35	c	516	DGD	O6E-C5E-C6E	2.78	113.58	106.38
20	D	404	CLA	C4A-NA-C1A	2.78	109.91	106.38
20	c	512	CLA	CMC-C2C-C1C	2.79	129.13	125.00
20	C	504	CLA	CAC-C3C-C4C	2.79	128.94	124.82
35	D	406	DGD	O1G-C1A-C2A	2.79	120.44	111.85
20	B	607	CLA	C4-C3-C5	2.80	119.63	115.37
20	c	513	CLA	O2A-CGA-CBA	2.80	120.45	111.85
20	B	611	CLA	C3B-C4B-NB	2.80	112.83	109.21
20	b	603	CLA	O2A-CGA-CBA	2.81	120.48	111.85
20	b	617	CLA	C4A-NA-C1A	2.81	109.94	106.38
32	D	417	HTG	O5-C5-C6	2.81	113.66	106.38
23	F	101	SQD	O48-C23-C24	2.81	120.50	111.85
20	a	404	CLA	C3B-C4B-NB	2.81	112.85	109.21
20	D	401	CLA	C4A-NA-C1A	2.81	109.95	106.38
24	c	518	LMG	C3-C4-C5	2.81	115.25	110.23
34	B	625	LMT	C1'-O5'-C5'	2.81	119.27	113.74
20	D	404	CLA	C3B-C4B-NB	2.82	112.86	109.21
21	a	406	PHO	C4A-NA-C1A	2.82	110.35	108.22
36	L	101	LHG	O4-P-O5	2.82	127.26	112.56
34	Z	101	LMT	C1'-O5'-C5'	2.84	119.31	113.74
20	B	604	CLA	CMD-C2D-C3D	2.84	130.63	125.09
20	B	610	CLA	CMC-C2C-C1C	2.84	129.20	125.00
20	D	401	CLA	C4-C3-C5	2.84	119.69	115.37
20	c	507	CLA	C4A-NA-C1A	2.84	109.98	106.38
20	B	615	CLA	CAC-C3C-C4C	2.84	129.01	124.82
27	a	415	PL9	C10-C9-C11	2.85	119.71	115.37
21	D	403	PHO	C4-C3-C5	2.85	119.71	115.37
32	B	621	HTG	O5-C5-C6	2.85	113.77	106.38
20	C	513	CLA	C4-C3-C5	2.85	119.72	115.37
20	C	513	CLA	C4A-NA-C1A	2.86	110.00	106.38
20	B	608	CLA	C3B-C4B-NB	2.86	112.91	109.21
20	A	402	CLA	C4-C3-C5	2.87	119.74	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	504	CLA	CAC-C3C-C4C	2.87	129.05	124.82
27	A	411	PL9	C25-C24-C26	2.87	119.75	115.37
32	C	521	HTG	O5-C5-C4	2.88	115.16	109.67
20	b	606	CLA	CMD-C2D-C3D	2.88	130.72	125.09
32	b	625	HTG	C1-O5-C5	2.88	118.29	112.73
20	D	404	CLA	C4-C3-C5	2.88	119.77	115.37
20	c	513	CLA	CMB-C2B-C3B	2.89	130.73	125.09
20	b	603	CLA	CMD-C2D-C3D	2.89	130.73	125.09
20	b	607	CLA	CMB-C2B-C3B	2.89	130.75	125.09
34	b	628	LMT	C1'-O5'-C5'	2.90	119.42	113.74
20	c	508	CLA	CMD-C2D-C3D	2.90	130.75	125.09
23	f	101	SQD	C1-O5-C5	2.90	119.43	113.74
20	B	602	CLA	CMC-C2C-C1C	2.90	129.30	125.00
20	B	616	CLA	CMB-C2B-C3B	2.90	130.77	125.09
36	E	103	LHG	O4-P-O5	2.91	120.11	110.63
20	B	609	CLA	CMB-C2B-C3B	2.91	130.78	125.09
20	C	504	CLA	C3B-C4B-NB	2.91	112.98	109.21
20	b	609	CLA	CMD-C2D-C3D	2.92	130.79	125.09
20	C	504	CLA	CMD-C2D-C3D	2.92	130.80	125.09
20	b	606	CLA	C4-C3-C5	2.92	119.82	115.37
20	B	612	CLA	C3B-C4B-NB	2.92	112.99	109.21
20	B	607	CLA	C4A-NA-C1A	2.93	110.09	106.38
20	b	612	CLA	CMC-C2C-C1C	2.93	129.34	125.00
34	a	418	LMT	C1B-O5B-C5B	2.93	119.50	113.74
20	b	617	CLA	C4-C3-C5	2.93	119.84	115.37
20	b	616	CLA	C4-C3-C5	2.94	119.84	115.37
20	b	618	CLA	CMB-C2B-C3B	2.94	130.84	125.09
20	a	403	CLA	CMD-C2D-C3D	2.94	130.84	125.09
20	B	608	CLA	CAC-C3C-C4C	2.94	129.16	124.82
20	b	611	CLA	O2D-CGD-CBD	2.95	115.47	111.22
20	B	602	CLA	C6-C5-C3	2.95	118.06	112.76
20	c	511	CLA	CMD-C2D-C3D	2.95	130.86	125.09
20	B	607	CLA	CMB-C2B-C1B	2.96	133.35	128.31
20	c	512	CLA	C4A-NA-C1A	2.96	110.14	106.38
23	a	401	SQD	O48-C23-C24	2.96	120.97	111.85
20	C	511	CLA	C3B-C4B-NB	2.97	113.05	109.21
35	d	416	DGD	C3D-C4D-C5D	2.97	115.53	110.23
23	A	406	SQD	O8-S-C6	2.97	111.17	104.99
27	d	412	PL9	C15-C14-C16	2.97	119.90	115.37
20	A	402	CLA	C3C-C4C-NC	2.98	113.23	110.21
20	B	603	CLA	C4A-NA-C1A	2.98	110.16	106.38
24	C	524	LMG	O8-C28-C29	2.98	121.03	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	612	CLA	CMD-C2D-C3D	2.99	130.93	125.09
20	D	402	CLA	CMB-C2B-C3B	2.99	130.94	125.09
27	a	415	PL9	C40-C39-C41	2.99	119.93	115.37
34	b	627	LMT	C4B-C3B-C2B	2.99	116.30	110.79
20	C	503	CLA	CMD-C2D-C3D	3.00	130.95	125.09
20	C	505	CLA	C3C-C4C-NC	3.00	113.25	110.21
20	d	402	CLA	O1D-CGD-CBD	3.00	129.30	124.64
20	C	507	CLA	CMC-C2C-C1C	3.00	129.45	125.00
21	a	406	PHO	CMB-C2B-C1B	3.01	129.87	125.06
20	B	603	CLA	CMD-C2D-C3D	3.01	130.97	125.09
20	C	508	CLA	C4A-NA-C1A	3.01	110.20	106.38
20	B	606	CLA	CMC-C2C-C1C	3.02	129.47	125.00
22	K	102	BCR	C34-C9-C8	3.02	123.01	118.08
20	c	505	CLA	CAC-C3C-C4C	3.02	129.28	124.82
34	z	102	LMT	O1'-C1'-C2'	3.03	111.73	108.00
23	a	409	SQD	O47-C7-C8	3.03	117.92	111.53
20	a	407	CLA	CMB-C2B-C3B	3.04	131.03	125.09
20	c	508	CLA	C4A-NA-C1A	3.04	110.24	106.38
20	c	503	CLA	CMD-C2D-C3D	3.04	131.04	125.09
34	E	101	LMT	C1'-C2'-C3'	3.04	116.02	109.98
20	C	509	CLA	C4A-NA-C1A	3.04	110.24	106.38
20	C	509	CLA	O2A-CGA-CBA	3.05	121.24	111.85
36	E	103	LHG	O8-C23-C24	3.05	121.25	111.85
20	b	610	CLA	CED-O2D-CGD	3.05	123.22	115.97
35	d	416	DGD	O1G-C1A-C2A	3.06	121.26	111.85
20	b	608	CLA	CMD-C2D-C3D	3.06	131.07	125.09
20	A	404	CLA	C3B-C4B-NB	3.06	113.17	109.21
20	d	403	CLA	C3B-C4B-NB	3.06	113.17	109.21
20	b	612	CLA	CMD-C2D-C3D	3.06	131.08	125.09
20	a	407	CLA	CMC-C2C-C1C	3.07	129.55	125.00
20	b	618	CLA	CAC-C3C-C4C	3.07	129.36	124.82
24	A	407	LMG	O7-C10-C11	3.08	118.01	111.53
35	C	517	DGD	O5D-C6D-C5D	3.08	114.63	109.14
20	b	618	CLA	CMD-C2D-C3D	3.08	131.12	125.09
20	D	404	CLA	CAC-C3C-C4C	3.09	129.38	124.82
20	b	604	CLA	OBD-CAD-CBD	3.09	130.60	125.94
20	D	402	CLA	C4-C3-C5	3.09	120.08	115.37
20	B	606	CLA	C4-C3-C5	3.10	120.09	115.37
20	B	616	CLA	O2D-CGD-CBD	3.10	115.69	111.22
20	c	507	CLA	O2A-CGA-CBA	3.10	121.39	111.85
34	b	627	LMT	C3'-C4'-C5'	3.11	117.96	110.85
20	C	506	CLA	CMC-C2C-C1C	3.11	129.61	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	406	PHO	C4-C3-C5	3.11	120.11	115.37
20	D	402	CLA	C3B-C4B-NB	3.12	113.24	109.21
20	C	510	CLA	C3B-C4B-NB	3.12	113.24	109.21
35	c	517	DGD	O2G-C1B-C2B	3.12	118.10	111.53
20	b	615	CLA	O2D-CGD-CBD	3.12	115.72	111.22
20	C	502	CLA	C4A-NA-C1A	3.12	110.34	106.38
20	B	609	CLA	CMC-C2C-C1C	3.13	129.64	125.00
20	b	606	CLA	C3B-C4B-NB	3.14	113.27	109.21
21	a	405	PHO	O2D-CGD-CBD	3.14	115.75	111.22
20	c	509	CLA	CAC-C3C-C4C	3.14	129.46	124.82
34	m	102	LMT	O1'-C1'-C2'	3.14	111.87	108.00
20	b	612	CLA	C3B-C4B-NB	3.15	113.28	109.21
20	b	610	CLA	C3C-C4C-NC	3.16	113.41	110.21
35	d	416	DGD	O3G-C1D-C2D	3.16	111.88	108.00
34	B	625	LMT	O5'-C5'-C4'	3.16	115.70	109.67
27	A	411	PL9	C45-C44-C46	3.16	120.19	115.37
20	D	401	CLA	O2D-CGD-CBD	3.16	115.78	111.22
22	T	101	BCR	C35-C13-C12	3.17	123.26	118.08
20	B	608	CLA	CMD-C2D-C3D	3.17	131.28	125.09
20	C	513	CLA	CMD-C2D-C3D	3.17	131.29	125.09
20	C	509	CLA	C3B-C4B-NB	3.17	113.31	109.21
24	c	518	LMG	C4-C3-C2	3.17	116.63	110.79
20	c	509	CLA	O2D-CGD-CBD	3.18	115.81	111.22
20	b	615	CLA	CAC-C3C-C4C	3.19	129.52	124.82
20	D	401	CLA	C3B-C4B-NB	3.19	113.33	109.21
32	B	631	HTG	O5-C5-C4	3.19	115.75	109.67
20	b	608	CLA	C3C-C4C-NC	3.19	113.44	110.21
20	c	504	CLA	C4-C3-C5	3.19	120.23	115.37
20	C	511	CLA	CMD-C2D-C3D	3.19	131.34	125.09
20	B	606	CLA	CMB-C2B-C3B	3.20	131.34	125.09
34	m	101	LMT	C1'-O5'-C5'	3.20	120.03	113.74
20	c	510	CLA	C3C-C4C-NC	3.20	113.46	110.21
20	d	404	CLA	O2D-CGD-CBD	3.20	115.84	111.22
20	B	615	CLA	C4A-NA-C1A	3.21	110.45	106.38
20	B	613	CLA	C3C-C4C-NC	3.21	113.46	110.21
20	B	608	CLA	C3C-C4C-NC	3.21	113.46	110.21
20	C	508	CLA	O2D-CGD-CBD	3.22	115.86	111.22
20	B	613	CLA	C4-C3-C5	3.22	120.28	115.37
20	B	606	CLA	C3B-C4B-NB	3.22	113.38	109.21
20	A	404	CLA	O2D-CGD-CBD	3.22	115.87	111.22
34	T	102	LMT	C1'-C2'-C3'	3.23	116.38	109.98
35	c	517	DGD	O1G-C1A-C2A	3.23	121.79	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	402	CLA	C4A-NA-C1A	3.24	110.49	106.38
20	B	614	CLA	O2A-CGA-CBA	3.26	121.87	111.85
21	D	403	PHO	C3C-C4C-NC	3.26	115.45	110.31
23	b	622	SQD	O48-C23-C24	3.26	121.88	111.85
20	C	506	CLA	C4-C3-C5	3.26	120.34	115.37
21	A	403	PHO	CMB-C2B-C1B	3.28	130.31	125.06
22	a	408	BCR	C29-C30-C25	3.29	115.37	110.48
34	b	627	LMT	O5B-C5B-C6B	3.29	114.90	106.38
23	l	101	SQD	O9-S-C6	3.30	109.25	106.92
35	c	516	DGD	O2G-C1B-C2B	3.30	118.48	111.53
20	C	510	CLA	C4-C3-C5	3.30	120.40	115.37
20	c	501	CLA	C3C-C4C-NC	3.30	113.55	110.21
20	B	601	CLA	CMD-C2D-C3D	3.30	131.55	125.09
20	b	615	CLA	C4A-NA-C1A	3.31	110.58	106.38
20	c	509	CLA	C3B-C4B-NB	3.31	113.49	109.21
20	c	509	CLA	CMC-C2C-C1C	3.32	129.91	125.00
20	c	513	CLA	CMC-C2C-C1C	3.32	129.92	125.00
21	a	406	PHO	C2C-C1C-NC	3.32	114.75	109.81
35	C	517	DGD	O2G-C1B-C2B	3.32	118.52	111.53
20	B	610	CLA	CMD-C2D-C3D	3.33	131.60	125.09
20	C	503	CLA	CMC-C2C-C1C	3.33	129.94	125.00
24	b	623	LMG	O8-C28-C29	3.34	122.12	111.85
20	b	616	CLA	C4A-NA-C1A	3.34	110.62	106.38
32	B	622	HTG	C1-C2-C3	3.34	118.06	110.58
20	B	609	CLA	C3B-C4B-NB	3.35	113.54	109.21
21	A	403	PHO	C4A-NA-C1A	3.36	110.75	108.22
20	B	609	CLA	C3C-C4C-NC	3.36	113.62	110.21
20	b	604	CLA	C4-C3-C5	3.36	120.49	115.37
32	B	621	HTG	C1-O5-C5	3.36	119.22	112.73
24	c	519	LMG	O8-C28-C29	3.36	122.20	111.85
20	C	506	CLA	C3C-C4C-NC	3.37	113.62	110.21
20	B	602	CLA	C4A-NA-C1A	3.37	110.65	106.38
20	C	502	CLA	C3C-C4C-NC	3.37	113.63	110.21
20	b	609	CLA	O2D-CGD-CBD	3.38	116.09	111.22
21	a	406	PHO	C3C-C4C-NC	3.38	115.64	110.31
22	B	619	BCR	C2-C1-C6	3.38	115.51	110.48
20	b	613	CLA	C6-C5-C3	3.39	118.84	112.76
20	B	607	CLA	C3C-C4C-NC	3.39	113.64	110.21
21	D	403	PHO	CAC-C3C-C4C	3.39	129.12	125.21
20	C	502	CLA	C3B-C4B-NB	3.39	113.59	109.21
20	C	509	CLA	C3C-C4C-NC	3.39	113.64	110.21
20	a	403	CLA	C4-C3-C5	3.39	120.53	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	505	CLA	CMC-C2C-C1C	3.39	130.03	125.00
36	d	406	LHG	C6-O8-C23	3.41	127.14	117.00
23	f	101	SQD	O48-C23-C24	3.41	122.33	111.85
20	b	616	CLA	C3B-C4B-NB	3.42	113.64	109.21
20	c	511	CLA	C4-C3-C5	3.43	120.60	115.37
20	C	512	CLA	C4-C3-C5	3.43	120.60	115.37
20	b	604	CLA	CMC-C2C-C1C	3.43	130.09	125.00
24	C	519	LMG	O7-C10-C11	3.45	118.79	111.53
24	C	519	LMG	O8-C28-C29	3.45	122.46	111.85
24	A	407	LMG	O1-C1-C2	3.45	112.24	108.00
20	B	610	CLA	CED-O2D-CGD	3.45	124.17	115.97
20	c	505	CLA	C3C-C4C-NC	3.48	113.73	110.21
20	B	604	CLA	C3C-C4C-NC	3.48	113.74	110.21
20	b	609	CLA	CAC-C3C-C4C	3.50	129.99	124.82
21	a	405	PHO	C2B-C1B-NB	3.50	115.03	109.81
20	b	606	CLA	C4A-NA-C1A	3.51	110.83	106.38
20	B	609	CLA	CMD-C2D-C3D	3.51	131.95	125.09
20	C	508	CLA	C4-C3-C5	3.51	120.72	115.37
22	B	618	BCR	C29-C30-C25	3.52	115.72	110.48
36	E	103	LHG	O7-C7-C8	3.52	122.69	111.85
20	c	507	CLA	C3C-C4C-NC	3.53	113.78	110.21
21	D	403	PHO	O2D-CGD-CBD	3.53	116.31	111.22
22	d	405	BCR	C29-C30-C25	3.54	115.75	110.48
20	d	404	CLA	C3B-C4B-NB	3.54	113.79	109.21
20	b	604	CLA	CMD-C2D-C3D	3.54	132.02	125.09
27	D	412	PL9	C10-C9-C11	3.55	120.77	115.37
36	d	406	LHG	O8-C23-C24	3.56	122.79	111.85
20	C	509	CLA	C4-C3-C5	3.56	120.80	115.37
21	D	403	PHO	C2C-C1C-NC	3.56	115.11	109.81
20	b	605	CLA	CMC-C2C-C1C	3.57	130.30	125.00
20	d	402	CLA	C3B-C4B-NB	3.58	113.83	109.21
20	a	404	CLA	CMC-C2C-C1C	3.58	130.30	125.00
20	c	513	CLA	C3C-C4C-NC	3.58	113.84	110.21
21	D	403	PHO	CED-O2D-CGD	3.58	124.49	115.97
20	b	604	CLA	O2D-CGD-CBD	3.59	116.40	111.22
20	c	501	CLA	C3B-C4B-NB	3.59	113.86	109.21
27	a	415	PL9	C25-C24-C26	3.59	120.84	115.37
20	B	610	CLA	CAC-C3C-C4C	3.60	130.13	124.82
20	b	611	CLA	CAC-C3C-C4C	3.60	130.13	124.82
20	c	511	CLA	CMC-C2C-C1C	3.61	130.35	125.00
20	B	606	CLA	CAC-C3C-C4C	3.61	130.15	124.82
20	b	611	CLA	C3C-C4C-NC	3.61	113.87	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	511	CLA	C4A-NA-C1A	3.61	110.96	106.38
20	b	618	CLA	C3B-C4B-NB	3.61	113.88	109.21
20	c	513	CLA	CMD-C2D-C3D	3.62	132.16	125.09
20	C	512	CLA	C4A-NA-C1A	3.62	110.97	106.38
20	D	401	CLA	CMB-C2B-C3B	3.63	132.18	125.09
22	b	620	BCR	C29-C30-C25	3.63	115.88	110.48
24	B	620	LMG	O8-C28-C29	3.63	123.02	111.85
36	D	409	LHG	O4-P-O5	3.63	131.46	112.56
20	C	507	CLA	C4-C3-C5	3.64	120.92	115.37
24	C	524	LMG	O1-C1-C2	3.65	112.49	108.00
23	A	412	SQD	O48-C23-C24	3.65	123.08	111.85
21	a	405	PHO	CAC-C3C-C4C	3.65	129.43	125.21
20	B	614	CLA	C3C-C4C-NC	3.65	113.91	110.21
34	c	523	LMT	O5'-C5'-C4'	3.66	117.58	109.78
20	B	616	CLA	CMD-C2D-C3D	3.66	132.25	125.09
20	B	606	CLA	O2D-CGD-CBD	3.67	116.51	111.22
23	b	622	SQD	C3-C4-C5	3.67	116.77	110.23
27	A	411	PL9	C30-C29-C31	3.67	120.96	115.37
20	C	506	CLA	C4A-NA-C1A	3.67	111.04	106.38
20	b	605	CLA	C3C-C4C-NC	3.67	113.93	110.21
20	B	611	CLA	C4A-NA-C1A	3.68	111.05	106.38
34	c	523	LMT	O1'-C1'-C2'	3.68	112.53	108.00
20	a	404	CLA	C3C-C4C-NC	3.69	113.94	110.21
20	C	512	CLA	CMD-C2D-C3D	3.69	132.31	125.09
35	h	101	DGD	O2G-C1B-C2B	3.69	119.31	111.53
35	c	515	DGD	O2G-C1B-C2B	3.69	119.31	111.53
20	B	614	CLA	C3B-C4B-NB	3.70	113.99	109.21
20	b	614	CLA	O2D-CGD-CBD	3.70	116.56	111.22
20	B	603	CLA	CMB-C2B-C3B	3.70	132.33	125.09
20	B	613	CLA	O2D-CGD-CBD	3.70	116.56	111.22
34	c	523	LMT	O5B-C5B-C4B	3.74	116.81	109.67
20	a	407	CLA	C3C-C4C-NC	3.74	114.00	110.21
20	b	617	CLA	CMC-C2C-C1C	3.76	130.58	125.00
20	A	401	CLA	C3C-C4C-NC	3.76	114.02	110.21
24	c	519	LMG	O7-C10-C11	3.77	119.48	111.53
23	l	101	SQD	O47-C7-C8	3.78	119.48	111.53
20	A	401	CLA	CAC-C3C-C4C	3.79	130.41	124.82
20	b	617	CLA	CAC-C3C-C4C	3.79	130.41	124.82
20	C	508	CLA	CAC-C3C-C4C	3.80	130.43	124.82
34	B	626	LMT	O1'-C1'-C2'	3.81	112.68	108.00
20	b	614	CLA	CMC-C2C-C1C	3.81	130.65	125.00
27	a	415	PL9	C53-C6-C1	3.81	122.78	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	a	403	CLA	CAC-C3C-C4C	3.82	130.46	124.82
21	a	406	PHO	C2B-C1B-NB	3.82	115.50	109.81
20	b	613	CLA	C3C-C4C-NC	3.84	114.10	110.21
34	b	628	LMT	O5'-C5'-C4'	3.85	117.99	109.78
20	C	511	CLA	O2D-CGD-CBD	3.86	116.79	111.22
32	B	631	HTG	C3-C4-C5	3.86	117.11	110.23
24	a	410	LMG	O7-C10-C11	3.86	119.67	111.53
20	d	404	CLA	C4-C3-C5	3.87	121.26	115.37
20	c	502	CLA	C4A-NA-C1A	3.87	111.29	106.38
34	a	418	LMT	O5B-C5B-C6B	3.89	116.46	106.38
20	b	605	CLA	C4-C3-C5	3.90	121.31	115.37
20	c	504	CLA	C3B-C4B-NB	3.90	114.25	109.21
34	z	102	LMT	C1B-O1B-C4'	3.90	128.38	118.00
20	A	401	CLA	C3B-C4B-NB	3.91	114.26	109.21
35	H	102	DGD	O1G-C1A-C2A	3.92	123.91	111.85
20	c	503	CLA	C4-C3-C5	3.92	121.34	115.37
20	B	606	CLA	CMD-C2D-C3D	3.93	132.76	125.09
20	B	601	CLA	CAC-C3C-C4C	3.93	130.62	124.82
20	B	612	CLA	C3C-C4C-NC	3.94	114.20	110.21
20	c	503	CLA	C4A-NA-C1A	3.94	111.38	106.38
20	b	618	CLA	C3C-C4C-NC	3.94	114.21	110.21
23	l	101	SQD	O48-C23-C24	3.95	124.01	111.85
20	a	404	CLA	CAC-C3C-C4C	3.95	130.66	124.82
20	c	510	CLA	C4-C3-C5	3.96	121.41	115.37
34	a	418	LMT	O1'-C1'-C2'	3.97	112.88	108.00
20	C	507	CLA	C4A-NA-C1A	3.97	111.42	106.38
20	B	607	CLA	C2C-C1C-NC	3.98	112.96	110.22
32	c	521	HTG	C1-O5-C5	3.98	120.41	112.73
20	B	605	CLA	C3C-C4C-NC	3.99	114.25	110.21
20	C	513	CLA	O2A-CGA-CBA	4.01	124.18	111.85
20	c	502	CLA	CMD-C2D-C3D	4.01	132.93	125.09
34	b	627	LMT	C1'-O5'-C5'	4.01	121.61	113.74
20	d	403	CLA	O2D-CGD-CBD	4.01	117.00	111.22
20	c	508	CLA	O2D-CGD-CBD	4.02	117.01	111.22
20	B	601	CLA	C3C-C4C-NC	4.02	114.28	110.21
21	a	406	PHO	C2D-C1D-ND	4.02	115.80	109.81
23	a	401	SQD	O9-S-C6	4.04	109.76	106.92
22	D	405	BCR	C29-C30-C25	4.05	116.50	110.48
20	C	502	CLA	O2D-CGD-CBD	4.07	117.09	111.22
20	c	509	CLA	C4A-NA-C1A	4.08	111.55	106.38
34	b	627	LMT	O5'-C5'-C4'	4.10	118.53	109.78
21	D	403	PHO	C2B-C1B-NB	4.11	115.92	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	415	PL9	C30-C29-C31	4.11	121.63	115.37
20	b	617	CLA	CMD-C2D-C3D	4.12	133.15	125.09
24	c	518	LMG	O1-C1-C2	4.12	113.08	108.00
20	c	513	CLA	O2D-CGD-CBD	4.17	117.23	111.22
35	C	516	DGD	O2G-C1B-C2B	4.17	120.31	111.53
20	b	610	CLA	CMD-C2D-C3D	4.17	133.24	125.09
24	b	623	LMG	O7-C10-C11	4.18	120.33	111.53
20	d	403	CLA	C3C-C4C-NC	4.18	114.45	110.21
23	a	401	SQD	O47-C7-C8	4.18	120.34	111.53
21	A	403	PHO	C2B-C1B-NB	4.18	116.04	109.81
20	B	606	CLA	C3C-C4C-NC	4.18	114.45	110.21
20	B	610	CLA	O2D-CGD-CBD	4.19	117.26	111.22
27	d	412	PL9	C40-C39-C41	4.19	121.75	115.37
20	B	609	CLA	O2D-CGD-CBD	4.19	117.27	111.22
20	D	402	CLA	CMD-C2D-C3D	4.19	133.29	125.09
20	B	602	CLA	O2A-CGA-CBA	4.21	124.81	111.85
20	B	611	CLA	C3C-C4C-NC	4.23	114.49	110.21
27	A	411	PL9	C20-C19-C21	4.25	121.84	115.37
20	B	604	CLA	C3B-C4B-NB	4.27	114.73	109.21
20	c	501	CLA	C4A-NA-C1A	4.30	111.84	106.38
21	D	403	PHO	C2D-C1D-ND	4.33	116.25	109.81
20	D	401	CLA	CMC-C2C-C1C	4.33	131.42	125.00
20	D	404	CLA	O2D-CGD-CBD	4.34	117.48	111.22
23	A	412	SQD	O47-C7-C8	4.34	120.68	111.53
24	B	620	LMG	O7-C10-C11	4.36	120.70	111.53
21	A	403	PHO	C3C-C4C-NC	4.36	117.19	110.31
20	b	618	CLA	C4-C3-C5	4.37	122.02	115.37
20	b	607	CLA	CMC-C2C-C1C	4.37	131.48	125.00
27	A	411	PL9	C53-C6-C1	4.38	123.98	114.66
20	b	607	CLA	C4-C3-C5	4.39	122.06	115.37
20	C	511	CLA	C4A-NA-C1A	4.42	111.99	106.38
23	b	622	SQD	O47-C7-C8	4.43	120.86	111.53
21	a	405	PHO	C3C-C4C-NC	4.44	117.32	110.31
20	a	407	CLA	CMD-C2D-C3D	4.46	133.81	125.09
20	A	401	CLA	C2C-C1C-NC	4.48	113.31	110.22
20	C	513	CLA	O2D-CGD-CBD	4.49	117.69	111.22
21	a	405	PHO	C2D-C1D-ND	4.49	116.49	109.81
20	b	610	CLA	CAC-C3C-C4C	4.50	131.46	124.82
35	d	416	DGD	O2G-C1B-C2B	4.50	121.02	111.53
20	D	402	CLA	CAC-C3C-C4C	4.52	131.49	124.82
20	c	502	CLA	CAC-C3C-C4C	4.55	131.54	124.82
20	c	504	CLA	O2D-CGD-CBD	4.56	117.79	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	504	CLA	C4A-NA-C1A	4.58	112.19	106.38
24	c	518	LMG	O7-C10-C11	4.58	121.18	111.53
20	B	612	CLA	O2D-CGD-CBD	4.58	117.83	111.22
20	A	401	CLA	C4-C3-C5	4.59	122.36	115.37
23	b	622	SQD	O6-C1-C2	4.61	113.67	108.00
20	B	603	CLA	O2D-CGD-CBD	4.61	117.87	111.22
20	a	407	CLA	CAC-C3C-C4C	4.61	131.63	124.82
20	c	510	CLA	O2D-CGD-CBD	4.62	117.89	111.22
20	B	605	CLA	O2D-CGD-CBD	4.63	117.90	111.22
20	b	604	CLA	CMB-C2B-C3B	4.64	134.15	125.09
20	B	601	CLA	O2D-CGD-CBD	4.64	117.91	111.22
36	D	407	LHG	O8-C23-C24	4.65	126.15	111.85
20	A	402	CLA	C3B-C4B-NB	4.66	115.23	109.21
21	a	405	PHO	CMD-C2D-C1D	4.68	132.55	125.06
21	a	406	PHO	O2D-CGD-CBD	4.70	117.99	111.22
20	c	506	CLA	O2D-CGD-CBD	4.72	118.03	111.22
23	A	406	SQD	O47-C7-C8	4.73	121.49	111.53
20	b	607	CLA	C3C-C4C-NC	4.73	115.00	110.21
20	b	610	CLA	O2D-CGD-CBD	4.73	118.04	111.22
20	b	614	CLA	CAC-C3C-C4C	4.73	131.81	124.82
20	C	505	CLA	O2D-CGD-CBD	4.74	118.05	111.22
20	c	505	CLA	O2D-CGD-CBD	4.74	118.05	111.22
20	B	602	CLA	C2C-C1C-NC	4.74	113.49	110.22
20	b	617	CLA	O2D-CGD-CBD	4.75	118.07	111.22
20	B	610	CLA	C3C-C4C-NC	4.75	115.03	110.21
20	d	402	CLA	C4-C3-C5	4.76	122.62	115.37
32	C	534	HTG	C1'-S1-C1	4.79	106.75	100.60
21	A	403	PHO	O2D-CGD-CBD	4.80	118.15	111.22
20	b	607	CLA	CAC-C3C-C4C	4.81	131.91	124.82
23	f	101	SQD	O8-S-C6	4.84	115.04	104.99
20	b	607	CLA	O2D-CGD-CBD	4.85	118.21	111.22
34	z	102	LMT	O1B-C4'-C3'	4.87	119.89	107.18
20	b	609	CLA	C4-C3-C5	4.89	122.81	115.37
21	a	405	PHO	C2C-C1C-NC	4.89	117.08	109.81
21	A	403	PHO	C2D-C1D-ND	4.92	117.13	109.81
20	b	606	CLA	C3C-C4C-NC	4.93	115.21	110.21
20	A	404	CLA	C4-C3-C5	4.94	122.90	115.37
20	b	618	CLA	C2C-C1C-NC	4.95	113.63	110.22
20	D	402	CLA	O2D-CGD-CBD	4.95	118.36	111.22
20	b	605	CLA	O2D-CGD-CBD	4.96	118.37	111.22
20	C	512	CLA	C2C-C1C-NC	5.04	113.69	110.22
20	B	615	CLA	C2C-C1C-NC	5.06	113.70	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	403	PHO	C2C-C1C-NC	5.06	117.34	109.81
20	c	502	CLA	O2D-CGD-CBD	5.08	118.55	111.22
32	C	521	HTG	C1-O5-C5	5.09	122.56	112.73
34	c	523	LMT	C1B-O5B-C5B	5.13	123.80	113.74
20	a	403	CLA	C2C-C1C-NC	5.14	113.76	110.22
23	a	401	SQD	O6-C1-C2	5.16	114.35	108.00
20	B	615	CLA	O2D-CGD-CBD	5.17	118.68	111.22
20	b	603	CLA	C2C-C1C-NC	5.20	113.80	110.22
34	I	101	LMT	O1B-C4'-C3'	5.20	120.75	107.18
32	B	632	HTG	C1'-S1-C1	5.20	107.28	100.60
20	C	509	CLA	O2D-CGD-CBD	5.20	118.72	111.22
34	b	627	LMT	C3B-C4B-C5B	5.24	119.58	110.23
20	b	613	CLA	O2D-CGD-CBD	5.25	118.80	111.22
27	D	412	PL9	C40-C39-C41	5.26	123.39	115.37
20	b	614	CLA	C3C-C4C-NC	5.29	115.57	110.21
20	C	504	CLA	O2D-CGD-CBD	5.31	118.87	111.22
32	B	621	HTG	C1'-S1-C1	5.31	107.43	100.60
20	C	503	CLA	O2D-CGD-CBD	5.35	118.93	111.22
20	C	506	CLA	C2C-C1C-NC	5.36	113.91	110.22
20	A	404	CLA	C2C-C1C-NC	5.36	113.91	110.22
20	b	606	CLA	O2D-CGD-CBD	5.37	118.96	111.22
20	b	616	CLA	O2D-CGD-CBD	5.38	118.98	111.22
20	B	612	CLA	C2C-C1C-NC	5.38	113.92	110.22
20	c	512	CLA	C2C-C1C-NC	5.40	113.94	110.22
20	D	404	CLA	C2C-C1C-NC	5.41	113.95	110.22
23	F	101	SQD	O6-C1-C2	5.43	114.68	108.00
20	B	607	CLA	O2D-CGD-CBD	5.43	119.05	111.22
20	c	510	CLA	C2C-C1C-NC	5.43	113.96	110.22
20	b	616	CLA	C2C-C1C-NC	5.45	113.97	110.22
35	D	406	DGD	O2G-C1B-C2B	5.46	123.04	111.53
20	c	509	CLA	C2C-C1C-NC	5.46	113.98	110.22
24	C	524	LMG	O7-C10-C11	5.46	123.04	111.53
20	A	402	CLA	CAC-C3C-C4C	5.49	132.92	124.82
34	c	523	LMT	C1'-O5'-C5'	5.51	124.55	113.74
20	C	510	CLA	O2D-CGD-CBD	5.54	119.21	111.22
20	A	401	CLA	CMD-C2D-C3D	5.55	135.94	125.09
20	B	613	CLA	CAC-C3C-C4C	5.57	133.04	124.82
23	b	622	SQD	O9-S-C6	5.59	110.86	106.92
20	C	502	CLA	C2C-C1C-NC	5.59	114.07	110.22
20	C	507	CLA	C2C-C1C-NC	5.59	114.07	110.22
20	c	511	CLA	O2D-CGD-CBD	5.60	119.30	111.22
20	C	512	CLA	O2D-CGD-CBD	5.62	119.33	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	608	CLA	O2D-CGD-CBD	5.64	119.35	111.22
20	D	401	CLA	C3C-C4C-NC	5.64	115.92	110.21
20	c	513	CLA	C2C-C1C-NC	5.65	114.11	110.22
21	D	403	PHO	CMD-C2D-C1D	5.77	134.28	125.06
20	A	402	CLA	O2D-CGD-CBD	5.77	119.55	111.22
23	f	101	SQD	O8-S-O7	5.79	124.09	111.26
20	a	404	CLA	O2D-CGD-CBD	5.83	119.62	111.22
20	c	511	CLA	C2C-C1C-NC	5.83	114.23	110.22
20	C	508	CLA	C2C-C1C-NC	5.84	114.24	110.22
20	c	504	CLA	C2C-C1C-NC	5.87	114.26	110.22
32	c	520	HTG	C1'-S1-C1	5.90	108.19	100.60
21	A	403	PHO	CMD-C2D-C1D	5.90	134.50	125.06
20	B	611	CLA	O2D-CGD-CBD	5.92	119.76	111.22
23	f	101	SQD	O47-C7-C8	5.98	122.47	111.09
20	c	508	CLA	C2C-C1C-NC	6.00	114.35	110.22
32	b	601	HTG	C1'-S1-C1	6.03	108.35	100.60
32	b	602	HTG	C1'-S1-C1	6.03	108.35	100.60
20	c	501	CLA	O2D-CGD-CBD	6.04	119.93	111.22
20	C	503	CLA	C2C-C1C-NC	6.04	114.38	110.22
21	a	406	PHO	CMD-C2D-C1D	6.05	134.74	125.06
20	b	617	CLA	C2C-C1C-NC	6.08	114.41	110.22
20	B	604	CLA	O2D-CGD-CBD	6.09	120.01	111.22
20	b	612	CLA	C2C-C1C-NC	6.11	114.42	110.22
20	c	506	CLA	C2C-C1C-NC	6.23	114.51	110.22
20	c	502	CLA	C2C-C1C-NC	6.28	114.54	110.22
20	c	512	CLA	O2D-CGD-CBD	6.33	120.35	111.22
20	C	513	CLA	C2C-C1C-NC	6.36	114.59	110.22
20	c	507	CLA	O2D-CGD-CBD	6.41	120.47	111.22
20	C	506	CLA	O2D-CGD-CBD	6.43	120.50	111.22
20	c	505	CLA	C2C-C1C-NC	6.46	114.67	110.22
20	b	604	CLA	C2C-C1C-NC	6.58	114.75	110.22
20	b	612	CLA	O2D-CGD-CBD	6.59	120.73	111.22
20	B	601	CLA	C2C-C1C-NC	6.60	114.76	110.22
20	a	407	CLA	O2D-CGD-CBD	6.60	120.74	111.22
20	C	501	CLA	C2C-C1C-NC	6.61	114.77	110.22
20	B	611	CLA	C2C-C1C-NC	6.65	114.80	110.22
20	B	606	CLA	C2C-C1C-NC	6.73	114.85	110.22
32	D	417	HTG	C1'-S1-C1	6.77	109.30	100.60
20	C	507	CLA	O2D-CGD-CBD	6.81	121.04	111.22
23	A	412	SQD	O6-C1-C2	6.83	116.40	108.00
23	A	406	SQD	O9-S-C6	6.86	111.75	106.92
20	c	503	CLA	C2C-C1C-NC	6.87	114.94	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	613	CLA	C2C-C1C-NC	6.88	114.95	110.22
20	b	608	CLA	C2C-C1C-NC	6.92	114.98	110.22
23	F	101	SQD	O9-S-C6	6.94	111.81	106.92
23	b	622	SQD	O7-S-C6	7.00	111.85	106.92
20	c	501	CLA	C2C-C1C-NC	7.09	115.10	110.22
23	A	406	SQD	O6-C1-C2	7.10	116.73	108.00
20	b	611	CLA	C2C-C1C-NC	7.13	115.12	110.22
20	b	609	CLA	C2C-C1C-NC	7.18	115.16	110.22
23	l	101	SQD	O6-C1-C2	7.20	116.86	108.00
20	d	404	CLA	C2C-C1C-NC	7.33	115.26	110.22
20	B	610	CLA	C2C-C1C-NC	7.36	115.28	110.22
20	B	616	CLA	C2C-C1C-NC	7.37	115.29	110.22
20	B	609	CLA	C2C-C1C-NC	7.37	115.29	110.22
32	B	622	HTG	C1'-S1-C1	7.38	110.09	100.60
20	b	603	CLA	O2D-CGD-CBD	7.41	121.91	111.22
20	C	505	CLA	C2C-C1C-NC	7.41	115.32	110.22
20	C	511	CLA	C2C-C1C-NC	7.42	115.33	110.22
20	b	610	CLA	C2C-C1C-NC	7.44	115.34	110.22
20	b	615	CLA	C2C-C1C-NC	7.50	115.38	110.22
20	a	407	CLA	C2C-C1C-NC	7.50	115.38	110.22
20	d	402	CLA	C2C-C1C-NC	7.55	115.41	110.22
20	c	507	CLA	C2C-C1C-NC	7.61	115.46	110.22
20	A	402	CLA	C2C-C1C-NC	7.65	115.48	110.22
20	B	613	CLA	C2C-C1C-NC	7.67	115.50	110.22
20	B	603	CLA	C2C-C1C-NC	7.76	115.56	110.22
32	b	624	HTG	C1'-S1-C1	7.86	110.71	100.60
20	C	501	CLA	O2D-CGD-CBD	8.04	122.82	111.22
20	D	402	CLA	C2C-C1C-NC	8.07	115.78	110.22
20	B	614	CLA	C2C-C1C-NC	8.09	115.79	110.22
20	C	509	CLA	C2C-C1C-NC	8.13	115.81	110.22
20	b	618	CLA	O2D-CGD-CBD	8.33	123.24	111.22
20	B	602	CLA	O2D-CGD-CBD	8.33	123.25	111.22
32	C	520	HTG	C1'-S1-C1	8.37	111.36	100.60
20	C	504	CLA	C2C-C1C-NC	8.38	115.98	110.22
32	B	623	HTG	C1'-S1-C1	8.46	111.47	100.60
20	B	605	CLA	C2C-C1C-NC	8.46	116.04	110.22
20	B	608	CLA	C2C-C1C-NC	8.51	116.08	110.22
20	b	606	CLA	C2C-C1C-NC	8.53	116.09	110.22
20	C	510	CLA	C2C-C1C-NC	8.56	116.11	110.22
20	D	401	CLA	C2C-C1C-NC	8.58	116.12	110.22
32	C	521	HTG	C1'-S1-C1	8.71	111.80	100.60
20	a	404	CLA	C2C-C1C-NC	8.90	116.34	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	607	CLA	C2C-C1C-NC	9.23	116.57	110.22
20	b	614	CLA	C2C-C1C-NC	9.24	116.58	110.22
32	C	522	HTG	C1'-S1-C1	9.41	112.70	100.60
32	B	631	HTG	C1'-S1-C1	9.59	112.92	100.60
23	A	412	SQD	O9-S-C6	9.59	113.67	106.92
20	d	403	CLA	C2C-C1C-NC	9.66	116.87	110.22
20	B	604	CLA	C2C-C1C-NC	9.86	117.00	110.22
20	b	605	CLA	C2C-C1C-NC	9.89	117.02	110.22
23	l	101	SQD	O7-S-C6	10.30	114.17	106.92
32	c	521	HTG	C1'-S1-C1	10.32	113.87	100.60
23	a	409	SQD	O6-C1-C2	12.01	122.78	108.00
23	a	409	SQD	O9-S-C6	13.02	116.09	106.92
32	d	401	HTG	C1'-S1-C1	14.04	118.65	100.60
23	f	101	SQD	O7-S-C6	17.19	119.03	106.92

All (170) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	c	502	CLA	NC
20	c	502	CLA	NA
20	b	614	CLA	NA
20	b	614	CLA	NC
20	b	614	CLA	ND
20	D	404	CLA	NC
20	D	404	CLA	ND
20	D	404	CLA	NA
20	C	505	CLA	ND
20	C	505	CLA	NA
20	B	605	CLA	NC
20	B	605	CLA	ND
20	B	605	CLA	NA
20	a	407	CLA	NC
20	c	507	CLA	NC
20	c	507	CLA	ND
20	c	507	CLA	NA
20	A	401	CLA	NC
20	A	401	CLA	ND
20	A	401	CLA	NA
20	C	504	CLA	NC
20	C	504	CLA	NA
20	B	608	CLA	NC
20	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	608	CLA	NA
20	C	506	CLA	NC
20	C	506	CLA	ND
20	C	506	CLA	NA
20	B	616	CLA	NC
20	B	616	CLA	ND
20	B	616	CLA	NA
20	B	603	CLA	NC
20	B	603	CLA	ND
20	B	603	CLA	NA
20	c	509	CLA	NC
20	c	509	CLA	ND
20	c	509	CLA	NA
20	c	503	CLA	NC
20	C	513	CLA	NC
20	b	611	CLA	NC
20	b	611	CLA	NA
20	C	508	CLA	NC
20	C	508	CLA	ND
20	C	508	CLA	NA
20	d	403	CLA	NA
20	a	404	CLA	NC
20	a	404	CLA	NA
20	c	504	CLA	NC
20	c	504	CLA	ND
20	c	504	CLA	NA
20	D	402	CLA	NA
20	c	513	CLA	NC
20	B	606	CLA	NC
20	B	606	CLA	ND
20	B	606	CLA	NA
20	b	603	CLA	NC
20	b	603	CLA	ND
20	b	603	CLA	NA
20	b	608	CLA	NC
20	b	608	CLA	ND
20	b	608	CLA	NA
20	d	402	CLA	ND
20	d	402	CLA	NA
20	B	601	CLA	NC
20	B	601	CLA	ND
20	B	601	CLA	NA

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Mol	Chain	Res	Type	Atom
20	b	617	CLA	NC
20	b	617	CLA	ND
20	b	617	CLA	NA
20	A	402	CLA	NC
20	A	402	CLA	NA
20	c	505	CLA	ND
20	c	505	CLA	NA
20	C	511	CLA	NC
20	C	511	CLA	NA
20	B	611	CLA	NC
20	B	611	CLA	ND
20	B	611	CLA	NA
20	c	512	CLA	NC
20	c	512	CLA	ND
20	c	512	CLA	NA
20	C	502	CLA	NA
20	B	610	CLA	NC
20	B	610	CLA	ND
20	C	510	CLA	NC
20	C	510	CLA	ND
20	C	510	CLA	NA
20	C	512	CLA	NC
20	C	512	CLA	NA
20	C	512	CLA	ND
20	c	511	CLA	NC
20	c	511	CLA	ND
20	c	511	CLA	NA
20	B	613	CLA	NA
20	B	613	CLA	NC
20	B	613	CLA	ND
20	b	606	CLA	NC
20	b	606	CLA	ND
20	b	606	CLA	NA
20	b	609	CLA	NC
20	b	609	CLA	ND
20	b	609	CLA	NA
20	C	501	CLA	NC
20	C	501	CLA	ND
20	C	501	CLA	NA
20	D	401	CLA	ND
20	B	602	CLA	NC
20	B	602	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	404	CLA	NC
20	a	403	CLA	NC
20	a	403	CLA	ND
20	a	403	CLA	NA
20	c	510	CLA	NC
20	c	510	CLA	ND
20	c	510	CLA	NA
20	b	607	CLA	NC
20	b	607	CLA	ND
20	b	607	CLA	NA
20	b	615	CLA	NC
20	b	615	CLA	ND
20	b	615	CLA	NA
20	b	616	CLA	NC
20	b	616	CLA	ND
20	b	616	CLA	NA
20	B	607	CLA	NC
20	B	607	CLA	ND
20	B	607	CLA	NA
20	B	614	CLA	NC
20	B	614	CLA	NA
20	B	614	CLA	ND
20	b	604	CLA	NC
20	b	604	CLA	ND
20	b	604	CLA	NA
20	d	404	CLA	NA
20	B	604	CLA	NC
20	B	604	CLA	ND
20	B	604	CLA	NA
20	C	503	CLA	NC
20	C	503	CLA	NA
20	b	610	CLA	NC
20	B	615	CLA	NC
20	B	615	CLA	ND
20	B	615	CLA	NA
20	b	618	CLA	NC
20	b	618	CLA	ND
20	b	618	CLA	NA
20	b	613	CLA	NC
20	c	508	CLA	NC
20	c	508	CLA	NA
20	b	605	CLA	NC

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Mol	Chain	Res	Type	Atom
20	b	605	CLA	ND
20	b	605	CLA	NA
20	C	509	CLA	NC
20	C	509	CLA	ND
20	C	509	CLA	NA
20	B	609	CLA	NC
20	c	501	CLA	NC
20	c	501	CLA	ND
20	c	501	CLA	NA
20	c	506	CLA	ND
20	c	506	CLA	NA
20	C	507	CLA	NC
20	C	507	CLA	ND
20	C	507	CLA	NA
20	b	612	CLA	NC
20	b	612	CLA	ND
20	b	612	CLA	NA
20	B	612	CLA	NC
20	B	612	CLA	ND
20	B	612	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	d	401	HTG	O5-C1-S1-C1'

There are no ring outliers.

102 monomers are involved in 348 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	401	CLA	5	0
20	A	402	CLA	3	0
21	A	403	PHO	2	0
20	A	404	CLA	3	0
22	A	405	BCR	4	0
23	A	406	SQD	3	0
24	A	407	LMG	4	0
27	A	411	PL9	11	0
23	A	412	SQD	2	0
28	A	416	DMS	1	0
31	A	421	BCT	5	0
20	B	601	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	602	CLA	2	0
20	B	603	CLA	2	0
20	B	604	CLA	6	0
20	B	605	CLA	4	0
20	B	606	CLA	9	0
20	B	607	CLA	6	0
20	B	608	CLA	2	0
20	B	609	CLA	1	0
20	B	610	CLA	2	0
20	B	611	CLA	5	0
20	B	612	CLA	4	0
20	B	613	CLA	4	0
20	B	614	CLA	5	0
20	B	615	CLA	3	0
20	B	616	CLA	2	0
22	B	618	BCR	3	0
22	B	619	BCR	3	0
32	B	622	HTG	8	0
34	B	625	LMT	1	0
34	B	626	LMT	1	0
34	B	627	LMT	1	0
32	B	631	HTG	1	0
32	B	632	HTG	2	0
28	B	634	DMS	1	0
28	B	635	DMS	3	0
28	B	637	DMS	1	0
28	B	639	DMS	6	0
28	B	640	DMS	2	0
28	B	641	DMS	7	0
28	B	642	DMS	5	0
28	B	644	DMS	4	0
20	C	501	CLA	5	0
20	C	502	CLA	5	0
20	C	503	CLA	2	0
20	C	504	CLA	6	0
20	C	505	CLA	2	0
20	C	506	CLA	5	0
20	C	507	CLA	4	0
20	C	508	CLA	6	0
20	C	509	CLA	5	0
20	C	510	CLA	8	0
20	C	511	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	512	CLA	4	0
20	C	513	CLA	3	0
22	C	514	BCR	3	0
22	C	515	BCR	2	0
35	C	516	DGD	2	0
35	C	517	DGD	2	0
24	C	519	LMG	3	0
32	C	520	HTG	2	0
24	C	524	LMG	2	0
28	C	527	DMS	2	0
28	C	530	DMS	9	0
28	C	531	DMS	4	0
28	C	532	DMS	4	0
28	C	533	DMS	1	0
32	C	534	HTG	1	0
20	D	401	CLA	1	0
20	D	402	CLA	4	0
21	D	403	PHO	2	0
20	D	404	CLA	2	0
22	D	405	BCR	3	0
35	D	406	DGD	5	0
36	D	408	LHG	18	0
36	D	409	LHG	19	0
28	D	413	DMS	1	0
28	D	414	DMS	13	0
28	D	415	DMS	2	0
32	D	417	HTG	3	0
36	E	103	LHG	6	0
37	E	104	HEM	2	0
23	F	101	SQD	3	0
28	F	102	DMS	3	0
35	H	102	DGD	2	0
34	I	101	LMT	2	0
34	J	103	LMT	1	0
22	K	101	BCR	5	0
22	K	102	BCR	3	0
28	O	303	DMS	3	0
28	O	305	DMS	1	0
28	O	306	DMS	3	0
28	O	307	DMS	6	0
28	O	308	DMS	2	0
28	O	310	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	T	101	BCR	7	0
28	U	902	DMS	1	0
28	U	903[B]	DMS	12	0
28	U	904	DMS	3	0
28	V	205	DMS	1	0
28	V	206	DMS	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.70	3 (0%) 85 85	16, 23, 46, 68	0
1	a	334/344 (97%)	-0.63	8 (2%) 62 60	18, 23, 48, 78	0
2	B	505/505 (100%)	-0.47	18 (3%) 46 44	19, 28, 54, 85	0
2	b	495/505 (98%)	-0.40	20 (4%) 42 39	19, 28, 53, 95	0
3	C	451/455 (99%)	-0.45	8 (1%) 71 71	21, 33, 49, 83	0
3	c	455/455 (100%)	-0.47	6 (1%) 79 79	22, 33, 46, 79	0
4	D	342/342 (100%)	-0.67	4 (1%) 81 81	17, 24, 44, 90	0
4	d	342/342 (100%)	-0.73	5 (1%) 76 76	18, 25, 42, 86	0
5	E	78/83 (93%)	0.76	19 (24%) 1 0	28, 47, 75, 87	0
5	e	78/83 (93%)	0.64	16 (20%) 1 1	29, 44, 67, 81	0
6	F	33/44 (75%)	-0.09	4 (12%) 6 6	28, 36, 63, 66	0
6	f	32/44 (72%)	-0.05	3 (9%) 11 10	28, 34, 72, 90	0
7	H	64/65 (98%)	0.07	3 (4%) 35 33	26, 37, 50, 78	0
7	h	62/65 (95%)	-0.24	0 100 100	25, 36, 48, 58	0
8	I	34/38 (89%)	-0.11	3 (8%) 12 12	29, 36, 60, 78	0
8	i	35/38 (92%)	-0.16	2 (5%) 27 26	29, 34, 52, 85	0
9	J	36/40 (90%)	-0.04	2 (5%) 28 26	26, 41, 74, 90	0
9	j	40/40 (100%)	-0.04	3 (7%) 17 16	27, 39, 56, 65	0
10	K	37/37 (100%)	-0.27	2 (5%) 29 28	33, 40, 52, 59	0
10	k	37/37 (100%)	-0.21	1 (2%) 58 55	32, 40, 56, 64	0
11	L	37/37 (100%)	-0.36	3 (8%) 15 14	18, 22, 65, 81	0
11	l	37/37 (100%)	-0.22	3 (8%) 15 14	18, 22, 76, 91	0
12	M	33/36 (91%)	-0.64	1 (3%) 54 51	21, 25, 39, 57	0
12	m	34/36 (94%)	-0.56	3 (8%) 12 12	20, 26, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.23	8 (3%) 50 47	18, 32, 56, 85	0
13	o	243/244 (99%)	-0.09	19 (7%) 16 15	19, 35, 67, 89	0
14	T	28/32 (87%)	-0.70	1 (3%) 46 44	19, 24, 37, 54	0
14	t	29/32 (90%)	-0.36	2 (6%) 20 18	20, 23, 49, 74	0
15	U	97/104 (93%)	-0.34	2 (2%) 67 65	22, 29, 49, 67	0
15	u	97/104 (93%)	-0.36	1 (1%) 84 84	24, 29, 44, 75	0
16	V	137/137 (100%)	-0.62	0 100 100	22, 28, 43, 60	0
16	v	137/137 (100%)	-0.25	5 (3%) 46 44	25, 36, 53, 74	0
17	Y	29/30 (96%)	1.08	6 (20%) 1 1	41, 51, 72, 79	0
17	y	29/30 (96%)	0.76	5 (17%) 2 2	41, 50, 66, 70	0
18	X	38/40 (95%)	0.26	5 (13%) 4 4	32, 42, 68, 72	0
18	x	35/40 (87%)	-0.09	2 (5%) 27 26	33, 40, 63, 67	0
19	Z	62/62 (100%)	0.66	14 (22%) 1 1	38, 48, 86, 98	0
19	z	61/62 (98%)	0.71	12 (19%) 1 1	45, 54, 86, 96	0
All	All	5230/5350 (97%)	-0.37	222 (4%) 40 37	16, 30, 57, 98	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	9.7
2	b	495	PHE	9.2
2	b	503	THR	8.4
13	o	246	ALA	8.3
2	b	502	VAL	7.2
2	b	504	THR	7.2
6	f	14	PRO	7.1
13	o	4	THR	6.8
7	H	64	ALA	6.8
5	e	61	ARG	6.7
3	C	23	ALA	6.3
11	l	3	PRO	6.2
17	y	19	ILE	5.9
2	b	484	PRO	5.9
17	Y	19	ILE	5.9
1	a	11	ALA	5.8
17	Y	18	VAL	5.5
13	O	60	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
2	b	500	GLY	5.2
5	e	59[A]	GLU	5.2
2	B	494	GLY	5.1
5	E	4	THR	5.1
2	B	486	LEU	5.1
15	u	8	GLU	5.0
4	D	240	ALA	5.0
19	z	32	ASP	5.0
11	l	1	MET	5.0
7	H	65	LEU	4.8
14	t	30	THR	4.8
18	X	2	THR	4.7
4	D	11	GLU	4.7
19	Z	32	ASP	4.7
19	Z	33	TRP	4.6
13	O	4	THR	4.6
9	J	5	GLY	4.6
1	A	11	ALA	4.6
2	b	499	VAL	4.6
19	Z	30	PRO	4.5
2	b	501	ASP	4.5
19	z	30	PRO	4.4
19	z	3	ILE	4.4
19	Z	31	GLN	4.4
16	v	16	GLY	4.3
4	d	11	GLU	4.3
9	j	6	GLY	4.3
13	o	35	SER	4.3
2	B	485	GLU	4.3
4	D	12	ARG	4.2
1	A	262	TYR	4.2
3	c	21	ILE	4.2
11	L	1	MET	4.2
19	z	60	PHE	4.2
5	E	17	VAL	4.2
6	F	16	PHE	4.2
11	l	2	GLU	4.1
6	F	13	TYR	4.1
11	L	3	PRO	4.1
1	a	262	TYR	4.1
5	E	78	THR	4.0
5	E	79	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	487	SER	3.9
2	B	506	LYS	3.8
5	e	25	ILE	3.8
2	B	503	THR	3.8
6	f	16	PHE	3.8
2	B	502	VAL	3.8
8	I	34	ARG	3.8
19	z	33	TRP	3.7
2	B	495	PHE	3.7
3	C	143	TYR	3.7
18	x	2	THR	3.7
19	z	34	ASP	3.7
5	E	6	GLY	3.6
12	M	33	GLN	3.6
5	e	62	SER	3.6
2	b	483	ASP	3.6
2	b	491	VAL	3.6
17	Y	20	ALA	3.5
19	Z	35	ARG	3.5
5	e	81	GLU	3.5
11	L	2	GLU	3.5
8	i	36	ASP	3.5
14	t	29	ILE	3.5
4	d	238	THR	3.4
5	E	74	GLN	3.4
19	Z	34	ASP	3.4
2	b	490	GLN	3.4
19	z	1	MET	3.4
19	Z	60	PHE	3.4
1	a	263	ALA	3.4
3	c	207	ARG	3.4
7	H	6	TRP	3.4
17	Y	22	LEU	3.3
19	z	31	GLN	3.3
3	c	20	SER	3.3
17	y	18	VAL	3.3
3	c	19	ASN	3.3
19	Z	3	ILE	3.2
2	B	293	ALA	3.2
9	J	6	GLY	3.2
13	o	60	ARG	3.2
9	j	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	81	GLU	3.1
5	e	60[A]	GLN	3.1
13	o	5	LEU	3.1
17	y	22	LEU	3.1
2	B	496	TYR	3.1
5	E	62	SER	3.1
17	y	20	ALA	3.1
4	D	238	THR	3.1
2	b	295	GLY	3.1
4	d	236	ASN	3.1
5	E	61	ARG	3.0
2	B	501	ASP	3.0
9	j	5	GLY	3.0
2	b	129	GLY	2.9
5	e	10	PHE	2.9
5	E	25	ILE	2.9
13	O	25	THR	2.9
13	o	25	THR	2.9
5	E	21	VAL	2.9
18	x	34	ILE	2.9
13	O	59	LYS	2.9
8	i	34[A]	ARG	2.8
13	o	36	GLN	2.8
1	a	260	PHE	2.8
2	B	504	THR	2.8
10	k	17	ILE	2.8
12	m	34	LYS	2.8
17	Y	43	ARG	2.8
5	e	6	GLY	2.8
13	O	61	GLN	2.8
3	C	191	PRO	2.8
19	z	61	VAL	2.8
3	C	25	ASN	2.8
5	E	5	THR	2.7
1	a	261	GLN	2.7
5	e	11	SER	2.7
4	d	240	ALA	2.7
2	B	85	GLY	2.7
2	b	85	GLY	2.7
1	a	13	LEU	2.7
13	O	62	GLU	2.7
1	A	12	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
13	o	27	ARG	2.7
10	K	17	ILE	2.6
19	z	59	PHE	2.6
13	o	24	ASP	2.6
5	E	80	LEU	2.6
19	Z	41	PHE	2.6
19	Z	62	VAL	2.6
2	b	497	GLN	2.6
12	m	33	GLN	2.6
5	e	71	GLU	2.6
4	d	237	PRO	2.6
2	b	86	ILE	2.6
6	f	15	ILE	2.6
19	z	41	PHE	2.5
1	a	242	GLU	2.5
2	B	488	PRO	2.5
8	I	35	LYS	2.5
3	C	24	THR	2.5
18	X	3	ILE	2.5
18	X	37	VAL	2.5
15	U	8	GLU	2.5
16	v	14	SER	2.5
5	E	73	LYS	2.5
6	F	15	ILE	2.4
2	B	374	ASN	2.4
2	b	126	PRO	2.4
6	F	14	PRO	2.4
19	z	35	ARG	2.4
5	E	72	ALA	2.4
12	m	5	GLN	2.4
16	v	106	ASN	2.4
13	o	23	ASP	2.4
5	e	82	GLN	2.4
14	T	29	ILE	2.4
19	Z	29	SER	2.3
16	v	72	LEU	2.3
19	Z	2	THR	2.3
13	O	56	PRO	2.3
13	o	34	SER	2.3
5	e	9	PRO	2.3
13	o	131	PRO	2.3
19	Z	36	SER	2.3

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Mol	Chain	Res	Type	RSRZ
13	o	132	ASN	2.3
13	o	61	GLN	2.2
2	B	505	ARG	2.2
5	e	21	VAL	2.2
8	I	33	LYS	2.2
13	o	136	ILE	2.2
13	O	132[A]	ASN	2.2
2	B	483	ASP	2.2
2	B	484	PRO	2.2
3	C	182	PHE	2.2
13	o	130	GLN	2.2
18	X	38	GLN	2.2
13	o	56	PRO	2.1
15	U	65	PRO	2.1
2	b	128	THR	2.1
5	e	80	LEU	2.1
5	e	83	LEU	2.1
16	v	18	THR	2.1
3	C	253	LEU	2.1
3	c	23	ALA	2.1
5	E	71	GLU	2.1
5	e	24	SER	2.1
13	o	59	LYS	2.1
18	X	39	ARG	2.1
19	Z	39	LEU	2.1
1	a	235	TYR	2.0
3	c	143	TYR	2.0
5	E	77	GLU	2.0
5	E	76	VAL	2.0
17	y	43	ARG	2.0
17	Y	21	GLN	2.0
2	b	293	ALA	2.0
10	K	16	ALA	2.0
5	E	68	ASP	2.0
3	C	145	SER	2.0
13	o	62	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.98	0.07	-	26,32,36,37	0
14	FME	T	1	10/11	0.97	0.07	-	23,29,48,51	0
8	FME	i	1	10/11	0.98	0.09	-	30,31,34,35	0
14	FME	t	1	10/11	0.96	0.07	-	23,27,49,50	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	LMT	b	627	32/35	0.71	0.24	21.38	42,67,84,87	0
26	UNL	T	103	13/-	0.69	0.17	19.83	64,68,72,72	0
28	DMS	B	641	4/4	0.95	0.31	17.73	68,69,75,80	0
28	DMS	b	636	4/4	0.90	0.15	16.16	66,71,72,79	0
26	UNL	h	103	16/-	0.75	0.29	15.91	61,69,73,76	0
34	LMT	E	101	24/35	0.81	0.26	13.84	64,78,84,90	0
28	DMS	A	416	4/4	0.91	0.23	12.08	59,60,69,77	0
28	DMS	c	530	4/4	0.97	0.16	11.95	36,43,45,49	0
28	DMS	A	418	4/4	0.90	0.32	11.89	68,74,80,85	0
26	UNL	B	630	14/-	0.70	0.20	11.54	67,74,83,84	0
34	LMT	T	102	24/35	0.80	0.20	11.40	36,53,78,85	0
28	DMS	C	531	4/4	0.92	0.24	10.97	53,54,58,74	0
34	LMT	f	102	24/35	0.59	0.26	10.92	62,77,94,98	0
34	LMT	a	418	35/35	0.73	0.21	10.82	45,69,78,81	0
26	UNL	C	523	34/-	0.75	0.22	10.58	59,80,92,101	0
32	HTG	d	401	19/19	0.58	0.29	10.40	58,99,111,120	0
28	DMS	O	309	4/4	0.81	0.23	10.35	58,65,72,73	0
32	HTG	C	522	19/19	0.81	0.27	10.11	66,83,104,107	0
28	DMS	d	413	4/4	0.95	0.17	10.04	47,53,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	DMS	B	639	4/4	0.90	0.24	9.77	65,70,71,76	0
35	DGD	D	406	51/66	0.60	0.30	9.56	57,74,100,108	0
28	DMS	C	532	4/4	0.87	0.19	9.54	33,40,41,48	0
28	DMS	D	415	4/4	0.85	0.25	9.05	57,58,63,65	0
26	UNL	t	102	16/-	0.77	0.17	8.66	61,71,80,80	0
28	DMS	B	638	4/4	0.86	0.19	8.64	53,61,63,68	0
34	LMT	B	626	24/35	0.74	0.20	8.62	37,54,86,95	0
28	DMS	B	642	4/4	0.77	0.30	8.15	43,51,68,71	0
34	LMT	B	627	16/35	0.81	0.18	7.80	52,60,78,78	0
35	DGD	d	416	51/66	0.64	0.27	7.75	56,75,96,103	0
28	DMS	o	307	4/4	0.95	0.17	7.60	53,58,63,65	0
28	DMS	O	305	4/4	0.68	0.30	7.38	64,66,77,86	0
26	UNL	J	105	12/-	0.79	0.23	7.31	63,67,71,71	0
28	DMS	C	525[A]	4/4	0.97	0.19	7.29	48,49,51,57	4
28	DMS	c	536	4/4	0.92	0.15	6.76	33,33,45,46	0
28	DMS	C	525[B]	4/4	0.97	0.19	6.54	32,33,35,35	4
26	UNL	E	102	15/-	0.68	0.28	6.49	55,62,76,77	0
28	DMS	A	417	4/4	0.93	0.17	6.34	70,72,77,81	0
28	DMS	b	631	4/4	0.96	0.10	6.24	23,24,27,35	0
28	DMS	V	205	4/4	0.81	0.25	6.09	67,76,77,79	0
23	SQD	a	401	54/54	0.81	0.16	5.57	39,58,82,86	0
26	UNL	d	410	16/-	0.82	0.18	5.54	33,45,63,63	0
26	UNL	d	409	36/-	0.79	0.18	5.48	36,60,91,102	0
28	DMS	O	306	4/4	0.89	0.29	5.39	66,73,73,75	0
28	DMS	v	202	4/4	0.98	0.15	5.09	50,51,53,55	0
28	DMS	O	304	4/4	0.92	0.28	5.04	63,68,72,73	0
28	DMS	U	902	4/4	0.88	0.23	5.03	35,44,49,58	0
24	LMG	C	524	45/55	0.52	0.33	5.03	22,46,51,56	45
32	HTG	c	521	19/19	0.55	0.35	4.97	57,85,102,105	0
24	LMG	B	620	51/55	0.87	0.12	4.89	33,43,55,58	0
28	DMS	O	310	4/4	0.84	0.33	4.87	76,78,82,94	0
28	DMS	c	528	4/4	0.96	0.18	4.73	58,62,63,65	0
27	PL9	A	411	55/55	0.79	0.20	4.69	43,67,89,92	0
26	UNL	B	633	16/-	0.81	0.25	4.46	53,61,69,70	0
32	HTG	O	302	19/19	0.94	0.11	4.39	34,42,50,53	0
28	DMS	C	527	4/4	0.89	0.17	4.27	73,76,79,87	0
32	HTG	C	521	19/19	0.67	0.26	4.27	46,78,89,90	0
26	UNL	d	411	16/-	0.92	0.12	4.25	33,42,55,55	0
32	HTG	b	625	19/19	0.85	0.20	4.05	30,44,66,70	0
32	HTG	B	621	19/19	0.93	0.12	4.01	36,41,48,52	0
26	UNL	A	410	36/-	0.64	0.25	3.93	57,78,84,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	DMS	o	304	4/4	0.86	0.33	3.93	68,79,82,83	0
26	UNL	D	411	16/-	0.89	0.16	3.93	39,45,58,62	0
36	LHG	E	103	48/49	0.65	0.29	3.92	44,99,108,119	0
26	UNL	j	106	6/-	0.82	0.18	3.81	52,55,58,59	0
22	BCR	K	102	40/40	0.92	0.13	3.78	31,36,40,41	0
28	DMS	b	633	4/4	0.97	0.13	3.68	45,48,49,53	0
28	DMS	C	526	4/4	0.97	0.15	3.61	59,60,63,65	0
34	LMT	J	103	24/35	0.60	0.23	3.59	53,61,81,85	0
28	DMS	c	535	4/4	0.91	0.18	3.59	58,59,65,68	0
32	HTG	V	202	13/19	0.86	0.21	3.54	45,49,70,82	0
28	DMS	D	413	4/4	0.96	0.10	3.37	50,56,60,61	0
23	SQD	l	101	54/54	0.75	0.20	3.26	47,68,101,106	0
28	DMS	d	414	4/4	0.95	0.16	3.23	57,62,64,68	0
28	DMS	o	306	4/4	0.84	0.25	3.18	55,58,65,77	0
28	DMS	C	530	4/4	0.96	0.16	3.17	44,44,46,50	0
28	DMS	u	202	4/4	0.91	0.18	3.15	40,46,52,54	0
27	PL9	a	415	55/55	0.77	0.22	3.13	52,67,89,94	0
26	UNL	U	901	14/-	0.74	0.27	3.10	40,49,59,59	0
24	LMG	b	623	49/55	0.89	0.12	3.09	33,42,54,61	0
24	LMG	A	407	51/55	0.87	0.13	3.07	40,55,70,78	0
24	LMG	a	410	51/55	0.88	0.15	3.07	44,55,65,67	0
23	SQD	b	622	54/54	0.80	0.17	3.04	46,63,95,100	0
28	DMS	v	206	4/4	0.93	0.20	3.01	52,53,61,66	0
32	HTG	B	622	19/19	0.84	0.16	2.95	28,46,54,54	0
28	DMS	U	903[B]	4/4	0.97	0.17	2.90	26,28,29,32	4
36	LHG	d	407	49/49	0.97	0.12	2.89	22,27,46,50	0
35	DGD	H	102	62/66	0.93	0.11	2.85	25,33,40,43	0
28	DMS	U	903[A]	4/4	0.97	0.17	2.85	32,34,40,41	4
26	UNL	X	101	16/-	0.81	0.17	2.82	37,40,59,59	0
24	LMG	c	518	51/55	0.72	0.21	2.62	37,72,84,87	0
26	UNL	b	630	11/-	0.82	0.21	2.61	55,60,67,68	0
20	CLA	B	602	65/65	0.88	0.14	2.61	29,42,77,81	0
35	DGD	h	101	62/66	0.93	0.10	2.55	25,34,41,49	0
34	LMT	m	101	35/35	0.63	0.25	2.48	48,94,110,114	0
20	CLA	b	603	65/65	0.89	0.15	2.40	30,45,75,82	0
20	CLA	a	404	60/65	0.96	0.09	2.39	18,22,66,75	0
36	LHG	D	409	49/49	0.95	0.12	2.23	27,33,81,83	0
28	DMS	B	634	4/4	0.98	0.08	2.16	23,24,25,26	0
23	SQD	f	101	40/54	0.83	0.25	2.13	57,86,102,107	0
28	DMS	B	637	4/4	0.96	0.16	2.11	53,53,54,60	0
20	CLA	D	404	65/65	0.95	0.10	2.10	26,29,77,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	UNL	D	410	37/-	0.83	0.15	2.10	42,57,93,98	0
34	LMT	b	628	25/35	0.64	0.23	2.03	54,79,95,96	0
32	HTG	D	417	19/19	0.53	0.31	2.02	67,105,119,120	0
32	HTG	v	210	14/19	0.69	0.27	2.02	60,80,92,100	0
20	CLA	d	404	65/65	0.94	0.10	1.93	24,29,78,87	0
28	DMS	b	632	4/4	0.90	0.15	1.92	55,58,66,70	0
34	LMT	c	523	35/35	0.81	0.23	1.88	67,77,83,85	0
23	SQD	A	412	54/54	0.82	0.16	1.86	41,60,78,81	0
28	DMS	b	638	4/4	0.75	0.28	1.85	67,75,77,86	0
22	BCR	d	405	40/40	0.89	0.12	1.85	24,30,56,58	0
35	DGD	C	516	62/66	0.97	0.09	1.84	22,32,74,79	0
34	LMT	I	101	35/35	0.77	0.24	1.81	67,82,91,92	0
35	DGD	c	515	62/66	0.95	0.10	1.80	23,32,71,75	0
34	LMT	Z	101	35/35	0.70	0.23	1.79	44,90,107,109	0
28	DMS	o	308	4/4	0.83	0.21	1.78	60,61,62,63	0
34	LMT	z	102	35/35	0.78	0.19	1.76	46,85,99,101	0
36	LHG	d	406	49/49	0.97	0.10	1.74	29,36,43,48	0
23	SQD	F	101	35/54	0.85	0.23	1.71	51,76,89,90	0
36	LHG	d	408	49/49	0.97	0.10	1.71	24,31,83,88	0
32	HTG	u	201	8/19	0.74	0.21	1.68	45,52,69,89	0
20	CLA	B	605	65/65	0.97	0.08	1.63	19,23,55,58	0
28	DMS	v	204	4/4	0.93	0.15	1.60	48,54,57,69	0
34	LMT	B	625	24/35	0.76	0.17	1.59	48,67,86,89	0
20	CLA	a	403	65/65	0.97	0.09	1.58	17,20,29,38	0
24	LMG	J	101	45/55	0.94	0.10	1.55	27,32,64,70	0
35	DGD	C	518	62/66	0.96	0.09	1.51	24,30,62,73	0
28	DMS	j	105	4/4	0.69	0.19	1.47	70,74,75,88	0
36	LHG	D	408	49/49	0.98	0.09	1.46	23,30,44,49	0
28	DMS	V	209	4/4	0.91	0.20	1.46	57,73,77,81	0
23	SQD	A	406	54/54	0.93	0.13	1.41	34,59,71,76	0
28	DMS	D	414	4/4	0.97	0.14	1.39	55,56,57,58	0
26	UNL	j	104	16/-	0.89	0.10	1.38	49,58,64,66	0
28	DMS	B	640	4/4	0.94	0.33	1.37	45,48,49,50	0
28	DMS	h	102	4/4	0.97	0.16	1.36	50,51,53,62	0
22	BCR	D	405	40/40	0.91	0.11	1.35	26,30,58,60	0
20	CLA	b	606	65/65	0.97	0.07	1.34	20,24,54,59	0
23	SQD	a	409	54/54	0.94	0.12	1.32	33,56,75,78	0
20	CLA	d	402	65/65	0.98	0.08	1.29	16,20,35,41	0
20	CLA	A	404	65/65	0.96	0.10	1.28	20,25,88,90	0
26	UNL	a	416	11/-	0.75	0.16	1.26	66,68,76,78	0
34	LMT	M	101	35/35	0.74	0.20	1.18	34,53,63,64	0
24	LMG	C	519	51/55	0.89	0.15	1.18	31,67,83,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	CLA	b	611	65/65	0.96	0.09	1.11	24,30,34,41	0
20	CLA	c	512	65/65	0.92	0.11	1.10	28,41,70,72	0
35	DGD	c	517	62/66	0.95	0.09	1.09	23,30,56,71	0
20	CLA	B	606	65/65	0.98	0.09	1.08	19,24,35,37	0
26	UNL	I	106	11/-	0.75	0.19	1.06	61,73,81,81	0
20	CLA	B	608	65/65	0.97	0.07	1.05	18,21,34,39	0
22	BCR	B	618	40/40	0.96	0.08	1.04	21,28,42,45	0
28	DMS	F	102	4/4	0.97	0.11	1.04	51,52,56,64	0
32	HTG	b	601	19/19	0.87	0.15	1.01	45,61,67,80	0
26	UNL	J	104	14/-	0.60	0.24	1.01	67,77,80,81	0
36	LHG	L	101	49/49	0.97	0.09	1.01	24,31,49,53	0
20	CLA	C	504	65/65	0.95	0.08	1.00	27,30,59,61	0
21	PHO	a	406	64/64	0.98	0.08	0.99	19,24,29,32	0
28	DMS	c	531	4/4	0.94	0.15	0.97	73,78,85,86	0
20	CLA	C	509	65/65	0.96	0.09	0.95	29,34,52,55	0
27	PL9	d	412	55/55	0.96	0.08	0.93	18,23,29,35	0
20	CLA	b	609	65/65	0.97	0.07	0.92	19,22,33,37	0
22	BCR	C	514	40/40	0.90	0.10	0.90	36,45,49,50	0
22	BCR	t	101	40/40	0.95	0.07	0.90	22,29,41,43	0
35	DGD	C	517	55/66	0.95	0.07	0.89	26,34,59,62	0
32	HTG	b	624	19/19	0.81	0.23	0.87	49,74,80,85	0
34	LMT	m	102	35/35	0.74	0.20	0.85	34,53,58,59	0
20	CLA	C	510	65/65	0.96	0.08	0.85	26,31,38,44	0
20	CLA	c	511	65/65	0.95	0.10	0.82	27,33,40,43	0
20	CLA	c	513	65/65	0.92	0.12	0.81	36,46,81,87	0
20	CLA	c	509	65/65	0.96	0.09	0.80	25,30,53,58	0
20	CLA	A	401	65/65	0.98	0.08	0.80	16,19,30,36	0
35	DGD	c	516	57/66	0.96	0.08	0.79	27,32,62,68	0
24	LMG	c	519	51/55	0.89	0.13	0.79	29,59,86,88	0
32	HTG	B	631	19/19	0.88	0.12	0.78	41,57,69,73	0
20	CLA	b	618	65/65	0.91	0.13	0.77	23,33,92,98	0
36	LHG	D	407	49/49	0.96	0.09	0.77	28,37,44,52	0
28	DMS	O	307	4/4	0.94	0.15	0.76	69,76,77,88	0
20	CLA	B	610	65/65	0.96	0.10	0.71	26,31,35,38	0
27	PL9	D	412	55/55	0.97	0.08	0.67	19,23,29,34	0
20	CLA	B	607	65/65	0.95	0.09	0.67	22,29,55,62	0
22	BCR	A	405	40/40	0.97	0.08	0.67	21,26,32,35	0
36	LHG	l	102	49/49	0.97	0.08	0.66	22,30,51,54	0
20	CLA	b	607	65/65	0.98	0.08	0.62	20,24,33,35	0
20	CLA	B	603	65/65	0.96	0.08	0.61	23,28,35,39	0
22	BCR	b	620	40/40	0.96	0.08	0.61	22,27,43,46	0
22	BCR	K	101	40/40	0.92	0.10	0.60	33,37,42,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	CLA	B	615	65/65	0.97	0.08	0.58	20,24,70,79	0
24	LMG	j	101	45/55	0.94	0.09	0.58	27,32,60,64	0
20	CLA	C	513	65/65	0.87	0.14	0.57	40,48,72,77	0
21	PHO	a	405	64/64	0.97	0.07	0.53	17,20,22,25	0
28	DMS	B	645	4/4	0.97	0.11	0.51	56,59,64,71	0
22	BCR	j	102	40/40	0.95	0.09	0.49	30,35,42,45	0
20	CLA	B	611	65/65	0.97	0.08	0.47	21,26,34,40	0
20	CLA	d	403	65/65	0.98	0.07	0.47	17,19,27,34	0
20	CLA	b	608	65/65	0.95	0.09	0.46	24,31,59,63	0
22	BCR	B	617	40/40	0.97	0.07	0.44	22,26,32,33	0
20	CLA	C	505	65/65	0.96	0.08	0.41	28,33,44,48	0
20	CLA	b	616	65/65	0.96	0.08	0.41	20,26,73,80	0
20	CLA	D	401	65/65	0.98	0.08	0.41	16,20,35,41	0
20	CLA	A	402	59/65	0.97	0.07	0.38	18,22,52,58	0
20	CLA	D	402	65/65	0.98	0.06	0.37	15,19,30,36	0
20	CLA	c	504	65/65	0.97	0.07	0.31	25,29,55,60	0
22	BCR	k	101	40/40	0.95	0.09	0.30	28,36,41,42	0
22	BCR	B	619	40/40	0.95	0.07	0.29	22,30,42,44	0
20	CLA	C	503	65/65	0.95	0.08	0.29	28,33,37,42	0
20	CLA	C	506	65/65	0.92	0.10	0.26	32,45,86,87	0
20	CLA	b	612	65/65	0.96	0.08	0.26	21,27,36,41	0
22	BCR	T	101	40/40	0.96	0.07	0.23	24,32,43,45	0
20	CLA	b	613	65/65	0.97	0.07	0.23	20,22,38,44	0
21	PHO	A	403	64/64	0.98	0.07	0.22	18,22,24,25	0
20	CLA	c	508	60/65	0.97	0.07	0.22	24,28,52,54	0
28	DMS	i	104	4/4	0.97	0.20	0.20	63,66,67,71	0
28	DMS	D	416	4/4	0.93	0.17	0.18	83,87,89,91	0
22	BCR	a	408	40/40	0.96	0.07	0.18	21,25,30,31	0
20	CLA	c	510	65/65	0.97	0.07	0.17	23,29,39,42	0
20	CLA	a	407	47/65	0.97	0.07	0.16	19,22,41,48	0
20	CLA	b	614	65/65	0.97	0.07	0.16	21,25,31,37	0
37	HEM	V	201	43/43	0.99	0.08	0.14	21,23,27,31	0
22	BCR	C	515	40/40	0.95	0.09	0.14	31,37,43,45	0
20	CLA	B	601	65/65	0.93	0.12	0.13	23,29,82,86	0
20	CLA	c	506	65/65	0.93	0.10	0.11	24,39,71,74	0
31	BCT	A	421	4/4	0.95	0.10	0.10	31,34,40,44	0
39	MG	j	103	1/1	1.00	0.08	0.04	31,31,31,31	0
28	DMS	v	203	4/4	0.93	0.16	0.03	67,69,76,79	0
21	PHO	D	403	64/64	0.97	0.07	0.01	18,24,29,35	0
20	CLA	b	604	65/65	0.96	0.08	-0.02	23,27,33,35	0
37	HEM	v	201	43/43	0.98	0.08	-0.03	25,29,34,37	0
20	CLA	c	503	65/65	0.96	0.08	-0.04	25,35,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	CLA	b	605	65/65	0.97	0.07	-0.05	21,25,34,37	0
38	RRX	x	101	41/41	0.92	0.10	-0.06	26,32,47,58	0
28	DMS	v	208	4/4	0.91	0.27	-0.06	89,92,92,95	0
20	CLA	C	507	65/65	0.95	0.09	-0.07	28,37,52,57	0
20	CLA	b	610	65/65	0.97	0.07	-0.07	20,26,31,33	0
20	CLA	B	612	65/65	0.98	0.07	-0.07	19,22,36,42	0
28	DMS	V	207	4/4	0.96	0.10	-0.10	62,63,63,70	0
20	CLA	B	613	65/65	0.98	0.07	-0.11	21,25,30,34	0
20	CLA	C	501	65/65	0.96	0.08	-0.11	27,33,45,52	0
22	BCR	k	102	40/40	0.93	0.09	-0.11	41,46,51,51	0
20	CLA	B	604	65/65	0.97	0.07	-0.12	21,24,33,39	0
38	RRX	H	101	41/41	0.94	0.10	-0.15	27,31,41,46	0
20	CLA	C	508	60/65	0.96	0.07	-0.17	23,31,47,51	0
20	CLA	c	501	65/65	0.96	0.08	-0.18	26,30,41,48	0
20	CLA	b	615	65/65	0.98	0.06	-0.19	18,22,53,59	0
20	CLA	c	507	65/65	0.97	0.08	-0.19	25,30,49,57	0
20	CLA	C	502	65/65	0.97	0.07	-0.21	24,29,41,48	0
28	DMS	V	208	4/4	0.95	0.12	-0.22	75,77,82,85	0
20	CLA	c	502	65/65	0.97	0.07	-0.22	22,26,39,48	0
20	CLA	B	614	65/65	0.98	0.06	-0.23	19,22,48,53	0
37	HEM	E	104	43/43	0.96	0.10	-0.25	39,44,52,56	0
20	CLA	c	505	65/65	0.97	0.06	-0.27	25,30,46,50	0
22	BCR	b	619	40/40	0.97	0.07	-0.28	23,26,32,35	0
20	CLA	B	616	65/65	0.97	0.07	-0.33	25,29,48,52	0
37	HEM	e	102	43/43	0.97	0.09	-0.34	34,41,56,68	0
20	CLA	C	512	55/65	0.93	0.09	-0.37	37,44,49,54	0
20	CLA	B	609	65/65	0.98	0.07	-0.38	22,25,31,33	0
20	CLA	C	511	65/65	0.95	0.08	-0.42	30,37,42,45	0
22	BCR	b	621	40/40	0.97	0.07	-0.46	27,32,42,44	0
22	BCR	c	514	40/40	0.96	0.07	-0.51	28,36,39,39	0
31	BCT	a	413	4/4	0.95	0.07	-0.55	32,32,38,42	0
25	CL	a	412	1/1	0.99	0.06	-0.67	24,24,24,24	0
25	CL	A	408	1/1	1.00	0.05	-0.87	22,22,22,22	0
20	CLA	b	617	65/65	0.97	0.07	-0.94	23,30,44,50	0
39	MG	J	102	1/1	0.97	0.05	-1.47	33,33,33,33	0
29	FE2	a	417	1/1	0.99	0.05	-1.56	27,27,27,27	0
29	FE2	A	419	1/1	0.99	0.03	-1.59	29,29,29,29	0
30	OEX	A	420	10/10	1.00	0.04	-1.61	21,23,24,24	0
33	CA	o	301	1/1	0.94	0.07	-1.61	48,48,48,48	0
33	CA	c	522	1/1	0.98	0.04	-1.88	41,41,41,41	0
33	CA	O	301	1/1	0.95	0.06	-2.01	47,47,47,47	0
25	CL	A	409	1/1	0.99	0.03	-2.20	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	OEX	a	419	10/10	1.00	0.03	-3.10	21,24,26,26	0
25	CL	a	411	1/1	1.00	0.02	-6.01	22,22,22,22	0
26	UNL	Z	102	4/-	0.53	0.17	-	59,61,62,63	0
28	DMS	b	641	4/4	0.83	0.17	-	63,65,75,80	0
28	DMS	V	206	4/4	0.96	0.20	-	59,61,63,65	0
28	DMS	c	532	4/4	0.94	0.23	-	65,70,76,77	0
28	DMS	O	311	4/4	0.90	0.26	-	57,65,69,72	0
33	CA	V	203	1/1	0.88	0.11	-	63,63,63,63	0
28	DMS	C	529	4/4	0.92	0.19	-	70,73,74,74	0
28	DMS	C	528	4/4	0.99	0.09	-	33,37,39,41	0
26	UNL	B	646	16/-	0.68	0.24	-	85,89,93,94	0
26	UNL	J	106	4/-	0.83	0.15	-	57,60,61,67	0
26	UNL	B	647	13/-	0.77	0.23	-	71,81,90,91	0
28	DMS	O	308	4/4	0.78	0.24	-	66,74,76,87	0
28	DMS	d	415	4/4	0.91	0.25	-	68,71,71,72	0
28	DMS	A	414	4/4	0.99	0.07	-	25,28,28,29	0
26	UNL	B	629	10/-	0.72	0.27	-	54,69,74,74	0
28	DMS	B	644	4/4	0.87	0.32	-	52,53,61,69	0
26	UNL	c	525	10/-	0.84	0.15	-	58,65,66,67	0
26	UNL	b	629	16/-	0.91	0.15	-	41,48,60,60	0
26	UNL	I	105	10/-	0.84	0.15	-	60,66,71,72	0
28	DMS	v	205	4/4	0.96	0.18	-	67,70,72,73	0
26	UNL	H	105	6/-	0.78	0.14	-	51,55,63,65	0
26	UNL	A	413	4/-	0.86	0.19	-	64,64,64,66	0
26	UNL	z	101	6/-	0.90	0.13	-	49,55,55,57	0
26	UNL	c	526	8/-	0.77	0.15	-	54,59,64,65	0
28	DMS	u	203	4/4	0.91	0.29	-	47,55,56,65	0
33	CA	B	624	1/1	0.99	0.16	-	43,43,43,43	0
26	UNL	i	102	11/-	0.80	0.16	-	48,54,64,65	0
26	UNL	H	104	4/-	0.88	0.21	-	60,62,65,67	0
28	DMS	v	207	4/4	0.68	0.20	-	53,66,72,87	0
28	DMS	V	204	4/4	0.91	0.32	-	58,64,64,72	0
28	DMS	C	533	4/4	0.94	0.28	-	72,73,73,74	0
26	UNL	i	103	11/-	0.90	0.27	-	58,61,65,66	0
32	HTG	B	623	19/19	0.59	0.35	-	53,88,93,94	0
26	UNL	M	102	12/-	0.84	0.22	-	49,53,95,98	0
28	DMS	o	303	4/4	0.92	0.39	-	66,69,75,79	0
26	UNL	a	414	28/-	0.67	0.23	-	59,68,84,87	0
32	HTG	C	520	19/19	0.86	0.22	-	64,70,76,79	0
28	DMS	b	634	4/4	0.91	0.29	-	59,67,67,75	0
26	UNL	e	101	7/-	0.82	0.25	-	54,58,64,65	0
26	UNL	b	646	6/-	0.86	0.14	-	54,58,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	DMS	c	529	4/4	0.93	0.23	-	79,82,86,87	0
26	UNL	I	103	13/-	0.88	0.13	-	47,53,84,87	0
26	UNL	b	642	13/-	0.56	0.22	-	71,80,87,90	0
26	UNL	i	101	16/-	0.85	0.17	-	41,45,65,65	0
28	DMS	B	636	4/4	0.61	0.40	-	77,86,90,96	0
26	UNL	c	524	30/-	0.71	0.19	-	59,74,86,87	0
28	DMS	b	640	4/4	0.77	0.27	-	49,58,71,73	0
32	HTG	c	520	19/19	0.78	0.22	-	77,88,99,100	0
28	DMS	B	643	4/4	0.94	0.14	-	51,53,62,71	0
26	UNL	b	643	9/-	0.68	0.18	-	67,67,74,74	0
28	DMS	A	415	4/4	0.94	0.20	-	55,58,65,71	0
26	UNL	J	107	3/-	0.74	0.21	-	61,61,63,64	0
28	DMS	B	635	4/4	0.86	0.24	-	90,94,95,96	0
32	HTG	C	534	19/19	0.39	0.38	-	68,110,128,130	0
26	UNL	I	104	11/-	0.84	0.19	-	53,56,59,62	0
28	DMS	u	204	4/4	0.84	0.19	-	71,78,83,86	0
32	HTG	B	632	19/19	0.65	0.23	-	51,97,108,114	0
26	UNL	I	102	16/-	0.85	0.19	-	38,47,63,64	0
26	UNL	L	102	14/-	0.85	0.22	-	56,60,84,84	0
26	UNL	b	644	7/-	0.90	0.18	-	64,65,70,70	0
28	DMS	c	527	4/4	0.99	0.05	-	33,33,34,38	0
33	CA	b	626	1/1	0.95	0.07	-	42,42,42,42	0
28	DMS	b	635	4/4	0.92	0.27	-	58,62,69,73	0
32	HTG	b	602	19/19	0.69	0.20	-	51,103,117,118	0
28	DMS	o	302	4/4	0.98	0.08	-	20,28,31,36	0
28	DMS	b	639	4/4	0.95	0.20	-	46,49,49,50	0
28	DMS	c	534	4/4	0.90	0.24	-	70,71,75,81	0
26	UNL	x	102	9/-	0.84	0.29	-	56,68,72,72	0
28	DMS	H	103	4/4	0.61	0.40	-	84,101,109,112	0
28	DMS	U	904	4/4	0.55	0.22	-	58,66,66,83	0
28	DMS	c	533	4/4	0.85	0.27	-	73,75,77,87	0
28	DMS	O	303	4/4	0.82	0.29	-	63,72,77,78	0
26	UNL	a	402	6/-	0.69	0.17	-	50,57,62,63	0
28	DMS	o	305	4/4	0.92	0.23	-	73,75,77,87	0
26	UNL	b	645	6/-	0.57	0.24	-	57,65,76,76	0
26	UNL	B	628	15/-	0.86	0.15	-	45,50,60,66	0
28	DMS	v	209	4/4	0.86	0.32	-	71,78,79,79	0
28	DMS	b	637	4/4	0.87	0.17	-	77,79,84,93	0

6.5 Other polymers (i)

There are no such residues in this entry.