Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:28 PM GMT

PDB ID	:	3WU2
Title	:	Crystal structure analysis of Photosystem II complex
Authors	:	Umena, Y.; Kawakami, K.; Shen, J.R.; Kamiya, N.
Deposited on	:	2014-04-21
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

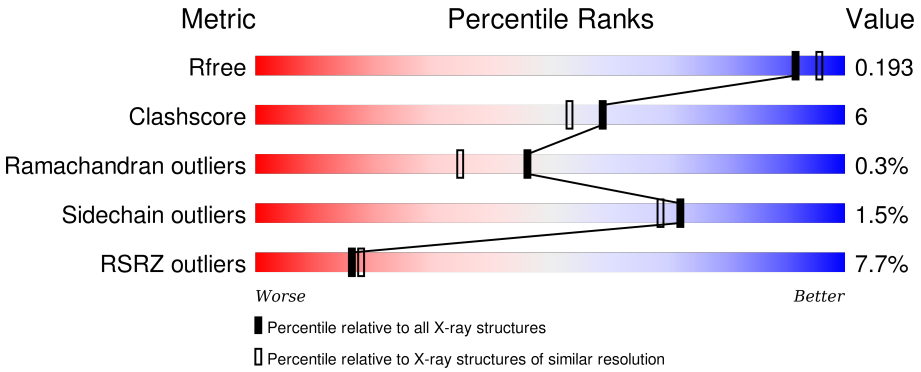
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	85% 10%
1	a	344	4% 93%
2	B	504	8% 87% 13%
2	b	504	9% 97%
3	C	455	3% 87% 11%

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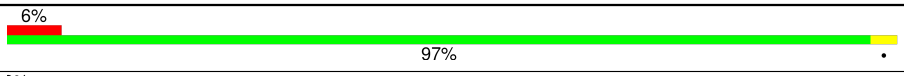
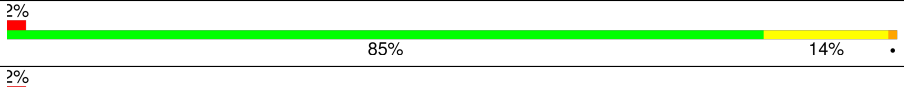
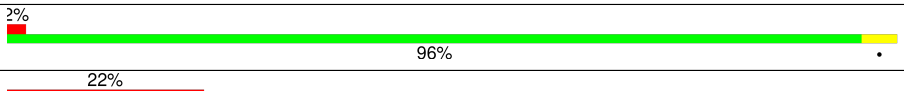
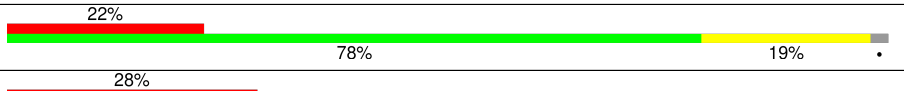
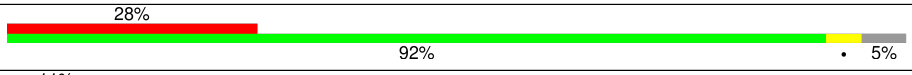
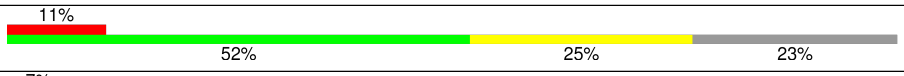
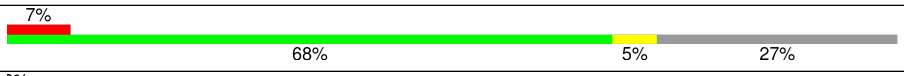
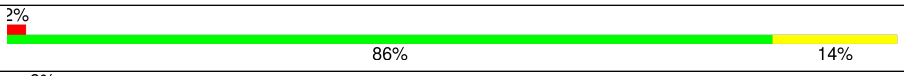
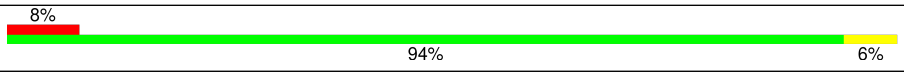
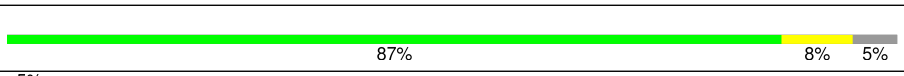
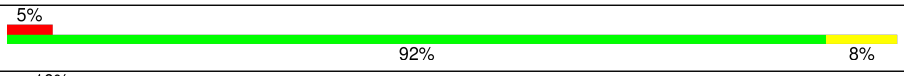
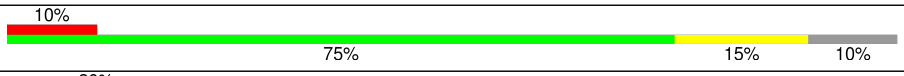
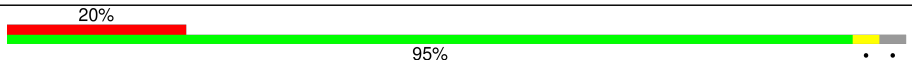
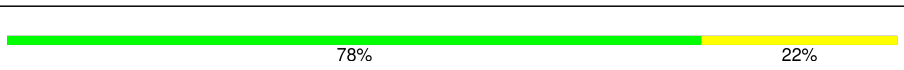
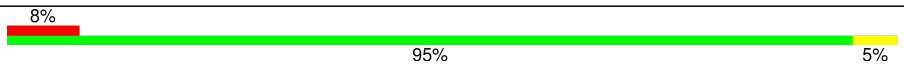
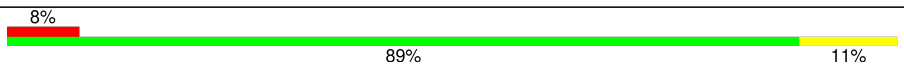
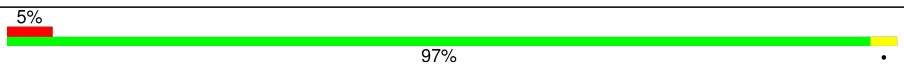
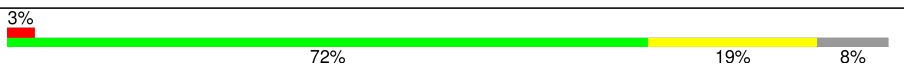
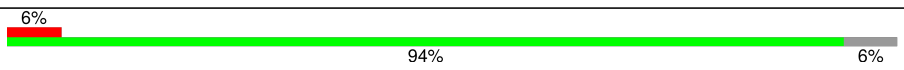
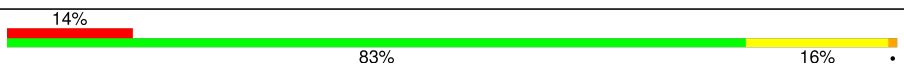
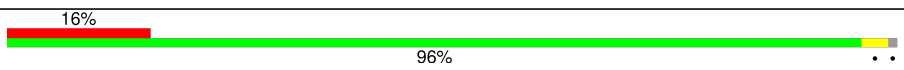
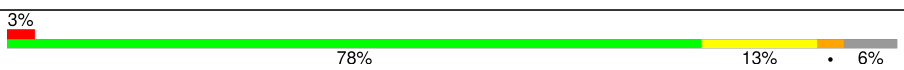
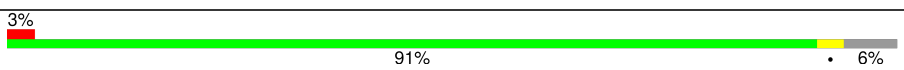
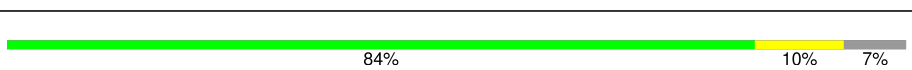
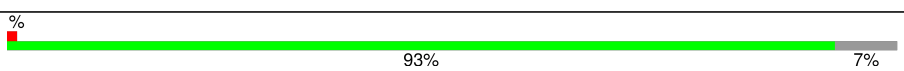
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	63	
7	h	63	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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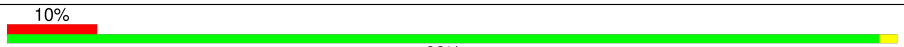
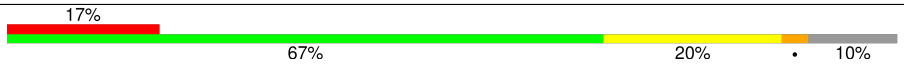
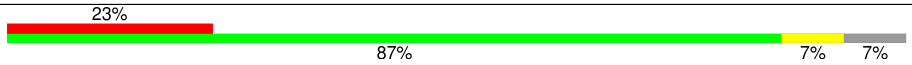
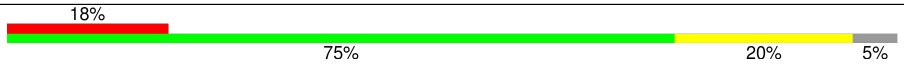
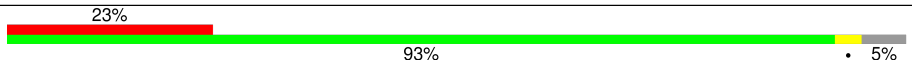
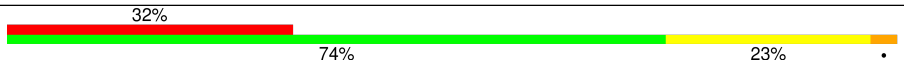
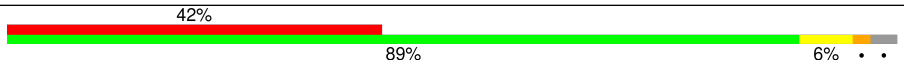
Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

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
12	FME	M	1	-	-	X	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	A	410	X	-	-	-
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	a	411	X	-	-	-
23	CLA	a	414	X	-	-	-
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	903	X	-	-	-
23	CLA	c	904	X	-	-	-
23	CLA	c	905	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	909	X	-	-	-
23	CLA	c	910	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	911	X	-	-	-
23	CLA	c	912	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	c	914	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	B	618	-	-	-	X
25	BCR	B	619	-	-	-	X
25	BCR	D	404	-	-	-	X
25	BCR	T	101	-	-	-	X
26	SQD	A	418	-	-	-	X
26	SQD	B	621	-	-	-	X
26	SQD	L	103	-	-	-	X
26	SQD	a	401	-	-	-	X
27	LMG	A	413	-	-	-	X
27	LMG	D	411	-	-	-	X
27	LMG	c	921	-	-	-	X
27	LMG	d	410	-	-	-	X
28	PL9	A	414	-	-	-	X
28	PL9	a	419	-	-	-	X
29	UNL	A	417	-	-	-	X
29	UNL	A	420	-	-	-	X
29	UNL	B	627	-	-	X	-
29	UNL	B	629	-	-	-	X
29	UNL	B	632	-	-	-	X
29	UNL	C	523	-	-	-	X
29	UNL	D	412	-	-	X	X
29	UNL	D	413	-	-	-	X
29	UNL	E	102	-	-	-	X
29	UNL	E	103	-	-	-	X
29	UNL	T	102	-	-	-	X
29	UNL	X	101	-	-	-	X
29	UNL	a	403	-	-	-	X
29	UNL	b	628	-	-	-	X
29	UNL	b	630	-	-	-	X
29	UNL	b	631	-	-	-	X
29	UNL	d	411	-	-	-	X
29	UNL	i	103	-	-	-	X
29	UNL	j	102	-	-	-	X
29	UNL	t	103	-	-	-	X
29	UNL	x	101	-	-	-	X
29	UNL	z	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	LMT	A	419	-	-	-	X
30	LMT	C	520	-	-	-	X
30	LMT	F	102	-	-	-	X
30	LMT	J	102	-	-	-	X
30	LMT	M	101	-	-	-	X
30	LMT	b	625	-	-	-	X
30	LMT	c	922	-	-	-	X
30	LMT	m	102	-	-	-	X
30	LMT	t	102	-	-	-	X
31	GOL	A	421	-	-	-	X
31	GOL	A	422	-	-	-	X
31	GOL	A	423	-	-	-	X
31	GOL	B	633	-	-	-	X
31	GOL	C	524	-	-	X	X
31	GOL	C	526	-	-	-	X
31	GOL	D	415	-	-	-	X
31	GOL	L	104	-	-	-	X
31	GOL	V	204	-	-	-	X
31	GOL	V	205	-	-	-	X
31	GOL	a	422	-	-	-	X
31	GOL	a	423	-	-	-	X
31	GOL	a	424	-	-	-	X
31	GOL	b	632	-	-	-	X
31	GOL	b	633	-	-	-	X
31	GOL	c	928	-	-	-	X
31	GOL	c	930	-	-	-	X
31	GOL	f	104	-	-	-	X
31	GOL	l	102	-	-	-	X
33	HTG	C	522	-	-	-	X
33	HTG	D	414	-	-	-	X
33	HTG	U	201	-	-	-	X
33	HTG	V	202	-	-	-	X
33	HTG	b	602	-	-	-	X
33	HTG	b	626	-	-	-	X
33	HTG	c	924	-	-	-	X
33	HTG	d	401	-	-	-	X
33	HTG	u	201	-	-	-	X
34	DGD	C	518	-	-	-	X
34	DGD	D	406	-	-	-	X
34	DGD	d	406	-	-	-	X
36	LHG	D	408	-	-	-	X
36	LHG	D	410	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	LHG	d	407	-	-	-	X
39	MG	j	101	-	-	-	X
40	SO4	O	302	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54036 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2633	1729	429	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2625	1722	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4009	2633	668	695	13			
2	b	501	Total	C	N	O	S	0	11	0
			3964	2605	658	688	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3502	2291	588	610	13			
3	c	455	Total	C	N	O	S	0	4	0
			3536	2315	593	615	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	SEE REMARK 999	UNP D0VWR7
C	20	SER	-	SEE REMARK 999	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	SEE REMARK 999	UNP D0VWR7
C	22	PHE	-	SEE REMARK 999	UNP D0VWR7
c	19	ASN	-	SEE REMARK 999	UNP D0VWR7
c	20	SER	-	SEE REMARK 999	UNP D0VWR7
c	21	ILE	-	SEE REMARK 999	UNP D0VWR7
c	22	PHE	-	SEE REMARK 999	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	2	0
			2726	1809	443	462	12			
4	d	341	Total	C	N	O	S	0	4	0
			2741	1817	449	463	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			657	429	106	122			
5	e	79	Total	C	N	O	0	0	0
			639	419	103	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			274	187	45	41	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	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			294	199	45	49	1			
8	i	38	Total	C	N	O	S	0	0	0
			311	210	48	52	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	39	Total	C	N	O	S	0	0	0
			271	182	40	48	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	1	0
			290	202	42	46			
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	SEE REMARK 999	UNP P19054
K	39	TRP	VAL	SEE REMARK 999	UNP P19054
k	33	LEU	PHE	SEE REMARK 999	UNP P19054
k	39	TRP	VAL	SEE REMARK 999	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	2	0
			300	204	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
			261	176	37	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			271	184	38	48	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	SEE REMARK 999	UNP P12312
m	8	LEU	PHE	SEE REMARK 999	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	5	0
			1878	1177	314	382	5			
13	o	241	Total	C	N	O	S	0	5	0
			1855	1163	305	381	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	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
			770	489	129	152			
15	u	97	Total	C	N	O	0	1	0
			772	490	129	153			

- 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	2	0
			1066	677	180	205	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			196	130	32	31	3			
17	y	28	Total	C	N	O	S	0	0	0
			196	128	33	32	3			

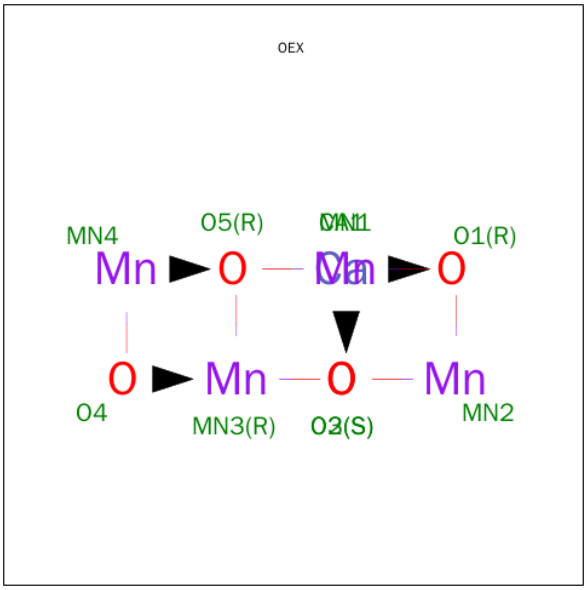
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	1	0
			280	190	44	46			
18	x	38	Total	C	N	O	0	1	0
			280	190	44	46			

- 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
			459	318	67	73	1			
19	z	60	Total	C	N	O	S	0	0	0
			431	301	64	65	1			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

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

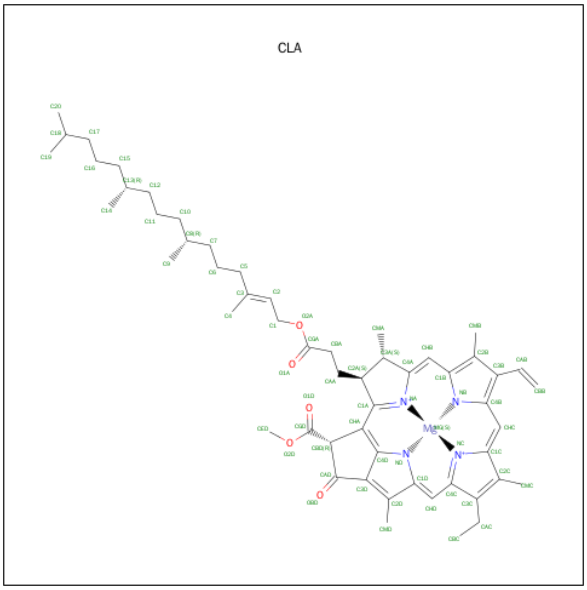
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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

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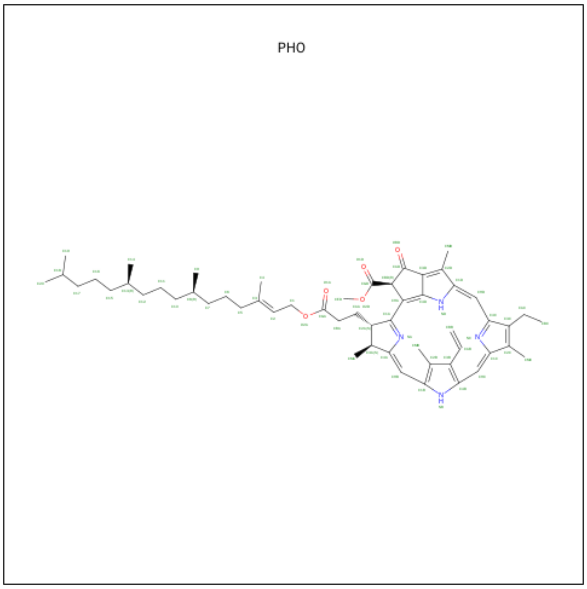
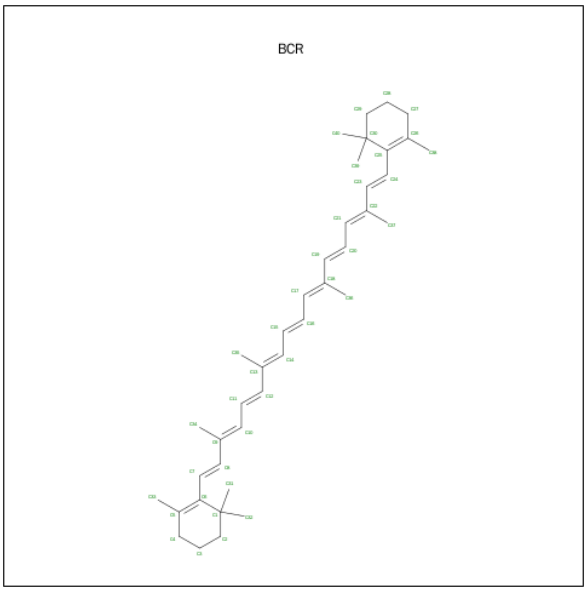
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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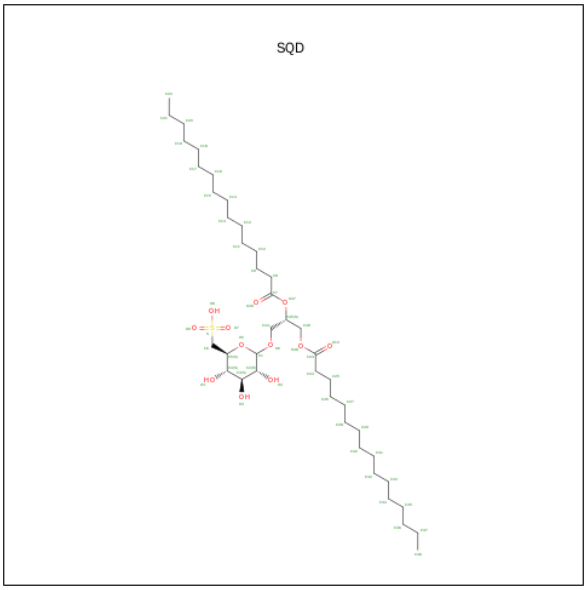
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 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
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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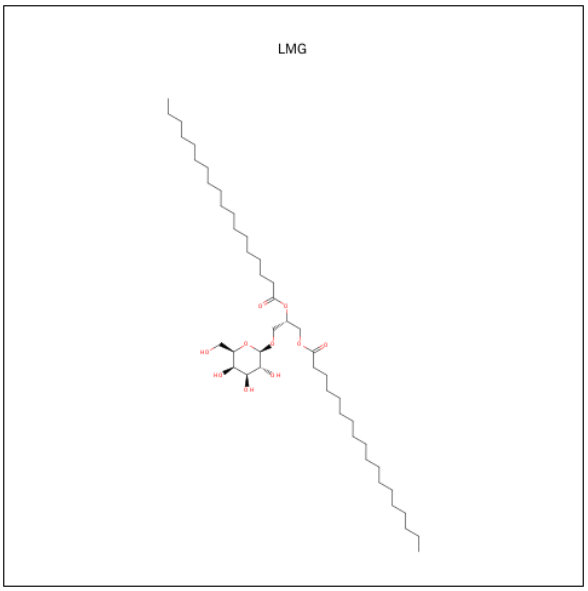
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	a	1	Total C O S 54 41 12 1	0	0
26	a	1	Total C O S 54 41 12 1	0	0
26	f	1	Total C O S 33 23 9 1	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 51 41 10	0	0
27	B	1	Total C O 51 41 10	0	0
27	C	1	Total C O 51 41 10	0	0
27	D	1	Total C O 51 41 10	0	0
27	Z	1	Total C O 51 41 10	0	0
27	a	1	Total C O 51 41 10	0	0
27	b	1	Total C O 51 41 10	0	0
27	c	1	Total C O 51 41 10	0	0

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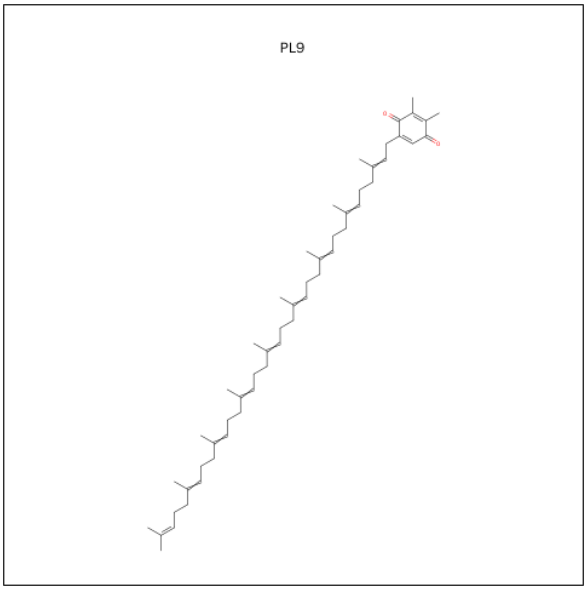
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 51 41 10	0	0
27	d	1	Total C O 51 41 10	0	0

- Molecule 28 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
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0
28	a	1	Total C O 55 53 2	0	0
28	d	1	Total C O 55 53 2	0	0

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	4	Total C 56 56	0	0
29	c	2	Total C O 40 35 5	0	0

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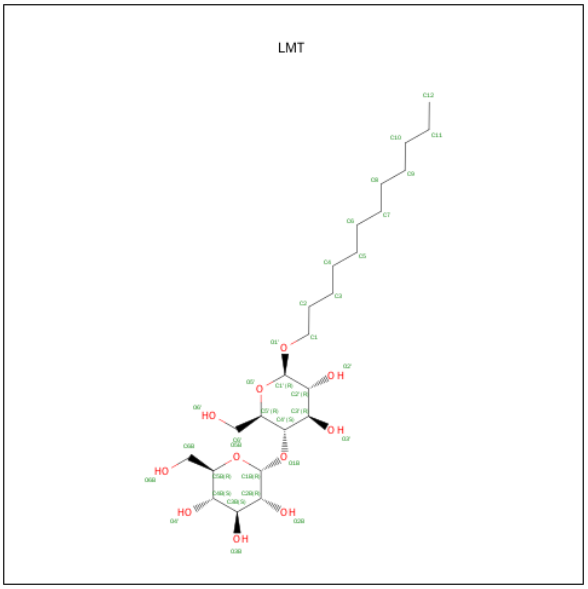
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	2	Total C 26 26	0	0
29	E	2	Total C 27 27	0	0
29	b	4	Total C O 84 79 5	0	0
29	A	4	Total C O 69 64 5	0	0
29	x	1	Total C 16 16	0	0
29	M	1	Total C 16 16	0	0
29	j	2	Total C 28 28	0	0
29	D	2	Total C O 56 51 5	0	0
29	e	1	Total C 11 11	0	0
29	I	2	Total C 24 24	0	0
29	Z	1	Total C 16 16	0	0
29	a	3	Total C O 56 51 5	0	0
29	L	1	Total C 14 14	0	0
29	d	1	Total C 16 16	0	0
29	H	1	Total C 10 10	0	0
29	i	4	Total C 55 55	0	0
29	C	1	Total C O 34 29 5	0	0
29	z	1	Total C 16 16	0	0
29	T	1	Total C 13 13	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 35 24 11	0	0
30	B	1	Total C O 35 24 11	0	0
30	C	1	Total C O 35 24 11	0	0
30	F	1	Total C O 35 24 11	0	0
30	J	1	Total C O 24 18 6	0	0
30	M	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	Z	1	Total C O 35 24 11	0	0
30	a	1	Total C O 35 24 11	0	0
30	b	1	Total C O 25 19 6	0	0
30	b	1	Total C O 24 18 6	0	0
30	c	1	Total C O 35 24 11	0	0

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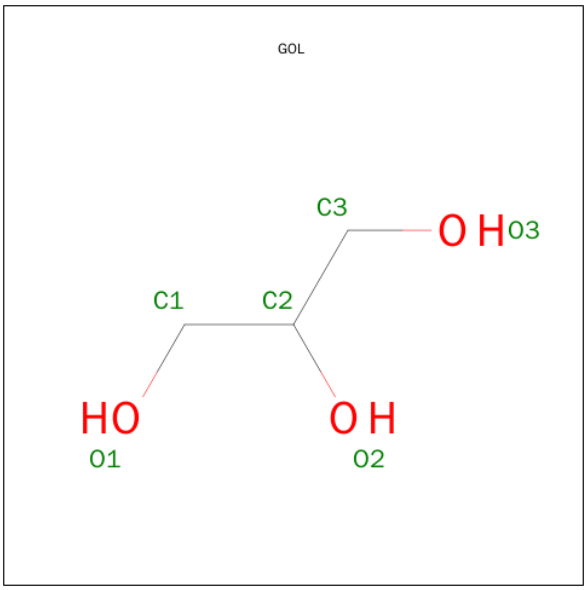
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	m	1	Total C O 35 24 11	0	0
30	m	1	Total C O 35 24 11	0	0
30	t	1	Total C O 24 18 6	0	0
30	z	1	Total C O 32 21 11	0	0

- Molecule 31 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 6 3 3	0	0
31	A	1	Total C O 6 3 3	0	0
31	A	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0
31	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			6	3	3		
31	B	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	C	1	Total	C	O	0	0
			6	3	3		
31	D	1	Total	C	O	0	0
			6	3	3		
31	L	1	Total	C	O	0	0
			6	3	3		
31	O	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	V	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	a	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	b	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		
31	c	1	Total	C	O	0	0
			6	3	3		

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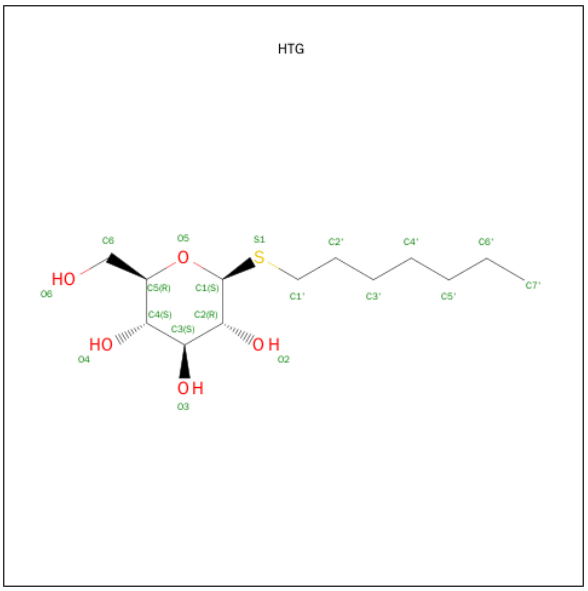
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 6 3 3	0	0
31	c	1	Total C O 6 3 3	0	0
31	f	1	Total C O 6 3 3	0	0
31	h	1	Total C O 6 3 3	0	0
31	l	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0
31	v	1	Total C O 6 3 3	0	0

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total Ca 1 1	0	0
32	c	1	Total Ca 1 1	0	0
32	F	1	Total Ca 1 1	0	0
32	o	1	Total Ca 1 1	0	0
32	O	1	Total Ca 1 1	0	0
32	b	1	Total Ca 1 1	0	0
32	f	1	Total Ca 1 1	0	0

- Molecule 33 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	C	1	Total C O S 19 13 5 1	0	0
33	C	1	Total C O S 19 13 5 1	0	0
33	D	1	Total C O S 19 13 5 1	0	0
33	O	1	Total C O S 19 13 5 1	0	0
33	U	1	Total C S 9 8 1	0	0
33	V	1	Total C O S 13 7 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0

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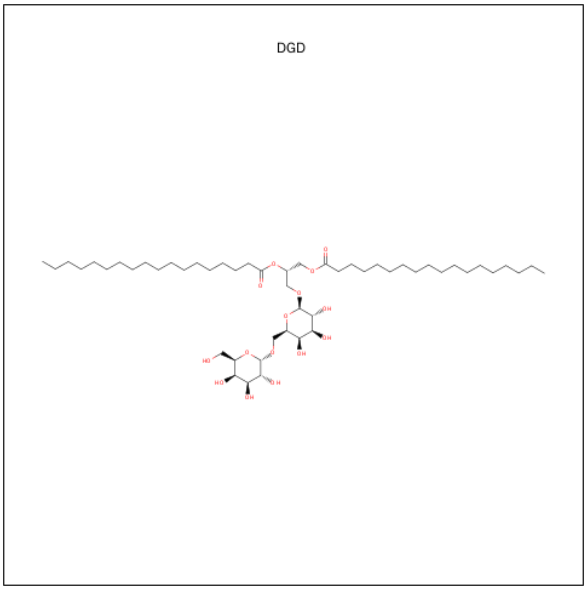
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	b	1	Total C O S 19 13 5 1	0	0
33	c	1	Total C O S 19 13 5 1	0	0
33	c	1	Total C O S 19 13 5 1	0	0
33	d	1	Total C O S 19 13 5 1	0	0
33	u	1	Total C O S 14 10 3 1	0	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	C	1	Total C O 62 47 15	0	0
34	C	1	Total C O 62 47 15	0	0
34	C	1	Total C O 62 47 15	0	0
34	D	1	Total C O 53 42 11	0	0
34	H	1	Total C O 62 47 15	0	0
34	c	1	Total C O 62 47 15	0	0

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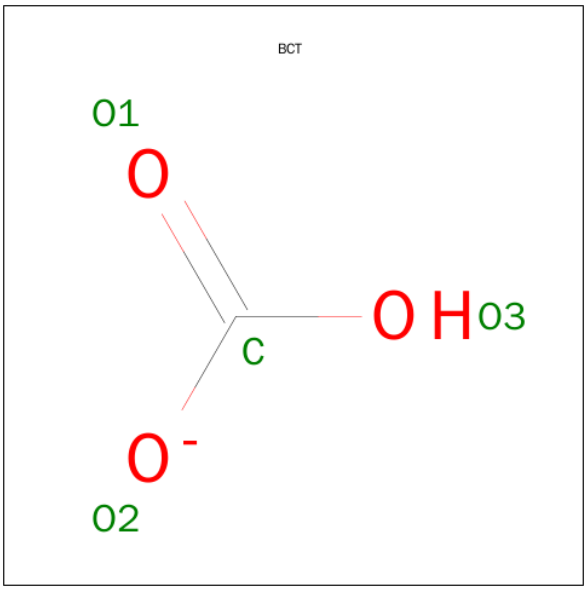
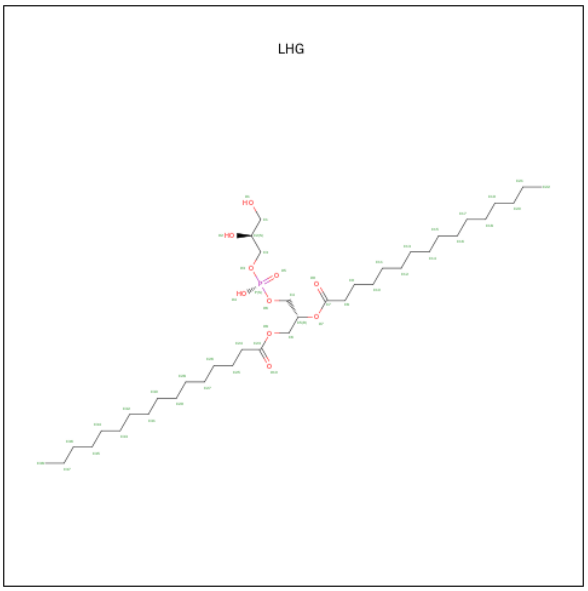
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	c	1	Total C O 62 47 15	0	0
34	c	1	Total C O 62 47 15	0	0
34	d	1	Total C O 50 41 9	0	0
34	h	1	Total C O 62 47 15	0	0

- Molecule 35 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



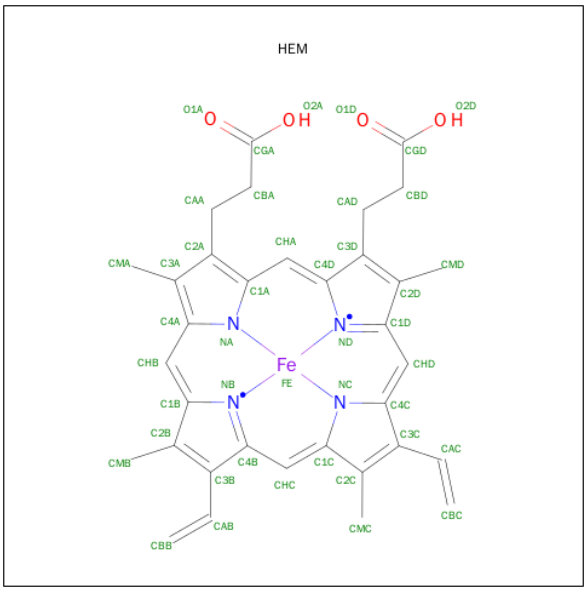
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	D	1	Total C O 4 1 3	0	0
35	a	1	Total C O 4 1 3	0	0

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



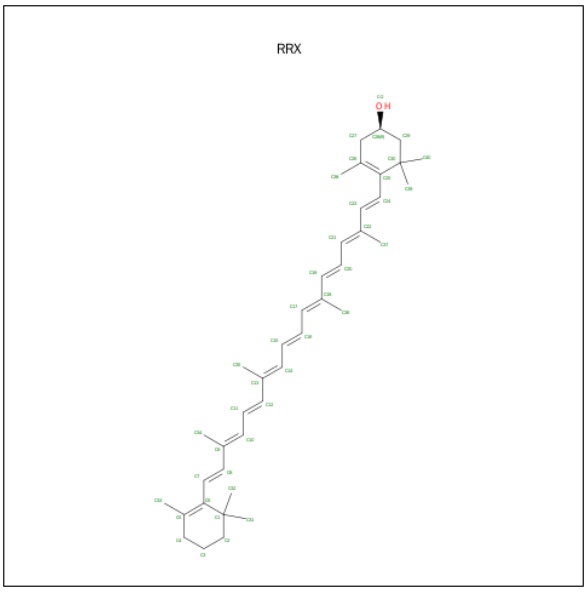
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			46	35	10	1		
36	E	1	Total	C	O	P	0	0
			49	38	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			40	29	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- 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	F	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	f	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: $C_{40}H_{56}O$).

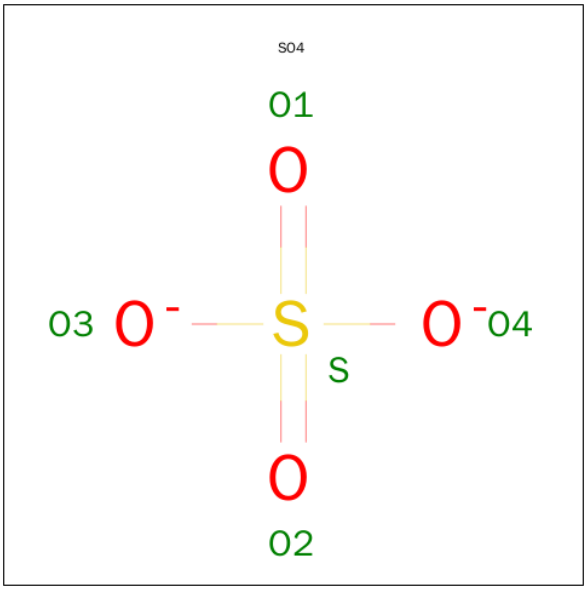


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	H	1	Total C O 41 40 1	0	0
38	h	1	Total C O 41 40 1	0	0

- 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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	O	1	Total O S 5 4 1	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	168	Total O 170 170	0	2
41	B	311	Total O 319 319	0	8

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	253	Total O 263 263	0	10
41	D	156	Total O 161 161	0	5
41	E	32	Total O 35 35	0	3
41	F	12	Total O 12 12	0	0
41	H	50	Total O 52 52	0	2
41	I	8	Total O 8 8	0	0
41	J	9	Total O 9 9	0	0
41	K	8	Total O 8 8	0	0
41	L	23	Total O 24 24	0	1
41	M	15	Total O 16 16	0	1
41	O	193	Total O 202 202	0	9
41	T	10	Total O 10 10	0	0
41	U	98	Total O 100 100	0	2
41	V	140	Total O 144 144	0	4
41	Y	6	Total O 6 6	0	0
41	X	13	Total O 14 14	0	1
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 155 155	0	2
41	b	295	Total O 306 306	0	11
41	c	238	Total O 245 245	0	7
41	d	156	Total O 160 160	0	4

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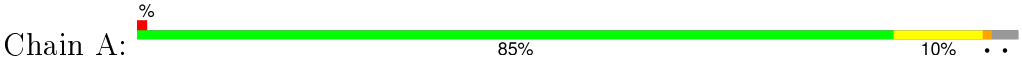
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	e	22	Total O 22 22	0	0
41	f	13	Total O 14 14	0	1
41	h	48	Total O 53 53	0	5
41	i	13	Total O 14 14	0	1
41	j	9	Total O 9 9	0	0
41	k	5	Total O 5 5	0	0
41	l	17	Total O 18 18	0	1
41	m	15	Total O 16 16	0	1
41	o	167	Total O 175 175	0	8
41	t	12	Total O 12 12	0	0
41	u	102	Total O 106 106	0	4
41	v	98	Total O 104 104	0	6
41	y	7	Total O 7 7	0	0
41	x	6	Total O 6 6	0	0
41	z	2	Total O 2 2	0	0

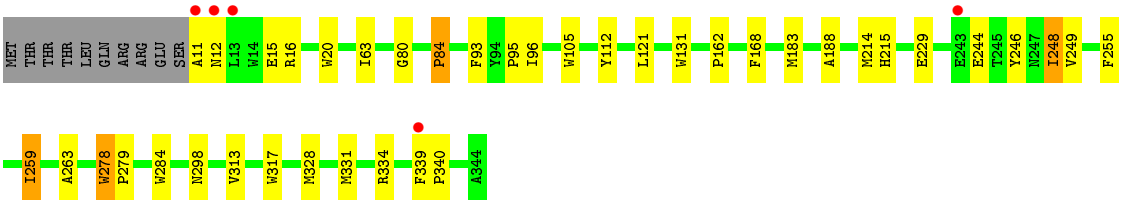
3 Residue-property plots (i)

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 Q(B) protein

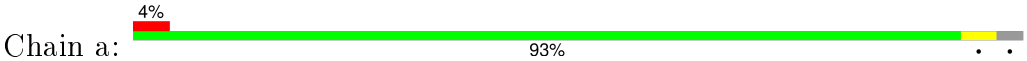
Chain A:





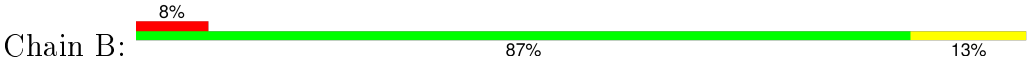
- Molecule 1: Photosystem Q(B) protein

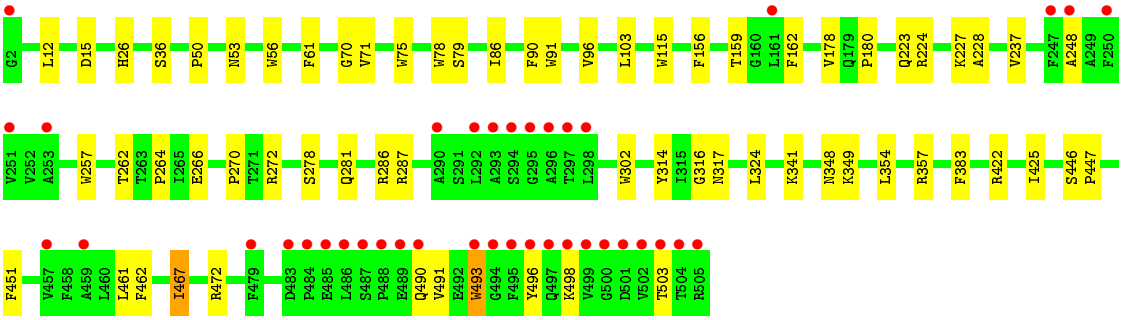
Chain a:



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

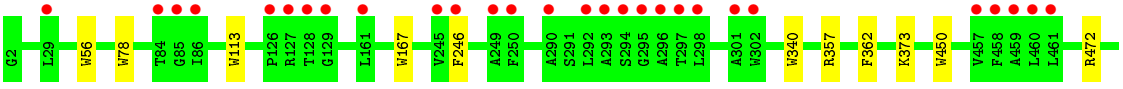
Chain B:

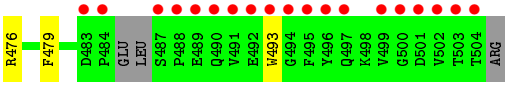




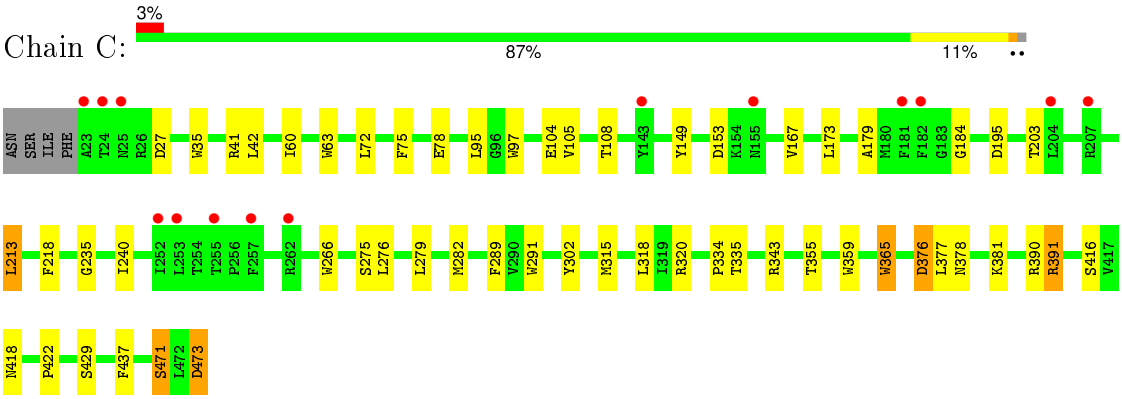
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

Chain b:

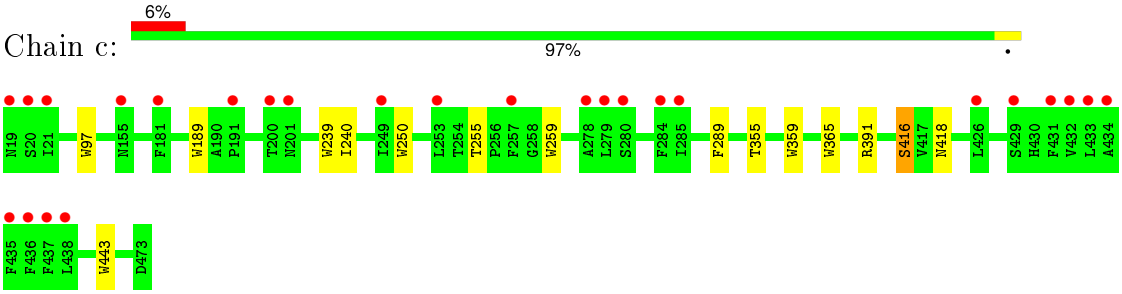




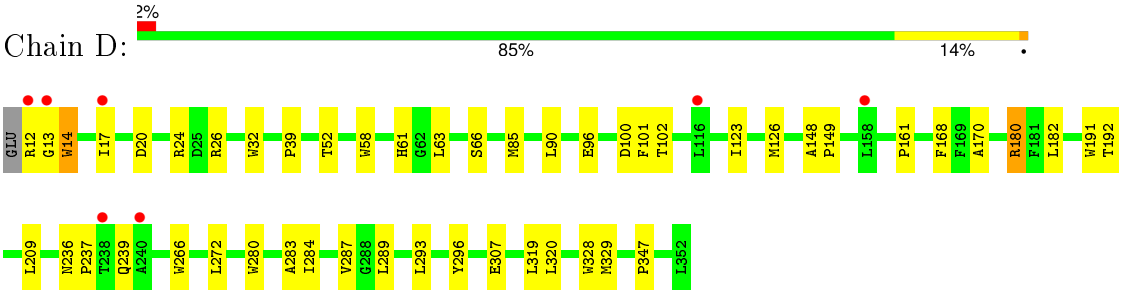
• Molecule 3: Photosystem II 44 kDa reaction center protein



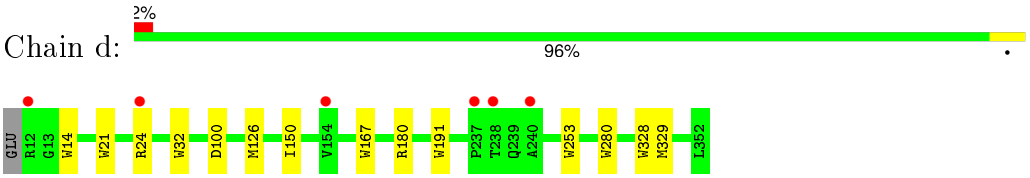
• Molecule 3: Photosystem II 44 kDa reaction center protein



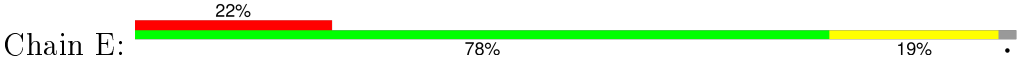
• Molecule 4: Photosystem II D2 protein

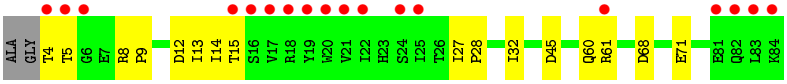


• Molecule 4: Photosystem II D2 protein

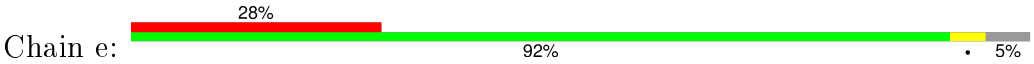


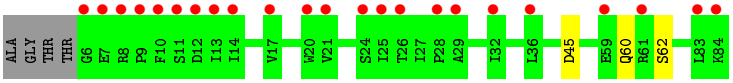
• Molecule 5: Cytochrome b559 subunit alpha



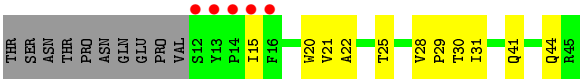


• Molecule 5: Cytochrome b559 subunit alpha

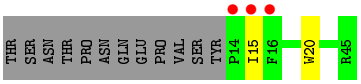




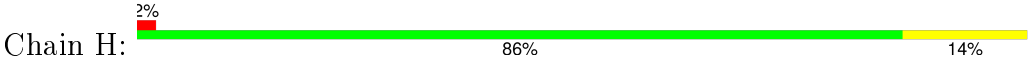
• Molecule 6: Cytochrome b559 subunit beta

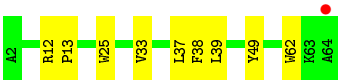


• Molecule 6: Cytochrome b559 subunit beta

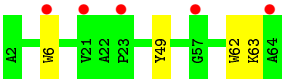


• Molecule 7: Photosystem II reaction center protein H

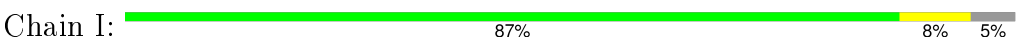




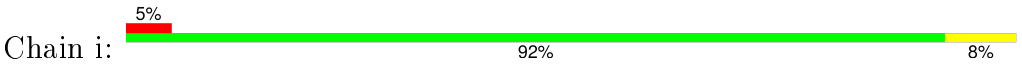
• Molecule 7: Photosystem II reaction center protein H

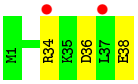


• Molecule 8: Photosystem II reaction center protein I



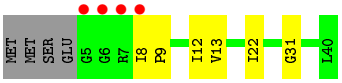
• Molecule 8: Photosystem II reaction center protein I





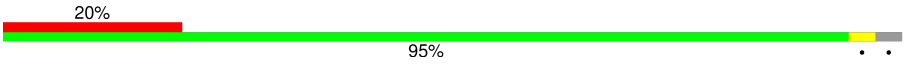
• Molecule 9: Photosystem II reaction center protein J

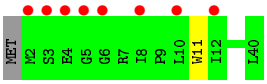
Chain J:



• Molecule 9: Photosystem II reaction center protein J

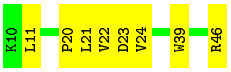
Chain j:





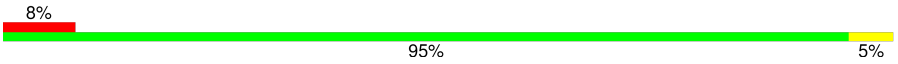
• Molecule 10: Photosystem II reaction center protein K

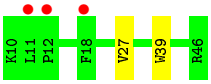
Chain K:



• Molecule 10: Photosystem II reaction center protein K

Chain k:



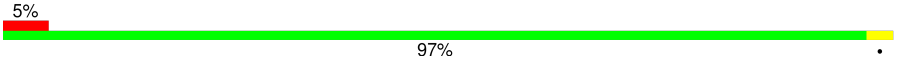


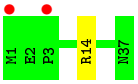
• Molecule 11: Photosystem II reaction center protein L

Chain L:

• Molecule 11: Photosystem II reaction center protein L

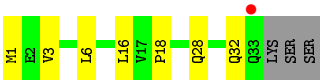
Chain l:





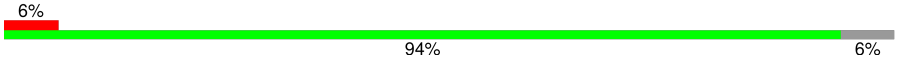
• Molecule 12: Photosystem II reaction center protein M

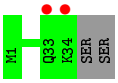
Chain M:



• Molecule 12: Photosystem II reaction center protein M

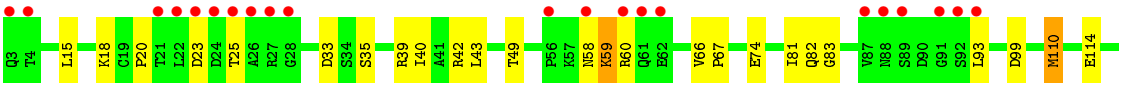
Chain m:





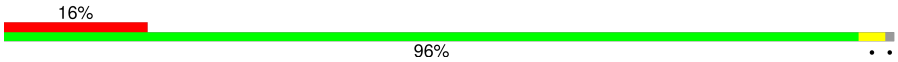
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

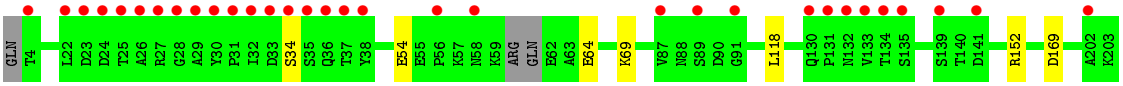
Chain O:

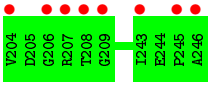


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

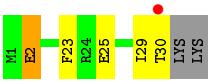






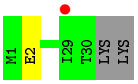
• Molecule 14: Photosystem II reaction center protein T

Chain T:



• Molecule 14: Photosystem II reaction center protein T

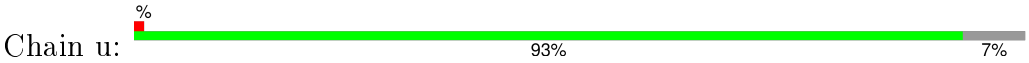
Chain t:

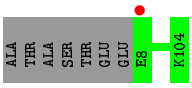


• Molecule 15: Photosystem II 12 kDa extrinsic protein

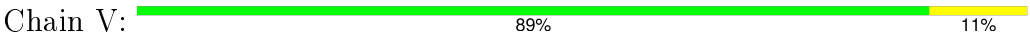
Chain U:

• Molecule 15: Photosystem II 12 kDa extrinsic protein

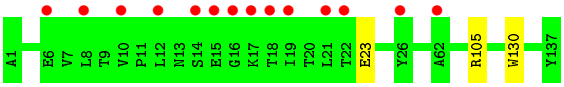




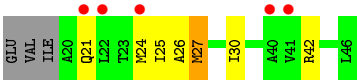
• Molecule 16: Cytochrome c-550



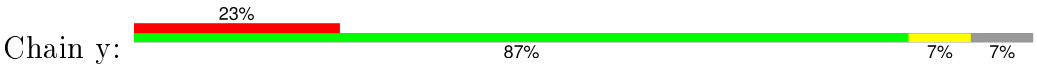
• Molecule 16: Cytochrome c-550

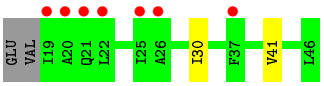


• Molecule 17: Photosystem II reaction center protein Ycf12

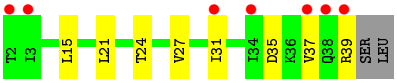


• Molecule 17: Photosystem II reaction center protein Ycf12

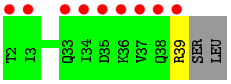




• Molecule 18: Photosystem II reaction center protein X

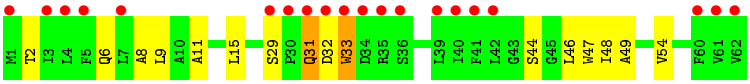


• Molecule 18: Photosystem II reaction center protein X



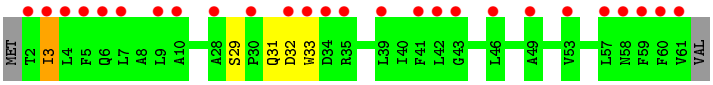
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 49.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (49.02-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.194 0.156 , 0.193	Depositor DCC
R_{free} test set	31204 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 67.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 623234 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	54036	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 1.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PL9, BCT, BCR, DGD, HSK, FE2, RRX, LHG, GOL, CL, CA, CLA, SO4, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, SQD, LMG

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	1.08	4/2730 (0.1%)	0.90	1/3723 (0.0%)
1	a	1.06	9/2721 (0.3%)	0.86	4/3711 (0.1%)
2	B	1.03	9/4179 (0.2%)	0.89	5/5693 (0.1%)
2	b	1.01	7/4134 (0.2%)	0.85	2/5633 (0.0%)
3	C	1.00	7/3624 (0.2%)	0.84	9/4933 (0.2%)
3	c	0.96	8/3662 (0.2%)	0.81	0/4986
4	D	1.13	5/2804 (0.2%)	0.93	3/3820 (0.1%)
4	d	1.05	8/2825 (0.3%)	0.87	2/3847 (0.1%)
5	E	0.81	0/676	0.82	0/924
5	e	0.81	0/658	0.78	1/899 (0.1%)
6	F	0.90	1/283 (0.4%)	0.71	0/386
6	f	0.92	1/265 (0.4%)	0.69	0/360
7	H	0.98	1/511 (0.2%)	0.79	0/697
7	h	0.94	2/511 (0.4%)	0.81	0/697
8	I	0.77	0/291	0.78	0/394
8	i	0.75	0/308	0.77	0/415
9	J	0.94	0/257	0.68	0/349
9	j	0.81	1/277 (0.4%)	0.69	0/376
10	K	0.76	1/303 (0.3%)	0.75	0/418
10	k	0.79	1/296 (0.3%)	0.77	0/408
11	L	1.05	0/312	0.88	0/425
11	l	1.00	0/313	0.84	1/428 (0.2%)
12	M	0.85	0/257	0.91	0/352
12	m	0.86	0/270	0.80	0/370
13	O	0.84	0/1924	0.89	0/2610
13	o	0.79	0/1900	0.86	3/2577 (0.1%)
14	T	0.93	0/255	0.86	0/346
14	t	0.99	0/255	0.92	0/346
15	U	0.93	0/781	0.90	1/1059 (0.1%)
15	u	0.95	0/786	0.91	0/1067
16	V	0.97	0/1093	0.89	1/1485 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.88	1/1084 (0.1%)	0.85	1/1475 (0.1%)
17	Y	0.55	0/197	0.66	0/263
17	y	0.50	0/197	0.75	0/264
18	X	0.72	0/286	0.75	0/387
18	x	0.67	0/286	0.75	0/387
19	Z	0.76	2/470 (0.4%)	0.74	0/645
19	z	0.68	1/442 (0.2%)	0.71	0/608
All	All	0.97	69/42423 (0.2%)	0.85	34/57763 (0.1%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	TRP	CD2-CE2	7.33	1.50	1.41
7	H	62	TRP	CD2-CE2	6.81	1.49	1.41
3	c	443	TRP	CD2-CE2	6.79	1.49	1.41
1	A	284	TRP	CD2-CE2	6.79	1.49	1.41
3	C	359	TRP	CD2-CE2	6.46	1.49	1.41
4	d	328	TRP	CD2-CE2	6.33	1.49	1.41
9	j	11	TRP	CD2-CE2	6.32	1.49	1.41
1	A	20	TRP	CD2-CE2	6.16	1.48	1.41
19	Z	33	TRP	CD2-CE2	6.13	1.48	1.41
4	D	328	TRP	CD2-CE2	6.13	1.48	1.41
2	b	113	TRP	CD2-CE2	6.00	1.48	1.41
3	c	189	TRP	CD2-CE2	5.95	1.48	1.41
4	d	167	TRP	CD2-CE2	5.94	1.48	1.41
2	B	56	TRP	CD2-CE2	5.94	1.48	1.41
16	v	130	TRP	CD2-CE2	5.86	1.48	1.41
7	h	6	TRP	CD2-CE2	5.79	1.48	1.41
2	b	340	TRP	CD2-CE2	5.75	1.48	1.41
3	c	239	TRP	CD2-CE2	5.75	1.48	1.41
10	k	39	TRP	CD2-CE2	5.74	1.48	1.41
6	F	20	TRP	CD2-CE2	5.66	1.48	1.41
2	B	75	TRP	CD2-CE2	5.66	1.48	1.41
6	f	20	TRP	CD2-CE2	5.65	1.48	1.41
1	a	32	TRP	CD2-CE2	5.63	1.48	1.41
4	D	32	TRP	CD2-CE2	5.62	1.48	1.41
1	a	161	TYR	CE1-CZ	5.59	1.45	1.38
19	z	33	TRP	CD2-CE2	5.56	1.48	1.41
7	h	62	TRP	CD2-CE2	5.55	1.48	1.41
3	c	365	TRP	CD2-CE2	5.53	1.48	1.41
4	d	21	TRP	CD2-CE2	5.53	1.48	1.41
19	Z	47	TRP	CD2-CE2	5.50	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	365	TRP	CD2-CE2	5.47	1.48	1.41
3	c	97	TRP	CD2-CE2	5.44	1.47	1.41
4	d	253	TRP	CD2-CE2	5.43	1.47	1.41
2	B	91	TRP	CD2-CE2	5.41	1.47	1.41
1	a	131	TRP	CD2-CE2	5.41	1.47	1.41
1	a	20	TRP	CD2-CE2	5.40	1.47	1.41
3	C	35	TRP	CD2-CE2	5.38	1.47	1.41
2	b	450	TRP	CD2-CE2	5.34	1.47	1.41
3	C	291	TRP	CD2-CE2	5.30	1.47	1.41
2	B	302	TRP	CD2-CE2	5.30	1.47	1.41
2	B	56	TRP	CG-CD1	5.29	1.44	1.36
2	b	56	TRP	CD2-CE2	5.28	1.47	1.41
1	a	142	TRP	CD2-CE2	5.27	1.47	1.41
3	c	259	TRP	CD2-CE2	5.26	1.47	1.41
4	D	58	TRP	CD2-CE2	5.26	1.47	1.41
2	B	115	TRP	CD2-CE2	5.26	1.47	1.41
3	c	250	TRP	CD2-CE2	5.24	1.47	1.41
2	b	78	TRP	CD2-CE2	5.23	1.47	1.41
3	C	97	TRP	CD2-CE2	5.23	1.47	1.41
1	a	105	TRP	CD2-CE2	5.22	1.47	1.41
2	B	493	TRP	CD2-CE2	5.21	1.47	1.41
4	d	32	TRP	CD2-CE2	5.20	1.47	1.41
2	b	493	TRP	CD2-CE2	5.18	1.47	1.41
3	C	266	TRP	CD2-CE2	5.16	1.47	1.41
3	C	63	TRP	CD2-CE2	5.13	1.47	1.41
2	b	167	TRP	CD2-CE2	5.12	1.47	1.41
4	D	280	TRP	CD2-CE2	5.12	1.47	1.41
2	B	257	TRP	CD2-CE2	5.11	1.47	1.41
10	K	39	TRP	CD2-CE2	5.10	1.47	1.41
4	D	14	TRP	CD2-CE2	5.10	1.47	1.41
4	d	280	TRP	CD2-CE2	5.09	1.47	1.41
1	A	278	TRP	CD2-CE2	5.08	1.47	1.41
1	a	169	SER	CA-CB	5.08	1.60	1.52
4	d	191	TRP	CD2-CE2	5.06	1.47	1.41
1	A	80	GLY	N-CA	5.05	1.53	1.46
1	a	317	TRP	CD2-CE2	5.05	1.47	1.41
3	c	359	TRP	CD2-CE2	5.03	1.47	1.41
1	a	278	TRP	CD2-CE2	5.02	1.47	1.41
4	d	14	TRP	CD2-CE2	5.02	1.47	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	272	ARG	NE-CZ-NH1	-7.88	116.36	120.30
13	o	152	ARG	NE-CZ-NH1	-7.53	116.54	120.30
2	B	357	ARG	NE-CZ-NH2	-7.36	116.62	120.30
3	C	153	ASP	CB-CG-OD1	7.03	124.63	118.30
4	D	100	ASP	CB-CG-OD2	7.02	124.62	118.30
3	C	153	ASP	CB-CG-OD2	-6.97	112.03	118.30
4	d	100	ASP	CB-CG-OD1	6.87	124.48	118.30
5	e	45	ASP	CB-CG-OD1	6.45	124.11	118.30
15	U	39	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	C	195	ASP	CB-CG-OD1	-6.39	112.55	118.30
3	C	195	ASP	CB-CG-OD2	6.16	123.84	118.30
1	a	342	ASP	CB-CG-OD1	6.08	123.77	118.30
3	C	343	ARG	NE-CZ-NH2	-5.91	117.34	120.30
3	C	473	ASP	CB-CG-OD2	5.88	123.60	118.30
4	D	329	MET	CG-SD-CE	5.83	109.54	100.20
16	v	105	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	b	357	ARG	NE-CZ-NH2	-5.67	117.46	120.30
13	o	169	ASP	CB-CG-OD2	5.67	123.41	118.30
13	o	69	LYS	CD-CE-NZ	-5.63	98.75	111.70
11	l	14	ARG	NE-CZ-NH1	-5.58	117.51	120.30
2	B	287[A]	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	B	287[B]	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	a	131	TRP	CA-CB-CG	-5.42	103.40	113.70
1	a	269	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	C	213	LEU	CB-CG-CD1	-5.40	101.82	111.00
4	d	126	MET	CG-SD-CE	-5.36	91.62	100.20
1	a	342	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	B	15	ASP	CB-CG-OD1	5.26	123.04	118.30
3	C	376	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	131	TRP	CA-CB-CG	-5.26	103.71	113.70
4	D	26	ARG	NE-CZ-NH2	-5.24	117.68	120.30
16	V	99	ASP	CB-CG-OD1	5.17	122.95	118.30
3	C	27	ASP	CB-CG-OD1	5.16	122.94	118.30
2	b	357	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2633	0	2544	37	0
1	a	2625	0	2538	0	0
2	B	4009	0	3879	59	0
2	b	3964	0	3817	0	0
3	C	3502	0	3431	43	0
3	c	3536	0	3460	0	0
4	D	2726	0	2629	45	0
4	d	2741	0	2654	0	0
5	E	657	0	637	22	0
5	e	639	0	617	0	0
6	F	274	0	279	7	0
6	f	257	0	269	0	0
7	H	498	0	518	7	0
7	h	498	0	518	0	0
8	I	294	0	304	6	0
8	i	311	0	326	0	0
9	J	251	0	257	5	0
9	j	271	0	270	0	0
10	K	290	0	294	7	0
10	k	286	0	285	0	0
11	L	302	0	316	7	0
11	l	300	0	314	0	0
12	M	261	0	280	21	0
12	m	271	0	293	0	0
13	O	1878	0	1853	34	0
13	o	1855	0	1823	0	0
14	T	256	0	256	4	0
14	t	256	0	256	0	0
15	U	770	0	769	6	0
15	u	772	0	766	0	0
16	V	1066	0	1075	12	0
16	v	1060	0	1053	0	0
17	Y	196	0	219	8	0
17	y	196	0	208	0	0
18	X	280	0	312	9	0
18	x	280	0	312	0	0
19	Z	459	0	484	7	0
19	z	431	0	438	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	10	0
23	B	1040	0	1152	61	0
23	C	845	0	936	36	0
23	D	130	0	144	7	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	128	0	148	5	0
24	a	128	0	148	0	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0
25	C	80	0	112	5	0
25	D	40	0	56	5	0
25	K	80	0	112	9	0
25	T	40	0	56	9	0
25	a	40	0	56	0	0
25	b	120	0	168	0	0
25	c	80	0	112	0	0
25	d	40	0	56	0	0
25	k	80	0	112	0	0
25	t	40	0	56	0	0
26	A	108	0	155	5	0
26	B	54	0	78	5	0
26	D	45	0	57	3	0
26	L	54	0	78	5	0
26	a	108	0	156	0	0
26	f	33	0	39	0	0
27	A	51	0	72	3	0
27	B	51	0	72	4	0
27	C	51	0	72	2	0
27	D	51	0	72	2	0
27	Z	51	0	72	0	0
27	a	51	0	72	0	0
27	b	51	0	72	0	0
27	c	102	0	144	0	0
27	d	51	0	72	0	0
28	A	55	0	80	10	0
28	D	55	0	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	69	0	0	0	0
29	B	56	0	0	4	0
29	C	34	0	0	0	0
29	D	56	0	0	2	0
29	E	27	0	0	0	0
29	H	10	0	0	0	0
29	I	24	0	0	0	0
29	J	26	0	0	0	0
29	L	14	0	0	1	0
29	M	16	0	0	1	0
29	T	13	0	0	0	0
29	X	16	0	0	1	0
29	Z	16	0	0	0	0
29	a	56	0	0	0	0
29	b	84	0	0	0	0
29	c	40	0	0	0	0
29	d	16	0	0	0	0
29	e	11	0	0	0	0
29	i	55	0	0	0	0
29	j	28	0	0	0	0
29	t	16	0	0	0	0
29	x	16	0	0	0	0
29	z	16	0	0	0	0
30	A	35	0	46	0	0
30	B	35	0	46	4	0
30	C	35	0	46	4	0
30	F	35	0	46	0	0
30	J	24	0	35	1	0
30	M	70	0	92	3	0
30	Z	35	0	46	3	0
30	a	35	0	46	0	0
30	b	49	0	70	0	0
30	c	35	0	46	0	0
30	m	70	0	92	0	0
30	t	24	0	35	0	0
30	z	32	0	36	0	0
31	A	18	0	22	4	0
31	B	36	0	48	3	0
31	C	18	0	24	4	0
31	D	6	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	L	6	0	8	1	0
31	O	6	0	8	0	0
31	V	18	0	24	0	0
31	a	18	0	24	0	0
31	b	30	0	40	0	0
31	c	24	0	32	0	0
31	f	6	0	6	0	0
31	h	6	0	8	0	0
31	l	6	0	8	0	0
31	v	18	0	24	0	0
32	B	1	0	0	0	0
32	F	1	0	0	0	0
32	O	1	0	0	0	0
32	b	1	0	0	0	0
32	c	1	0	0	0	0
32	f	1	0	0	0	0
32	o	1	0	0	0	0
33	B	95	0	130	3	0
33	C	38	0	52	1	0
33	D	19	0	26	2	0
33	O	19	0	26	0	0
33	U	9	0	15	1	0
33	V	13	0	11	0	0
33	b	76	0	104	0	0
33	c	38	0	52	0	0
33	d	19	0	26	0	0
33	u	14	0	19	0	0
34	C	186	0	246	2	0
34	D	53	0	71	9	0
34	H	62	0	82	1	0
34	c	186	0	246	0	0
34	d	50	0	69	0	0
34	h	62	0	82	0	0
35	D	4	0	0	0	0
35	a	4	0	0	0	0
36	D	144	0	213	24	0
36	E	49	0	74	3	0
36	L	49	0	74	2	0
36	a	40	0	53	0	0
36	d	147	0	222	0	0
36	l	49	0	74	0	0
37	F	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	V	43	0	30	1	0
37	f	43	0	30	0	0
37	v	43	0	30	0	0
38	H	41	0	56	4	0
38	h	41	0	56	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	O	5	0	0	0	0
41	A	170	0	0	1	0
41	B	319	0	0	4	0
41	C	263	0	0	4	0
41	D	161	0	0	2	0
41	E	35	0	0	4	0
41	F	12	0	0	0	0
41	H	52	0	0	0	0
41	I	8	0	0	0	0
41	J	9	0	0	0	0
41	K	8	0	0	1	0
41	L	24	0	0	0	0
41	M	16	0	0	1	0
41	O	202	0	0	5	0
41	T	10	0	0	0	0
41	U	100	0	0	2	0
41	V	144	0	0	3	0
41	X	14	0	0	0	0
41	Y	6	0	0	0	0
41	Z	1	0	0	0	0
41	a	155	0	0	0	0
41	b	306	0	0	0	0
41	c	245	0	0	0	0
41	d	160	0	0	0	0
41	e	22	0	0	0	0
41	f	14	0	0	0	0
41	h	53	0	0	0	0
41	i	14	0	0	0	0
41	j	9	0	0	0	0
41	k	5	0	0	0	0
41	l	18	0	0	0	0
41	m	16	0	0	0	0
41	o	175	0	0	0	0
41	t	12	0	0	0	0
41	u	106	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	v	104	0	0	0	0
41	x	6	0	0	0	0
41	y	7	0	0	0	0
41	z	2	0	0	0	0
All	All	54036	0	51777	461	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 6.

All (461) 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[A]:LEU:CD2	12:M:16[A]:LEU:HD23	0.97	1.49
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:CD2	0.00	1.21
36:D:409:LHG:H112	36:D:409:LHG:C38	13.80	1.17
26:L:103:SQD:H1	26:L:103:SQD:H462	1.28	1.12
36:D:409:LHG:H372	36:D:409:LHG:H131	13.21	1.10
1:A:214:MET:CG	28:A:414:PL9:H102	1.84	1.07
5:E:9:PRO:HA	36:E:101:LHG:HC32	1.32	1.07
1:A:214:MET:HG2	28:A:414:PL9:C10	1.84	1.06
36:D:409:LHG:H112	36:D:409:LHG:H381	14.54	1.04
13:O:33:ASP:OD1	13:O:35:SER:HB3	3.18	1.01
30:C:520:LMT:H6'1	8:I:26:GLY:HA3	1.42	0.99
26:B:621:SQD:H462	26:B:621:SQD:H1	1.44	0.99
12:M:16[A]:LEU:HD23	12:M:16[A]:LEU:HD21	1.58	0.99
31:C:524:GOL:H11	41:C:706:HOH:O	1.63	0.98
36:D:410:LHG:H152	36:D:410:LHG:C33	1.94	0.98
15:U:86:GLU:H	15:U:86:GLU:CD	1.66	0.97
23:B:615:CLA:H18	27:B:622:LMG:H421	1.46	0.96
1:A:214:MET:HG2	28:A:414:PL9:H102	0.98	0.96
23:B:617:CLA:C19	29:B:627:UNL:C16	2.43	0.96
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.48	0.94
31:A:423:GOL:H11	12:M:1:FME:HG2	59.12	0.90
36:D:410:LHG:H152	36:D:410:LHG:H332	1.54	0.89
12:M:16[A]:LEU:HD23	12:M:16[A]:LEU:HD23	0.00	0.88
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.75	0.87
12:M:16[A]:LEU:HD21	12:M:16[A]:LEU:HG	2.34	0.86
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.88	0.86
4:D:236:ASN:O	4:D:239:GLN:HG2	2.38	0.86
23:B:617:CLA:H191	29:B:627:UNL:C16	2.05	0.86
5:E:9:PRO:HA	36:E:101:LHG:C3	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:612:CLA:HMB1	23:B:612:CLA:HBB1	1.58	0.85
26:L:103:SQD:C1	26:L:103:SQD:H462	2.06	0.84
23:D:403:CLA:HBB1	23:D:403:CLA:HMB1	1.80	0.83
23:C:504:CLA:H201	36:D:410:LHG:C35	2.08	0.82
13:O:179:GLU:HG2	41:O:569:HOH:O	1.82	0.80
36:D:410:LHG:H152	36:D:410:LHG:H331	1.62	0.79
5:E:45:ASP:OD1	41:E:228[A]:HOH:O	1.99	0.79
25:T:101:BCR:HC8	25:T:101:BCR:H321	1.65	0.78
4:D:102:THR:OG1	34:D:406:DGD:HG31	1.82	0.78
3:C:279:LEU:HD12	3:C:282:MET:CE	2.33	0.78
12:M:16[A]:LEU:HD21	12:M:16[A]:LEU:CG	2.06	0.78
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.66	0.76
41:B:799:HOH:O	13:O:58:ASN:HA	64.81	0.76
31:D:415:GOL:H11	12:M:1:FME:HG2	1.67	0.75
36:D:409:LHG:H372	36:D:409:LHG:C13	12.99	0.75
36:D:409:LHG:H322	36:D:409:LHG:H151	7.02	0.75
26:L:103:SQD:H371	29:M:103:UNL:C16	2.17	0.75
2:B:503:THR:O	18:X:39:ARG:HG2	2.27	0.75
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.70	0.74
23:C:504:CLA:H191	36:D:410:LHG:C35	2.17	0.73
4:D:13:GLY:HA3	33:D:414:HTG:H62	1.69	0.73
23:C:512:CLA:HMB1	23:C:512:CLA:HBB1	1.71	0.73
23:C:506:CLA:HMC2	23:C:507:CLA:H102	1.71	0.73
23:A:406:CLA:HBB1	23:A:406:CLA:HMB1	1.71	0.72
2:B:462:PHE:CZ	23:B:616:CLA:HMB3	24.25	0.71
13:O:58:ASN:C	13:O:60:ARG:H	1.94	0.71
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:HD21	0.97	0.71
23:B:616:CLA:HMB1	23:B:616:CLA:HBB1	1.90	0.70
23:B:617:CLA:HED2	23:B:617:CLA:H43	1.73	0.70
23:A:405:CLA:HBB1	23:A:405:CLA:HMB1	1.72	0.70
26:B:621:SQD:C46	26:B:621:SQD:H1	2.21	0.70
36:D:409:LHG:C11	36:D:409:LHG:C38	14.58	0.70
23:B:617:CLA:H193	29:B:627:UNL:C16	2.22	0.70
23:B:606:CLA:C14	23:B:611:CLA:HED2	2.22	0.69
12:M:16[A]:LEU:CD2	12:M:16[A]:LEU:CG	1.52	0.69
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.75	0.69
34:D:406:DGD:HD4	5:E:45:ASP:HB3	1.73	0.69
16:V:2:GLU:HB2	41:V:384:HOH:O	40.09	0.69
3:C:320:ARG:HG3	31:C:524:GOL:H2	1.75	0.68
34:D:406:DGD:HD3	5:E:45:ASP:HB3	3.03	0.68
3:C:72:LEU:HD11	3:C:108:THR:HB	2.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:74[A]:GLU:OE1	41:O:550:HOH:O	2.11	0.68
1:A:183:MET:HA	23:A:405:CLA:HMD2	1.76	0.68
5:E:61:ARG:O	41:E:214[A]:HOH:O	2.10	0.67
34:D:406:DGD:O1B	34:D:406:DGD:O2D	2.13	0.67
5:E:60:GLN:O	41:E:214[B]:HOH:O	2.12	0.66
1:A:248[A]:ILE:HD11	4:D:237:PRO:O	1.96	0.66
25:D:404:BCR:H313	34:D:406:DGD:HAW1	5.23	0.66
1:A:248[A]:ILE:HD13	1:A:249:VAL:H	1.59	0.66
28:A:414:PL9:H403	6:F:22:ALA:HB2	1.78	0.65
23:B:611:CLA:HBB1	23:B:611:CLA:HHC	1.77	0.65
15:U:86:GLU:N	15:U:86:GLU:CD	2.46	0.65
23:C:506:CLA:H18	23:C:506:CLA:H122	1.76	0.65
25:K:102:BCR:C8	25:K:102:BCR:H331	2.25	0.65
23:C:511:CLA:HBB1	23:C:511:CLA:HMB1	1.78	0.65
4:D:14:TRP:CD1	33:D:414:HTG:H61	2.32	0.65
13:O:82:GLN:NE2	41:O:563:HOH:O	2.29	0.65
25:C:515:BCR:C8	25:C:515:BCR:H331	2.25	0.64
8:I:35:LYS:HB2	8:I:35:LYS:NZ	4.94	0.64
23:B:615:CLA:HBB1	23:B:615:CLA:HMB1	2.16	0.64
30:M:101:LMT:O6'	41:M:211[B]:HOH:O	2.15	0.64
4:D:85:MET:HE1	4:D:96:GLU:HG2	2.15	0.63
2:B:462:PHE:CE1	23:B:616:CLA:HMB3	23.63	0.63
10:K:24[A]:VAL:HG13	17:Y:25:ILE:HD13	1.81	0.62
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.33	0.62
23:C:506:CLA:HBB1	23:C:506:CLA:HMB1	1.81	0.62
13:O:203:LYS:HE3	41:O:584:HOH:O	2.00	0.62
4:D:85:MET:CE	4:D:96:GLU:HG2	2.53	0.62
26:B:621:SQD:H45	14:T:23:PHE:CD1	36.10	0.62
19:Z:15:LEU:HD22	19:Z:46:LEU:HD23	2.77	0.62
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.17	0.62
23:C:508:CLA:HBB1	23:C:508:CLA:HMB1	1.82	0.61
11:L:24[A]:ILE:CD1	12:M:18:PRO:HB2	2.30	0.61
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.35	0.61
23:A:410:CLA:HBB1	23:A:410:CLA:HMB1	2.12	0.61
24:A:409:PHO:HBB1	24:A:409:PHO:HMB1	1.83	0.61
10:K:24[A]:VAL:CG1	17:Y:25:ILE:HD13	2.31	0.61
9:J:9:PRO:HD2	9:J:12:ILE:HD12	2.09	0.60
31:A:423:GOL:H11	12:M:1:FME:CG	59.33	0.60
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.60
13:O:33:ASP:C	13:O:35:SER:H	2.60	0.60
4:D:272:LEU:C	4:D:272:LEU:HD23	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:404:BCR:C8	25:D:404:BCR:H331	2.41	0.59
23:C:513:CLA:HMB1	23:C:513:CLA:HBB1	1.83	0.59
23:B:617:CLA:HMB1	23:B:617:CLA:HBB1	1.84	0.59
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.99	0.59
13:O:42:ARG:O	13:O:241:ALA:HA	2.19	0.59
23:B:607:CLA:H43	23:B:608:CLA:H2	25.33	0.59
30:B:623:LMT:H122	29:D:412:UNL:C22	2.33	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.59
2:B:103:LEU:HD21	23:B:606:CLA:HMC3	1.84	0.58
2:B:467:ILE:HG13	4:D:126:MET:CE	2.33	0.58
26:A:412:SQD:H383	9:J:22:ILE:HD11	1.86	0.58
3:C:318:LEU:C	3:C:318:LEU:HD23	2.27	0.58
25:K:101:BCR:HC8	25:K:101:BCR:H321	1.90	0.58
30:C:520:LMT:C6B	8:I:26:GLY:HA3	2.28	0.58
5:E:61:ARG:HG3	41:E:214[B]:HOH:O	2.04	0.58
25:K:102:BCR:H331	25:K:102:BCR:HC8	1.86	0.58
1:A:259:ILE:HD12	28:A:414:PL9:C25	2.34	0.57
13:O:129:THR:HA	13:O:141:ASP:O	2.25	0.57
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.75	0.57
5:E:15:THR:HB	9:J:8:ILE:O	2.04	0.57
25:T:101:BCR:H23C	25:T:101:BCR:H382	1.87	0.57
30:C:520:LMT:H6'1	8:I:26:GLY:CA	2.27	0.56
4:D:12:ARG:HG3	4:D:17:ILE:HD11	4.27	0.56
23:A:410:CLA:H91	30:C:520:LMT:H123	1.88	0.56
30:Z:102:LMT:H2B	30:Z:102:LMT:O3'	2.05	0.56
24:A:408:PHO:HBB1	24:A:408:PHO:HMB1	1.87	0.56
34:D:406:DGD:HB21	34:D:406:DGD:HA22	1.86	0.56
19:Z:44:SER:O	19:Z:48:ILE:HG13	2.35	0.56
15:U:86:GLU:HG2	41:U:328:HOH:O	7.42	0.55
13:O:207:ARG:NH1	41:O:536:HOH:O	31.84	0.55
23:C:502:CLA:H193	33:C:521:HTG:H3'1	1.87	0.55
2:B:462:PHE:CE1	23:B:614:CLA:HMB3	2.42	0.55
3:C:203:THR:O	3:C:235:GLY:HA3	2.22	0.55
3:C:279:LEU:HD22	23:C:509:CLA:HED2	1.89	0.55
2:B:50:PRO:HB2	31:B:633:GOL:H12	26.53	0.55
36:D:410:LHG:H342	36:D:410:LHG:H302	1.89	0.54
23:C:513:CLA:HMD1	30:Z:102:LMT:H5'	1.88	0.54
3:C:391[A]:ARG:HD3	41:C:825[A]:HOH:O	2.05	0.54
23:B:612:CLA:H142	36:L:101:LHG:H361	1.90	0.54
31:A:423:GOL:C1	12:M:1:FME:HG2	59.91	0.54
2:B:446:SER:HB2	2:B:447:PRO:CD	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:B:956:HOH:O	12:M:6:LEU:HD12	28.85	0.54
6:F:15:ILE:HD12	6:F:15:ILE:H	4.07	0.54
25:K:101:BCR:C8	25:K:101:BCR:H311	2.37	0.54
33:U:201:HTG:H1'1	41:U:372:HOH:O	2.07	0.54
15:U:73:GLN:O	15:U:77:GLU:HG3	2.07	0.54
23:B:605:CLA:HMB1	23:B:605:CLA:HBB1	1.88	0.53
3:C:376:ASP:OD1	3:C:378[A]:ASN:HB3	2.08	0.53
23:B:607:CLA:HMD2	23:B:615:CLA:H203	35.85	0.53
4:D:123:ILE:HD11	34:H:102:DGD:HAE1	1.89	0.53
2:B:26:HIS:HB2	23:B:613:CLA:HMB2	1.90	0.53
2:B:237:VAL:HG12	23:B:615:CLA:HMD1	24.54	0.53
3:C:167:VAL:HG21	23:C:512:CLA:HHB	1.91	0.53
4:D:307:GLU:HG3	41:D:611:HOH:O	34.46	0.53
5:E:28:PRO:O	5:E:32:ILE:HG12	2.09	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
23:B:613:CLA:H203	23:B:613:CLA:H152	5.89	0.52
23:D:403:CLA:H192	18:X:15[A]:LEU:HD11	1.92	0.52
2:B:341:LYS:HZ1	33:B:626:HTG:C2	54.30	0.52
28:A:414:PL9:H502	4:D:39:PRO:HG3	1.91	0.52
3:C:429:SER:HB3	34:C:517:DGD:HBT2	1.92	0.52
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.06	0.52
26:A:412:SQD:H141	36:D:410:LHG:H172	1.91	0.52
23:A:407:CLA:HMD3	4:D:182:LEU:HD11	1.91	0.52
2:B:341:LYS:NZ	33:B:626:HTG:O2	54.23	0.52
23:C:501:CLA:H42	23:C:502:CLA:HMD1	1.91	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.52
31:D:415:GOL:C1	12:M:1:FME:HG2	2.38	0.51
25:B:619:BCR:C8	25:B:619:BCR:H331	2.39	0.51
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.93	0.51
2:B:223[A]:GLN:NE2	2:B:227:LYS:HD2	2.24	0.51
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.44	0.51
16:V:55[B]:ARG:NH1	41:V:357:HOH:O	22.75	0.51
4:D:266:TRP:CD1	36:D:408:LHG:HC31	9.37	0.51
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.91	0.51
2:B:266:GLU:HB3	31:B:635:GOL:H31	1.92	0.51
2:B:286:ARG:HH11	2:B:286:ARG:HG2	1.76	0.51
31:C:524:GOL:H12	37:V:201:HEM:HMD1	1.93	0.51
13:O:49[B]:THR:OG1	13:O:236:GLN:HB2	2.11	0.51
23:B:607:CLA:H202	33:B:631:HTG:H61	1.92	0.51
23:C:510:CLA:H192	23:C:510:CLA:HBC3	1.93	0.51
5:E:8:ARG:HB3	5:E:13:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:334:PRO:HA	13:O:153:THR:OG1	2.11	0.51
23:B:611:CLA:H203	23:B:611:CLA:H151	1.93	0.51
2:B:79:SER:HB3	2:B:86:ILE:HG12	2.06	0.51
10:K:21:LEU:HB2	17:Y:24:MET:HE2	5.96	0.51
2:B:248:ALA:HA	23:B:604:CLA:H42	1.93	0.50
4:D:102:THR:OG1	34:D:406:DGD:HD1	2.11	0.50
23:C:512:CLA:H121	23:C:513:CLA:H142	1.93	0.50
27:C:519:LMG:O10	30:J:102:LMT:H42	2.10	0.50
5:E:27:ILE:HG12	37:F:101:HEM:HMC3	1.92	0.50
13:O:58:ASN:C	13:O:60:ARG:N	2.63	0.50
23:C:505:CLA:HMD2	25:C:515:BCR:H343	1.92	0.50
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.27	0.50
27:D:411:LMG:H412	6:F:30:THR:HG21	1.93	0.50
3:C:381:LYS:NZ	13:O:99[A]:ASP:OD2	2.32	0.50
3:C:78:GLU:OE2	16:V:106[A]:ASN:ND2	2.34	0.50
16:V:106[B]:ASN:ND2	41:V:432:HOH:O	2.42	0.50
4:D:101:PHE:HB3	34:D:406:DGD:HG2	1.94	0.49
8:I:29:ALA:O	8:I:35:LYS:HG2	2.12	0.49
4:D:236:ASN:OD1	4:D:237:PRO:HD2	2.60	0.49
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.94	0.49
13:O:23:ASP:HB3	13:O:25:THR:HG23	1.94	0.49
1:A:11:ALA:HB1	1:A:15:GLU:HB3	1.94	0.49
2:B:162:PHE:O	23:B:609:CLA:HHD	33.29	0.49
23:A:405:CLA:CBD	23:A:406:CLA:HAC2	2.42	0.49
17:Y:42:ARG:HD2	19:Z:29:SER:OG	4.76	0.49
1:A:96:ILE:HD12	23:A:410:CLA:HMD1	1.94	0.49
27:A:413:LMG:H111	3:C:218:PHE:HE2	1.77	0.49
25:C:514:BCR:C8	25:C:514:BCR:H331	2.43	0.49
2:B:237:VAL:HG11	23:B:613:CLA:H201	12.93	0.49
7:H:38:PHE:HB2	38:H:101:RRX:C10	2.57	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
4:D:101:PHE:H	34:D:406:DGD:HA22	4.36	0.49
25:K:101:BCR:HC8	25:K:101:BCR:H311	1.95	0.49
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.95	0.49
36:D:409:LHG:H112	36:D:409:LHG:C37	12.95	0.49
11:L:24[A]:ILE:HD13	12:M:18:PRO:HB2	1.93	0.49
16:V:102:PRO:HA	16:V:105:ARG:HG3	2.59	0.49
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.41	0.48
2:B:324:LEU:HA	4:D:293[A]:LEU:HG	2.13	0.48
13:O:33:ASP:O	13:O:35:SER:N	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:TRP:HB3	3:C:391[B]:ARG:HG2	2.24	0.48
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.53	0.48
1:A:263:ALA:HA	36:E:101:LHG:H291	1.95	0.48
18:X:21:LEU:HD11	29:X:101:UNL:C16	3.29	0.48
1:A:63:ILE:HB	3:C:335:THR:HG21	1.94	0.48
2:B:467:ILE:HG13	4:D:126:MET:HE2	1.95	0.48
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.56	0.48
2:B:12:LEU:HB2	23:B:615:CLA:HMC2	14.44	0.48
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.96	0.48
26:B:621:SQD:O7	11:L:7:ARG:NH1	2.47	0.48
23:B:614:CLA:H72	23:B:614:CLA:H112	1.64	0.47
3:C:437:PHE:CE1	23:C:510:CLA:HMB3	2.48	0.47
23:C:503:CLA:HMB1	23:C:503:CLA:HBB1	1.96	0.47
34:C:517:DGD:HB22	27:C:519:LMG:H302	1.96	0.47
23:B:617:CLA:H171	25:B:620:BCR:H331	1.96	0.47
23:B:609:CLA:HBB1	23:B:609:CLA:HMB1	1.95	0.47
7:H:39:LEU:C	7:H:39:LEU:HD23	2.49	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.47
26:L:103:SQD:H341	26:L:103:SQD:H311	1.56	0.47
24:A:408:PHO:ND	24:A:408:PHO:NC	2.62	0.47
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.78	0.47
13:O:110:MET:HG3	13:O:114:GLU:HB3	1.95	0.47
13:O:33:ASP:C	13:O:35:SER:N	3.02	0.47
13:O:15:LEU:HD23	13:O:18:LYS:HD2	1.95	0.47
1:A:11:ALA:HA	1:A:15:GLU:OE1	3.48	0.47
31:D:415:GOL:H11	12:M:1:FME:CG	2.39	0.47
12:M:1:FME:HCN	30:M:101:LMT:O6B	18.16	0.47
1:A:248[A]:ILE:HD13	1:A:249:VAL:N	2.26	0.47
23:A:406:CLA:H162	23:A:406:CLA:H203	1.46	0.47
23:C:511:CLA:H191	30:Z:102:LMT:H122	1.97	0.47
1:A:313:VAL:O	31:A:422:GOL:H31	2.15	0.47
23:B:612:CLA:NC	38:H:101:RRX:H56	25.21	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
3:C:60:ILE:HG22	23:C:503:CLA:HHD	1.97	0.47
23:B:617:CLA:H91	23:B:617:CLA:H112	1.72	0.46
26:A:418:SQD:H212	25:T:101:BCR:H323	1.96	0.46
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	2.50	0.46
2:B:237:VAL:HG12	23:B:613:CLA:HMD1	1.96	0.46
2:B:451:PHE:CZ	23:B:605:CLA:HED1	2.51	0.46
31:C:524:GOL:C1	41:C:706:HOH:O	2.38	0.46
11:L:14:ARG:HH12	26:L:103:SQD:H3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TYR:CZ	1:A:248[A]:ILE:HG22	2.50	0.46
2:B:493:TRP:HB3	5:E:5:THR:HG23	1.97	0.46
23:B:613:CLA:H203	23:B:613:CLA:C15	5.02	0.46
25:T:101:BCR:H321	25:T:101:BCR:C8	2.42	0.46
23:C:504:CLA:C20	36:D:410:LHG:C35	2.87	0.46
5:E:61:ARG:HH12	16:V:127:GLY:HA3	2.70	0.46
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.56	0.46
23:B:602:CLA:CBB	23:B:602:CLA:HHC	2.46	0.46
25:T:101:BCR:HC8	25:T:101:BCR:H311	2.18	0.46
5:E:60:GLN:HB2	5:E:60:GLN:HE21	4.41	0.46
23:B:605:CLA:H43	23:B:606:CLA:H2	1.98	0.45
27:B:622:LMG:H242	4:D:284:ILE:HD13	1.97	0.45
25:K:102:BCR:H11C	25:K:102:BCR:H341	1.77	0.45
6:F:21:VAL:O	6:F:25:THR:HG23	2.39	0.45
4:D:24:ARG:NH2	18:X:35:ASP:O	4.34	0.45
4:D:283:ALA:O	4:D:287:VAL:HG23	2.16	0.45
23:A:405:CLA:HBD	23:A:406:CLA:HAC2	1.98	0.45
3:C:377:LEU:HG	3:C:381:LYS:HE3	3.17	0.45
1:A:298:ASN:ND2	41:A:636:HOH:O	33.52	0.45
36:D:410:LHG:H342	36:D:410:LHG:C30	2.47	0.45
24:A:409:PHO:HBC2	24:A:409:PHO:HHD	1.98	0.45
2:B:71:VAL:HG23	23:B:607:CLA:HMA2	1.97	0.45
26:A:412:SQD:H211	26:A:412:SQD:H181	1.61	0.45
23:B:606:CLA:HAB	23:B:608:CLA:H171	34.16	0.45
3:C:149:TYR:CZ	23:C:509:CLA:H191	2.52	0.45
13:O:58:ASN:O	13:O:60:ARG:N	2.46	0.45
3:C:318:LEU:O	3:C:318:LEU:HD23	2.30	0.45
23:B:611:CLA:CBB	23:B:611:CLA:HHC	2.45	0.45
25:B:620:BCR:C8	25:B:620:BCR:H331	2.47	0.45
36:D:410:LHG:C15	36:D:410:LHG:H331	2.40	0.45
23:C:511:CLA:HBD	23:C:511:CLA:HAA1	1.98	0.45
2:B:266:GLU:HB3	31:B:633:GOL:H31	25.17	0.45
2:B:224:ARG:HH21	30:B:623:LMT:H2'	1.82	0.45
2:B:248:ALA:HA	23:B:606:CLA:H42	8.71	0.45
18:X:27:VAL:O	18:X:31:ILE:HG13	2.22	0.45
23:D:403:CLA:H161	7:H:37:LEU:HD21	7.82	0.45
8:I:35:LYS:HZ2	8:I:35:LYS:HB2	4.98	0.45
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.18	0.45
24:A:409:PHO:NC	24:A:409:PHO:ND	2.65	0.45
13:O:39:ARG:HG3	13:O:246:ALA:HB2	3.40	0.45
4:D:52:THR:O	4:D:66:SER:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:617:CLA:H62	23:B:617:CLA:H41	3.01	0.44
2:B:461:LEU:HD22	36:D:408:LHG:H301	1.99	0.44
25:T:101:BCR:C23	25:T:101:BCR:H382	2.53	0.44
41:C:822:HOH:O	13:O:149:PRO:HB2	2.17	0.44
4:D:293[B]:LEU:HD23	4:D:293[B]:LEU:HA	2.10	0.44
28:A:414:PL9:H202	28:A:414:PL9:H162	1.98	0.44
23:B:615:CLA:C9	30:M:101:LMT:H112	11.89	0.44
13:O:39:ARG:HB2	13:O:83:GLY:O	2.17	0.44
31:L:104:GOL:H2	14:T:25:GLU:HB3	1.98	0.44
13:O:93:LEU:O	13:O:128:SER:HA	2.23	0.44
2:B:36[A]:SER:OG	25:B:619:BCR:H362	2.18	0.44
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.99	0.44
1:A:12:ASN:HB3	1:A:15:GLU:HB3	5.22	0.44
23:B:604:CLA:HMB1	23:B:604:CLA:HBB1	1.99	0.44
30:B:623:LMT:C12	29:D:412:UNL:C22	2.95	0.44
3:C:377:LEU:O	3:C:381:LYS:HG3	2.18	0.44
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.52	0.44
2:B:224:ARG:HD2	41:B:894:HOH:O	2.16	0.44
4:D:266:TRP:CD1	36:D:409:LHG:HC31	2.53	0.44
6:F:31:ILE:HG13	37:F:101:HEM:HMC1	2.00	0.44
26:B:621:SQD:H442	26:B:621:SQD:O9	2.18	0.44
3:C:41:ARG:NH1	23:C:511:CLA:HMD1	2.33	0.44
29:B:628:UNL:C6	41:B:913:HOH:O	65.42	0.44
27:A:413:LMG:H111	3:C:218:PHE:CE2	2.53	0.43
2:B:228:ALA:HB2	30:B:623:LMT:H21	2.00	0.43
23:C:504:CLA:C19	36:D:410:LHG:C35	2.94	0.43
23:B:612:CLA:HMB2	23:B:613:CLA:C2B	4.08	0.43
36:D:410:LHG:H132	36:D:410:LHG:H332	2.01	0.43
4:D:24:ARG:NH1	41:D:643:HOH:O	2.51	0.43
19:Z:46:LEU:O	19:Z:49:ALA:HB3	2.76	0.43
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.55	0.43
10:K:46:ARG:NH1	41:K:207:HOH:O	2.50	0.43
27:B:622:LMG:H332	11:L:35:PHE:CE2	2.53	0.43
28:A:414:PL9:H512	26:D:407:SQD:H301	1.98	0.43
5:E:8:ARG:HA	5:E:9:PRO:HD3	2.17	0.43
11:L:24[A]:ILE:HD11	12:M:18:PRO:HB2	1.98	0.43
13:O:180:GLU:CD	13:O:180:GLU:H	2.22	0.43
23:D:403:CLA:HBB1	23:D:403:CLA:CMB	2.61	0.43
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.48	0.43
3:C:275:SER:HB3	23:C:509:CLA:HED3	1.99	0.43
23:D:403:CLA:CBB	23:D:403:CLA:HMB1	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:39:ARG:HG2	13:O:246:ALA:HB2	2.01	0.43
1:A:121[B]:LEU:HG	27:A:413:LMG:H181	2.00	0.43
23:B:616:CLA:OBD	23:B:617:CLA:HHC	5.99	0.43
23:B:609:CLA:H161	23:B:609:CLA:H141	1.91	0.43
19:Z:31:GLN:O	19:Z:33:TRP:N	2.52	0.43
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.35	0.43
25:T:101:BCR:C38	25:T:101:BCR:C23	2.99	0.43
11:L:7:ARG:HH12	29:L:102:UNL:C4	2.32	0.43
17:Y:26:ALA:O	17:Y:30:ILE:HB	2.51	0.43
1:A:214:MET:CE	1:A:255:PHE:CE1	4.93	0.43
38:H:101:RRX:H46	38:H:101:RRX:H55	2.02	0.43
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.01	0.43
23:D:403:CLA:H162	7:H:33:VAL:HG13	10.84	0.43
25:K:101:BCR:C23	25:K:101:BCR:H382	2.62	0.43
2:B:156:PHE:HB3	2:B:162:PHE:HB3	2.30	0.43
2:B:462:PHE:CZ	23:B:614:CLA:HMB3	2.53	0.43
23:B:607:CLA:HBB1	23:B:607:CLA:HMB1	2.01	0.43
19:Z:8:ALA:O	19:Z:11:ALA:HB3	2.48	0.43
1:A:259:ILE:HD12	28:A:414:PL9:H251	2.00	0.42
2:B:61:PHE:CE1	23:B:610:CLA:HMB3	26.36	0.42
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.01	0.42
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.14	0.42
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.49	0.42
1:A:331:MET:SD	4:D:347:PRO:HB2	2.73	0.42
23:C:510:CLA:HBB1	23:C:510:CLA:HMB1	1.99	0.42
1:A:248[A]:ILE:CD1	4:D:237:PRO:O	2.67	0.42
1:A:215:HIS:ND1	28:A:414:PL9:O1	2.42	0.42
25:B:619:BCR:H363	25:T:101:BCR:H19C	35.17	0.42
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.75	0.42
23:C:501:CLA:H192	23:C:506:CLA:C1B	2.49	0.42
26:D:407:SQD:H241	18:X:31:ILE:HD13	2.01	0.42
5:E:8:ARG:HH21	5:E:12:ASP:HB3	2.98	0.42
3:C:302:TYR:O	3:C:422:PRO:HD2	2.59	0.42
3:C:179:ALA:O	3:C:184:GLY:HA2	2.30	0.42
3:C:390:ARG:HD3	16:V:90:GLU:O	2.19	0.42
12:M:28:GLN:O	12:M:32:GLN:HG3	2.19	0.42
38:H:101:RRX:H36	38:H:101:RRX:H40	1.86	0.42
25:D:404:BCR:C38	27:D:411:LMG:H231	2.50	0.42
25:A:411:BCR:C8	25:A:411:BCR:H331	2.48	0.42
23:B:612:CLA:HMB1	23:B:612:CLA:CBB	2.41	0.42
26:A:412:SQD:H271	36:D:410:LHG:H162	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:TRP:HD1	5:E:5:THR:CG2	2.32	0.42
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.02	0.42
4:D:61:HIS:HB3	4:D:63:LEU:HG	2.19	0.42
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.42
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.51	0.42
1:A:12:ASN:O	1:A:16:ARG:HG3	2.48	0.42
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.08	0.42
4:D:209:LEU:HD23	4:D:209:LEU:C	2.40	0.42
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.01	0.41
25:D:404:BCR:H11C	25:D:404:BCR:H341	1.99	0.41
3:C:279:LEU:HA	3:C:282:MET:HE3	2.34	0.41
4:D:61:HIS:CE1	4:D:168:PHE:CE2	3.08	0.41
5:E:14:ILE:HD12	9:J:13:VAL:HG11	2.09	0.41
2:B:270:PRO:HG2	2:B:317:ASN:O	2.36	0.41
3:C:471:SER:HB3	3:C:473:ASP:OXT	2.19	0.41
5:E:13:ILE:HG21	37:F:101:HEM:HAD2	2.08	0.41
2:B:90:PHE:CE1	23:B:609:CLA:H162	46.96	0.41
4:D:192:THR:HG23	23:D:402:CLA:HBC2	2.25	0.41
13:O:20:PRO:HB2	13:O:240:TYR:CD1	2.56	0.41
23:B:606:CLA:H41	23:B:606:CLA:H62	1.80	0.41
23:B:617:CLA:H41	23:B:617:CLA:H61	1.76	0.41
23:C:506:CLA:HMB2	23:C:507:CLA:NB	2.36	0.41
3:C:95:LEU:HD21	23:C:501:CLA:OBD	2.21	0.41
2:B:498:LYS:HA	4:D:24:ARG:HA	2.23	0.41
2:B:103:LEU:HD21	23:B:608:CLA:HMC3	16.02	0.41
36:D:409:LHG:H272	36:D:409:LHG:H242	4.29	0.41
16:V:122:GLU:HG3	16:V:126:LEU:HD12	2.22	0.41
23:B:615:CLA:H161	27:B:622:LMG:C43	2.51	0.41
3:C:377:LEU:HG	3:C:381:LYS:HE2	2.02	0.41
2:B:349:LYS:HE2	2:B:349:LYS:HB3	1.91	0.41
23:B:617:CLA:H11	23:B:617:CLA:H43	4.62	0.41
25:D:404:BCR:H361	25:D:404:BCR:H20C	1.86	0.41
3:C:276:LEU:HD21	23:C:508:CLA:CAB	2.51	0.41
3:C:390:ARG:HD3	16:V:100:ILE:HD12	2.11	0.41
25:A:411:BCR:H351	25:A:411:BCR:H15C	1.93	0.41
25:K:101:BCR:C23	25:K:101:BCR:C38	3.11	0.41
2:B:278:SER:HB3	2:B:281:GLN:HE21	1.86	0.41
23:B:605:CLA:H161	23:B:605:CLA:H141	1.89	0.41
37:F:101:HEM:CMB	37:F:101:HEM:HBB2	2.57	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.21	0.41
3:C:173:LEU:HD23	3:C:173:LEU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:29:ILE:O	14:T:30:THR:CB	3.22	0.41
13:O:133:VAL:O	13:O:133:VAL:HG12	2.30	0.41
4:D:296:TYR:CE2	4:D:319:LEU:HD22	2.81	0.41
13:O:33:ASP:OD1	13:O:35:SER:CB	3.29	0.40
18:X:15[A]:LEU:HA	18:X:15[A]:LEU:HD23	1.85	0.40
17:Y:27:MET:HE2	17:Y:27:MET:HB3	1.97	0.40
3:C:240:ILE:HD13	3:C:240:ILE:HA	2.02	0.40
3:C:213:LEU:HD11	25:C:515:BCR:C20	2.52	0.40
26:D:407:SQD:H321	18:X:24:THR:HA	2.03	0.40
3:C:78:GLU:CD	16:V:106[A]:ASN:HD21	2.21	0.40
36:L:101:LHG:H142	36:L:101:LHG:H171	1.93	0.40
2:B:262:THR:C	2:B:264:PRO:HD3	2.42	0.40
2:B:159:THR:O	2:B:180:PRO:HB3	2.22	0.40
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.03	0.40
16:V:123:PRO:HD3	16:V:130:TRP:CD1	2.69	0.40
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.03	0.40
1:A:246:TYR:CE2	1:A:248[A]:ILE:HG22	2.56	0.40
25:C:515:BCR:C33	25:C:515:BCR:C8	2.97	0.40
25:K:102:BCR:H371	25:K:102:BCR:H24C	1.88	0.40
15:U:68:THR:O	15:U:72:LYS:HG3	2.21	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	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	46 35
1	a	336/344 (98%)	329 (98%)	7 (2%)	0	100 100
2	B	512/504 (102%)	503 (98%)	9 (2%)	0	100 100
2	b	508/504 (101%)	497 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	452/455 (99%)	442 (98%)	9 (2%)	1 (0%)	52 42
3	c	457/455 (100%)	442 (97%)	13 (3%)	2 (0%)	39 27
4	D	339/342 (99%)	332 (98%)	7 (2%)	0	100 100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100 100
5	E	79/83 (95%)	78 (99%)	1 (1%)	0	100 100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100 100
6	F	32/44 (73%)	32 (100%)	0	0	100 100
6	f	30/44 (68%)	30 (100%)	0	0	100 100
7	H	61/63 (97%)	57 (93%)	4 (7%)	0	100 100
7	h	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	12 3
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100 100
8	i	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2 0
9	J	34/40 (85%)	34 (100%)	0	0	100 100
9	j	37/40 (92%)	35 (95%)	2 (5%)	0	100 100
10	K	36/37 (97%)	36 (100%)	0	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	37/37 (100%)	37 (100%)	0	0	100 100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100 100
12	m	34/36 (94%)	34 (100%)	0	0	100 100
13	O	247/244 (101%)	238 (96%)	8 (3%)	1 (0%)	39 27
13	o	242/244 (99%)	232 (96%)	9 (4%)	1 (0%)	39 27
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100 100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100 100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100 100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100 100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100 100
16	v	136/137 (99%)	129 (95%)	7 (5%)	0	100 100
17	Y	25/30 (83%)	25 (100%)	0	0	100 100
17	y	26/30 (87%)	25 (96%)	1 (4%)	0	100 100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	3 0
19	z	58/62 (94%)	50 (86%)	5 (9%)	3 (5%)	2 0
All	All	5224/5344 (98%)	5075 (97%)	134 (3%)	15 (0%)	46 35

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
19	Z	31	GLN
19	Z	32	ASP
8	i	36	ASP
19	z	31	GLN
3	C	416	SER
19	Z	2	THR
3	c	416[A]	SER
3	c	416[B]	SER
19	z	3	ILE
19	z	32	ASP
8	i	34	ARG
13	o	34	SER
7	h	63	LYS
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	272/279 (98%)	267 (98%)	5 (2%)	66 61
1	a	271/279 (97%)	269 (99%)	2 (1%)	88 88
2	B	407/402 (101%)	404 (99%)	3 (1%)	88 88
2	b	399/402 (99%)	393 (98%)	6 (2%)	72 69
3	C	355/356 (100%)	347 (98%)	8 (2%)	58 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	c	358/356 (101%)	349 (98%)	9 (2%)	55 47
4	D	275/276 (100%)	273 (99%)	2 (1%)	88 88
4	d	278/276 (101%)	274 (99%)	4 (1%)	74 71
5	E	71/72 (99%)	70 (99%)	1 (1%)	74 71
5	e	68/72 (94%)	66 (97%)	2 (3%)	50 40
6	F	27/38 (71%)	26 (96%)	1 (4%)	41 29
6	f	26/38 (68%)	25 (96%)	1 (4%)	40 28
7	H	53/53 (100%)	52 (98%)	1 (2%)	65 59
7	h	53/53 (100%)	52 (98%)	1 (2%)	65 59
8	I	31/34 (91%)	31 (100%)	0	100 100
8	i	33/34 (97%)	32 (97%)	1 (3%)	48 38
9	J	23/28 (82%)	23 (100%)	0	100 100
9	j	25/28 (89%)	25 (100%)	0	100 100
10	K	29/30 (97%)	29 (100%)	0	100 100
10	k	28/30 (93%)	27 (96%)	1 (4%)	42 30
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	34/35 (97%)	34 (100%)	0	100 100
12	M	29/32 (91%)	29 (100%)	0	100 100
12	m	30/32 (94%)	30 (100%)	0	100 100
13	O	207/207 (100%)	203 (98%)	4 (2%)	65 59
13	o	206/207 (100%)	203 (98%)	3 (2%)	72 69
14	T	25/28 (89%)	24 (96%)	1 (4%)	38 26
14	t	25/28 (89%)	24 (96%)	1 (4%)	38 26
15	U	83/89 (93%)	81 (98%)	2 (2%)	57 49
15	u	83/89 (93%)	83 (100%)	0	100 100
16	V	116/117 (99%)	116 (100%)	0	100 100
16	v	115/117 (98%)	114 (99%)	1 (1%)	84 83
17	Y	19/23 (83%)	18 (95%)	1 (5%)	28 16
17	y	18/23 (78%)	16 (89%)	2 (11%)	8 2
18	X	30/33 (91%)	30 (100%)	0	100 100
18	x	30/33 (91%)	29 (97%)	1 (3%)	45 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	Z	47/52 (90%)	46 (98%)	1 (2%)	61 55
19	z	40/52 (77%)	38 (95%)	2 (5%)	30 18
All	All	4253/4368 (97%)	4186 (98%)	67 (2%)	72 66

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	229	GLU
1	A	244	GLU
1	A	248[A]	ILE
1	A	248[B]	ILE
2	B	53	ASN
2	B	467	ILE
2	B	472	ARG
3	C	104	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	391[A]	ARG
3	C	391[B]	ARG
3	C	418	ASN
3	C	471	SER
4	D	90	LEU
4	D	180	ARG
5	E	4	THR
6	F	44	GLN
7	H	49	TYR
13	O	59	LYS
13	O	110	MET
13	O	118	LEU
13	O	207	ARG
14	T	2	GLU
15	U	24	LYS
15	U	70	ARG
17	Y	27	MET
19	Z	6	GLN
1	a	244	GLU
1	a	261	GLN
2	b	246	PHE
2	b	362	PHE

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Mol	Chain	Res	Type
2	b	373	LYS
2	b	472	ARG
2	b	476	ARG
2	b	479	PHE
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	355	THR
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN
4	d	24	ARG
4	d	150	ILE
4	d	180	ARG
4	d	329	MET
5	e	60	GLN
5	e	62	SER
6	f	15	ILE
7	h	49	TYR
8	i	38	GLU
10	k	27	VAL
13	o	54	GLU
13	o	64	GLU
13	o	118	LEU
14	t	2	GLU
16	v	23	GLU
17	y	30	ILE
17	y	41	VAL
18	x	39	ARG
19	z	3	ILE
19	z	29	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
2	B	53	ASN
2	B	281	GLN
2	B	331	ASN
2	B	497	GLN

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Mol	Chain	Res	Type
3	C	311	GLN
11	L	6	ASN
13	O	82	GLN
13	O	104	GLN
16	V	34	GLN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
2	b	338	GLN
3	c	311	GLN
4	d	332	GLN
13	o	36	GLN
13	o	82	GLN
13	o	104	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

10 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	$\#\|Z\|>2$
4	HSK	D	336[A]	-	5,10,12	0.49	0	3,12,16	2.04	2 (66%)
4	HSK	D	336[B]	-	6,11,12	0.74	0	5,14,16	2.89	3 (60%)
8	FME	I	1	8	8,9,10	0.62	0	6,9,11	1.35	0
12	FME	M	1	12	8,9,10	0.77	0	6,9,11	1.81	2 (33%)
14	FME	T	1	14	8,9,10	0.47	0	6,9,11	1.50	2 (33%)
4	HSK	d	336[A]	-	5,10,12	0.51	0	3,12,16	1.83	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HSK	d	336[B]	-	6,11,12	0.70	0	5,14,16	3.01	4 (80%)
8	FME	i	1	8	8,9,10	0.41	0	6,9,11	1.56	3 (50%)
12	FME	m	1	12	8,9,10	0.77	0	6,9,11	2.09	3 (50%)
14	FME	t	1	14	8,9,10	0.77	0	6,9,11	1.97	2 (33%)

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
4	HSK	D	336[A]	-	-	0/4/6/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/4/6/8	0/1/1/1
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
4	HSK	d	336[A]	-	-	0/4/6/8	0/1/1/1
4	HSK	d	336[B]	-	-	0/4/6/8	0/1/1/1
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	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 (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O1-CN-N	-3.70	119.43	124.76
12	m	1	FME	O1-CN-N	-2.44	121.24	124.76
8	i	1	FME	O-C-CA	-2.42	119.04	125.44
4	d	336[B]	HSK	CD2-CG-ND1	-2.33	104.96	108.24
14	t	1	FME	O-C-CA	-2.31	119.35	125.44
14	T	1	FME	O-C-CA	-2.28	119.41	125.44
4	d	336[A]	HSK	OXT-C-CA	-2.19	119.78	125.49
4	d	336[B]	HSK	OXT-C-CA	-2.18	119.82	125.49
4	D	336[A]	HSK	OXT-C-CA	-2.10	120.03	125.49
14	T	1	FME	O1-CN-N	-2.03	121.84	124.76
4	D	336[B]	HSK	OXT-C-CA	-2.03	120.21	125.49
8	i	1	FME	CG-CB-CA	-2.03	107.11	113.06
8	i	1	FME	O1-CN-N	-2.02	121.85	124.76
4	D	336[A]	HSK	CD2-NE2-CE1	2.45	109.58	105.71
4	d	336[B]	HSK	CD2-NE2-CE1	2.46	109.58	105.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	336[B]	HSK	CD2-NE2-CE1	2.48	109.62	105.71
12	m	1	FME	CE-SD-CG	2.48	108.84	100.37
12	m	1	FME	CG-CB-CA	2.60	120.69	113.06
12	M	1	FME	CG-CB-CA	2.63	120.80	113.06
12	M	1	FME	CE-SD-CG	2.97	110.49	100.37
4	D	336[B]	HSK	CE1-ND1-CG	5.18	112.47	104.70
4	d	336[B]	HSK	CE1-ND1-CG	5.34	112.71	104.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	7	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 276 ligands modelled in this entry, 43 are unknown and 15 are monoatomic - leaving 218 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	OEX	A	401	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
23	CLA	A	405	-	55,73,73	1.67	11 (20%)	61,113,113	1.96	18 (29%)
23	CLA	A	406	41	55,73,73	1.68	12 (21%)	61,113,113	2.57	24 (39%)
23	CLA	A	407	41	55,73,73	1.49	9 (16%)	61,113,113	2.21	17 (27%)
24	PHO	A	408	-	67,69,69	1.69	11 (16%)	84,99,99	2.16	23 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	PHO	A	409	-	67,69,69	1.86	13 (19%)	84,99,99	2.16	26 (30%)
23	CLA	A	410	-	55,73,73	1.69	11 (20%)	61,113,113	2.17	17 (27%)
25	BCR	A	411	-	41,41,41	1.01	0	56,56,56	1.49	11 (19%)
26	SQD	A	412	-	53,54,54	1.35	3 (5%)	61,65,65	2.50	16 (26%)
27	LMG	A	413	-	51,51,55	0.96	2 (3%)	59,59,63	1.32	4 (6%)
28	PL9	A	414	-	55,55,55	1.00	3 (5%)	68,69,69	1.58	13 (19%)
26	SQD	A	418	-	53,54,54	1.35	3 (5%)	61,65,65	1.88	12 (19%)
30	LMT	A	419	-	36,36,36	0.81	1 (2%)	47,47,47	1.39	5 (10%)
31	GOL	A	421	-	5,5,5	0.84	0	5,5,5	0.51	0
31	GOL	A	422	-	5,5,5	0.39	0	5,5,5	0.53	0
31	GOL	A	423	32	5,5,5	0.34	0	5,5,5	0.72	0
23	CLA	B	602	41	55,73,73	1.88	13 (23%)	61,113,113	2.19	15 (24%)
23	CLA	B	603	-	55,73,73	1.86	11 (20%)	61,113,113	1.78	14 (22%)
23	CLA	B	604	-	55,73,73	1.70	11 (20%)	61,113,113	2.54	19 (31%)
23	CLA	B	605	-	55,73,73	1.46	10 (18%)	61,113,113	2.27	18 (29%)
23	CLA	B	606	-	55,73,73	1.64	9 (16%)	61,113,113	2.00	16 (26%)
23	CLA	B	607	-	55,73,73	1.80	11 (20%)	61,113,113	2.17	14 (22%)
23	CLA	B	608	41	55,73,73	1.69	12 (21%)	61,113,113	1.93	17 (27%)
23	CLA	B	609	-	55,73,73	1.52	9 (16%)	61,113,113	2.44	17 (27%)
23	CLA	B	610	-	55,73,73	1.57	10 (18%)	61,113,113	2.09	15 (24%)
23	CLA	B	611	41	55,73,73	1.73	12 (21%)	61,113,113	2.12	17 (27%)
23	CLA	B	612	-	55,73,73	1.39	10 (18%)	61,113,113	2.38	18 (29%)
23	CLA	B	613	-	55,73,73	1.59	11 (20%)	61,113,113	1.95	16 (26%)
23	CLA	B	614	-	55,73,73	1.57	12 (21%)	61,113,113	1.72	15 (24%)
23	CLA	B	615	-	55,73,73	1.63	8 (14%)	61,113,113	2.01	14 (22%)
23	CLA	B	616	-	55,73,73	1.77	12 (21%)	61,113,113	2.00	16 (26%)
23	CLA	B	617	-	55,73,73	1.70	12 (21%)	61,113,113	2.03	13 (21%)
25	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.58	9 (16%)
25	BCR	B	619	-	41,41,41	1.16	3 (7%)	56,56,56	1.21	7 (12%)
25	BCR	B	620	-	41,41,41	0.99	1 (2%)	56,56,56	1.68	9 (16%)
26	SQD	B	621	-	53,54,54	1.30	4 (7%)	61,65,65	2.19	11 (18%)
27	LMG	B	622	-	51,51,55	0.91	2 (3%)	59,59,63	1.61	10 (16%)
30	LMT	B	623	-	36,36,36	0.97	2 (5%)	47,47,47	1.43	8 (17%)
33	HTG	B	624	-	19,19,19	1.07	1 (5%)	22,24,24	1.52	5 (22%)
33	HTG	B	625	-	19,19,19	0.91	1 (5%)	22,24,24	1.66	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	HTG	B	626	-	19,19,19	0.87	1 (5%)	22,24,24	2.25	2 (9%)
33	HTG	B	630	-	19,19,19	1.00	2 (10%)	22,24,24	1.80	2 (9%)
33	HTG	B	631	-	19,19,19	0.78	1 (5%)	22,24,24	2.38	3 (13%)
31	GOL	B	633	-	5,5,5	0.34	0	5,5,5	1.34	1 (20%)
31	GOL	B	634	-	5,5,5	0.80	0	5,5,5	0.65	0
31	GOL	B	635	-	5,5,5	0.52	0	5,5,5	1.02	0
31	GOL	B	636	-	5,5,5	0.42	0	5,5,5	0.67	0
31	GOL	B	637	-	5,5,5	0.47	0	5,5,5	1.04	0
31	GOL	B	638	-	5,5,5	0.46	0	5,5,5	0.82	0
23	CLA	C	501	-	55,73,73	1.68	12 (21%)	61,113,113	2.69	14 (22%)
23	CLA	C	502	-	55,73,73	1.70	11 (20%)	61,113,113	2.10	16 (26%)
23	CLA	C	503	-	55,73,73	1.79	11 (20%)	61,113,113	1.93	13 (21%)
23	CLA	C	504	41	55,73,73	1.70	11 (20%)	61,113,113	2.14	16 (26%)
23	CLA	C	505	-	55,73,73	1.73	12 (21%)	61,113,113	2.04	15 (24%)
23	CLA	C	506	-	55,73,73	1.79	11 (20%)	61,113,113	2.27	18 (29%)
23	CLA	C	507	41	55,73,73	1.93	13 (23%)	61,113,113	1.90	14 (22%)
23	CLA	C	508	-	55,73,73	2.02	14 (25%)	61,113,113	1.85	15 (24%)
23	CLA	C	509	-	55,73,73	1.72	12 (21%)	61,113,113	2.05	17 (27%)
23	CLA	C	510	-	55,73,73	1.75	12 (21%)	61,113,113	1.95	17 (27%)
23	CLA	C	511	3	55,73,73	1.83	14 (25%)	61,113,113	1.98	15 (24%)
23	CLA	C	512	-	55,73,73	1.82	12 (21%)	61,113,113	1.95	18 (29%)
23	CLA	C	513	-	55,73,73	1.90	11 (20%)	61,113,113	1.85	15 (24%)
25	BCR	C	514	-	41,41,41	0.87	0	56,56,56	1.30	8 (14%)
25	BCR	C	515	-	41,41,41	0.91	1 (2%)	56,56,56	1.46	4 (7%)
34	DGD	C	516	-	63,63,67	0.89	3 (4%)	77,77,81	1.39	13 (16%)
34	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	4 (5%)
34	DGD	C	518	-	63,63,67	0.77	2 (3%)	77,77,81	1.31	9 (11%)
27	LMG	C	519	-	51,51,55	0.99	3 (5%)	59,59,63	1.49	9 (15%)
30	LMT	C	520	-	36,36,36	0.60	1 (2%)	47,47,47	1.53	8 (17%)
33	HTG	C	521	-	19,19,19	0.84	1 (5%)	22,24,24	1.73	1 (4%)
33	HTG	C	522	-	19,19,19	0.93	1 (5%)	22,24,24	2.58	3 (13%)
31	GOL	C	524	-	5,5,5	0.33	0	5,5,5	1.55	1 (20%)
31	GOL	C	525	-	5,5,5	0.77	0	5,5,5	0.84	0
31	GOL	C	526	-	5,5,5	0.63	0	5,5,5	0.48	0
35	BCT	D	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	D	402	-	55,73,73	1.73	11 (20%)	61,113,113	2.31	24 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	D	403	-	55,73,73	1.78	13 (23%)	61,113,113	1.86	17 (27%)
25	BCR	D	404	-	41,41,41	1.15	3 (7%)	56,56,56	2.07	20 (35%)
28	PL9	D	405	-	55,55,55	1.38	10 (18%)	68,69,69	1.71	15 (22%)
34	DGD	D	406	-	53,53,67	1.15	3 (5%)	60,61,81	1.40	8 (13%)
26	SQD	D	407	-	44,45,54	1.36	4 (9%)	52,56,65	2.45	15 (28%)
36	LHG	D	408	-	48,48,48	0.78	1 (2%)	49,54,54	1.50	6 (12%)
36	LHG	D	409	-	48,48,48	0.81	2 (4%)	49,54,54	1.13	5 (10%)
36	LHG	D	410	-	45,45,48	0.99	3 (6%)	46,51,54	1.02	3 (6%)
27	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	1.05	2 (3%)
33	HTG	D	414	-	19,19,19	1.01	1 (5%)	22,24,24	1.39	1 (4%)
31	GOL	D	415	-	5,5,5	0.69	0	5,5,5	1.19	0
36	LHG	E	101	-	48,48,48	0.98	2 (4%)	49,54,54	0.96	3 (6%)
37	HEM	F	101	5,6	30,50,50	2.12	6 (20%)	24,82,82	2.88	9 (37%)
30	LMT	F	102	-	36,36,36	0.73	0	47,47,47	1.18	3 (6%)
38	RRX	H	101	-	42,42,42	1.08	3 (7%)	58,58,58	1.57	11 (18%)
34	DGD	H	102	-	63,63,67	1.09	3 (4%)	77,77,81	1.37	12 (15%)
30	LMT	J	102	-	24,24,36	0.81	1 (4%)	29,29,47	1.18	3 (10%)
25	BCR	K	101	-	41,41,41	0.87	0	56,56,56	1.69	13 (23%)
25	BCR	K	102	-	41,41,41	0.93	1 (2%)	56,56,56	1.69	11 (19%)
36	LHG	L	101	-	48,48,48	0.80	2 (4%)	49,54,54	1.52	7 (14%)
26	SQD	L	103	-	53,54,54	1.25	3 (5%)	61,65,65	2.10	11 (18%)
31	GOL	L	104	-	5,5,5	0.48	0	5,5,5	0.59	0
30	LMT	M	101	-	36,36,36	0.84	1 (2%)	47,47,47	1.30	6 (12%)
30	LMT	M	102	-	36,36,36	0.62	0	47,47,47	1.36	7 (14%)
40	SO4	O	302	-	4,4,4	0.67	0	6,6,6	0.35	0
33	HTG	O	303	-	19,19,19	1.10	2 (10%)	22,24,24	1.52	1 (4%)
31	GOL	O	304	-	5,5,5	0.50	0	5,5,5	0.58	0
25	BCR	T	101	-	41,41,41	0.87	0	56,56,56	1.62	13 (23%)
33	HTG	U	201	-	8,8,19	0.27	0	7,7,24	1.26	1 (14%)
37	HEM	V	201	16	30,50,50	2.47	10 (33%)	24,82,82	2.76	10 (41%)
33	HTG	V	202	-	13,13,19	0.69	0	16,18,24	2.89	6 (37%)
31	GOL	V	203	-	5,5,5	0.97	0	5,5,5	0.81	0
31	GOL	V	204	-	5,5,5	0.29	0	5,5,5	0.37	0
31	GOL	V	205	-	5,5,5	0.61	0	5,5,5	0.32	0
27	LMG	Z	101	-	51,51,55	1.06	3 (5%)	59,59,63	1.37	7 (11%)
30	LMT	Z	102	-	36,36,36	0.65	1 (2%)	47,47,47	0.91	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	SQD	a	401	-	53,54,54	1.45	3 (5%)	61,65,65	1.76	9 (14%)
30	LMT	a	402	-	36,36,36	0.74	1 (2%)	47,47,47	1.65	10 (21%)
20	OEX	a	404	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
35	BCT	a	408	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	a	409	-	55,73,73	1.65	9 (16%)	61,113,113	1.97	16 (26%)
23	CLA	a	410	41	55,73,73	1.61	11 (20%)	61,113,113	2.01	14 (22%)
23	CLA	a	411	41	55,73,73	1.58	12 (21%)	61,113,113	2.35	23 (37%)
24	PHO	a	412	-	67,69,69	1.83	14 (20%)	84,99,99	1.97	21 (25%)
24	PHO	a	413	-	67,69,69	1.93	16 (23%)	84,99,99	2.11	22 (26%)
23	CLA	a	414	-	55,73,73	1.68	8 (14%)	61,113,113	2.49	20 (32%)
25	BCR	a	415	-	41,41,41	1.20	3 (7%)	56,56,56	1.46	7 (12%)
26	SQD	a	416	-	53,54,54	1.32	3 (5%)	61,65,65	2.62	14 (22%)
36	LHG	a	417	-	39,39,48	1.13	2 (5%)	40,45,54	1.03	3 (7%)
27	LMG	a	418	-	51,51,55	0.90	2 (3%)	59,59,63	1.35	4 (6%)
28	PL9	a	419	-	55,55,55	0.92	3 (5%)	68,69,69	1.83	20 (29%)
31	GOL	a	422	-	5,5,5	0.64	0	5,5,5	0.74	0
31	GOL	a	423	-	5,5,5	0.58	0	5,5,5	0.52	0
31	GOL	a	424	-	5,5,5	0.61	0	5,5,5	0.76	0
33	HTG	b	601	-	19,19,19	0.93	2 (10%)	22,24,24	1.33	1 (4%)
33	HTG	b	602	-	19,19,19	0.72	0	22,24,24	1.33	2 (9%)
23	CLA	b	604	41	55,73,73	1.96	12 (21%)	61,113,113	2.10	15 (24%)
23	CLA	b	605	-	55,73,73	1.85	10 (18%)	61,113,113	2.08	16 (26%)
23	CLA	b	606	-	55,73,73	1.67	9 (16%)	61,113,113	2.40	18 (29%)
23	CLA	b	607	-	55,73,73	1.59	11 (20%)	61,113,113	2.25	19 (31%)
23	CLA	b	608	-	55,73,73	1.60	8 (14%)	61,113,113	2.38	19 (31%)
23	CLA	b	609	-	55,73,73	1.79	13 (23%)	61,113,113	1.88	15 (24%)
23	CLA	b	610	41	55,73,73	1.68	10 (18%)	61,113,113	1.84	16 (26%)
23	CLA	b	611	-	55,73,73	1.70	11 (20%)	61,113,113	2.00	13 (21%)
23	CLA	b	612	-	55,73,73	1.89	11 (20%)	61,113,113	2.00	16 (26%)
23	CLA	b	613	41	55,73,73	1.81	11 (20%)	61,113,113	1.86	13 (21%)
23	CLA	b	614	-	55,73,73	1.62	8 (14%)	61,113,113	2.01	19 (31%)
23	CLA	b	615	-	55,73,73	1.56	9 (16%)	61,113,113	2.27	18 (29%)
23	CLA	b	616	-	55,73,73	1.71	9 (16%)	61,113,113	2.03	18 (29%)
23	CLA	b	617	-	55,73,73	1.61	10 (18%)	61,113,113	2.30	21 (34%)
23	CLA	b	618	-	55,73,73	1.77	11 (20%)	61,113,113	2.32	20 (32%)
23	CLA	b	619	-	55,73,73	1.85	13 (23%)	61,113,113	2.27	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	b	620	-	41,41,41	1.04	2 (4%)	56,56,56	1.76	14 (25%)
25	BCR	b	621	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	8 (14%)
25	BCR	b	622	-	41,41,41	0.96	1 (2%)	56,56,56	1.25	5 (8%)
27	LMG	b	623	-	51,51,55	0.83	2 (3%)	59,59,63	1.46	9 (15%)
30	LMT	b	624	-	25,25,36	0.72	1 (4%)	30,30,47	1.39	5 (16%)
30	LMT	b	625	-	24,24,36	0.53	0	29,29,47	1.26	4 (13%)
33	HTG	b	626	-	19,19,19	0.96	1 (5%)	22,24,24	1.38	4 (18%)
33	HTG	b	627	-	19,19,19	1.06	2 (10%)	22,24,24	1.99	1 (4%)
31	GOL	b	632	-	5,5,5	0.52	0	5,5,5	1.29	0
31	GOL	b	633	-	5,5,5	0.36	0	5,5,5	0.89	0
31	GOL	b	634	-	5,5,5	0.45	0	5,5,5	0.20	0
31	GOL	b	635	-	5,5,5	0.76	0	5,5,5	0.87	0
31	GOL	b	636	-	5,5,5	0.52	0	5,5,5	0.93	0
23	CLA	c	902	-	55,73,73	1.83	12 (21%)	61,113,113	2.06	15 (24%)
23	CLA	c	903	-	55,73,73	1.82	13 (23%)	61,113,113	2.04	19 (31%)
23	CLA	c	904	-	55,73,73	1.82	12 (21%)	61,113,113	1.85	18 (29%)
23	CLA	c	905	41	55,73,73	1.82	11 (20%)	61,113,113	1.93	18 (29%)
23	CLA	c	906	-	55,73,73	1.67	11 (20%)	61,113,113	2.06	19 (31%)
23	CLA	c	907	-	55,73,73	1.77	12 (21%)	61,113,113	1.91	16 (26%)
23	CLA	c	908	41	55,73,73	1.78	14 (25%)	61,113,113	2.29	19 (31%)
23	CLA	c	909	-	55,73,73	1.90	13 (23%)	61,113,113	1.65	13 (21%)
23	CLA	c	910	-	55,73,73	1.97	12 (21%)	61,113,113	1.99	18 (29%)
23	CLA	c	911	-	55,73,73	1.81	11 (20%)	61,113,113	1.74	14 (22%)
23	CLA	c	912	3	55,73,73	1.87	10 (18%)	61,113,113	2.12	18 (29%)
23	CLA	c	913	-	55,73,73	1.96	11 (20%)	61,113,113	1.86	16 (26%)
23	CLA	c	914	-	55,73,73	2.01	12 (21%)	61,113,113	1.81	12 (19%)
25	BCR	c	915	-	41,41,41	0.85	1 (2%)	56,56,56	1.29	5 (8%)
25	BCR	c	916	-	41,41,41	0.95	1 (2%)	56,56,56	1.39	7 (12%)
34	DGD	c	917	-	63,63,67	0.88	3 (4%)	77,77,81	1.30	10 (12%)
34	DGD	c	918	-	63,63,67	0.97	4 (6%)	77,77,81	1.25	10 (12%)
34	DGD	c	919	-	63,63,67	1.03	6 (9%)	77,77,81	1.39	11 (14%)
27	LMG	c	920	-	51,51,55	1.08	4 (7%)	59,59,63	1.29	8 (13%)
27	LMG	c	921	-	51,51,55	1.06	3 (5%)	59,59,63	1.27	6 (10%)
30	LMT	c	922	-	36,36,36	0.73	1 (2%)	47,47,47	1.04	4 (8%)
33	HTG	c	923	-	19,19,19	0.94	2 (10%)	22,24,24	1.97	1 (4%)
33	HTG	c	924	-	19,19,19	0.94	1 (5%)	22,24,24	2.60	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	GOL	c	927	-	5,5,5	0.59	0	5,5,5	0.43	0
31	GOL	c	928	-	5,5,5	0.27	0	5,5,5	0.77	0
31	GOL	c	929	-	5,5,5	0.48	0	5,5,5	0.79	0
31	GOL	c	930	-	5,5,5	0.41	0	5,5,5	0.68	0
33	HTG	d	401	-	19,19,19	1.01	2 (10%)	22,24,24	1.73	2 (9%)
23	CLA	d	402	-	55,73,73	1.62	7 (12%)	61,113,113	2.33	17 (27%)
23	CLA	d	403	-	55,73,73	1.82	13 (23%)	61,113,113	2.16	16 (26%)
25	BCR	d	404	-	41,41,41	0.99	3 (7%)	56,56,56	1.82	15 (26%)
28	PL9	d	405	-	55,55,55	1.37	9 (16%)	68,69,69	1.70	14 (20%)
34	DGD	d	406	-	50,50,67	1.16	3 (6%)	58,58,81	1.37	11 (18%)
36	LHG	d	407	-	48,48,48	0.78	2 (4%)	49,54,54	1.44	6 (12%)
36	LHG	d	408	-	48,48,48	0.77	2 (4%)	49,54,54	1.32	8 (16%)
36	LHG	d	409	-	48,48,48	0.90	3 (6%)	49,54,54	1.07	4 (8%)
27	LMG	d	410	39	51,51,55	0.98	3 (5%)	59,59,63	1.15	8 (13%)
37	HEM	f	101	5,6	30,50,50	2.00	7 (23%)	24,82,82	3.07	12 (50%)
26	SQD	f	102	-	30,32,54	1.51	3 (10%)	33,36,65	1.95	7 (21%)
31	GOL	f	104	32	5,5,5	0.49	0	5,5,5	0.42	0
38	RRX	h	101	-	42,42,42	0.94	0	58,58,58	1.30	8 (13%)
34	DGD	h	102	-	63,63,67	0.96	3 (4%)	77,77,81	1.29	9 (11%)
31	GOL	h	103	-	5,5,5	0.32	0	5,5,5	0.27	0
25	BCR	k	101	-	41,41,41	0.84	1 (2%)	56,56,56	1.48	10 (17%)
25	BCR	k	102	-	41,41,41	0.97	2 (4%)	56,56,56	1.31	4 (7%)
36	LHG	l	101	-	48,48,48	0.82	2 (4%)	49,54,54	1.10	5 (10%)
31	GOL	l	102	-	5,5,5	0.45	0	5,5,5	1.01	0
30	LMT	m	101	-	36,36,36	0.73	0	47,47,47	1.43	9 (19%)
30	LMT	m	102	-	36,36,36	0.71	1 (2%)	47,47,47	1.17	3 (6%)
25	BCR	t	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.85	13 (23%)
30	LMT	t	102	-	24,24,36	0.66	0	29,29,47	1.43	4 (13%)
33	HTG	u	201	-	10,13,19	0.75	1 (10%)	8,14,24	3.03	2 (25%)
37	HEM	v	201	16	30,50,50	2.54	11 (36%)	24,82,82	2.58	10 (41%)
31	GOL	v	202	-	5,5,5	0.56	0	5,5,5	0.47	0
31	GOL	v	203	-	5,5,5	0.71	0	5,5,5	0.45	0
31	GOL	v	204	-	5,5,5	0.32	0	5,5,5	0.60	0
30	LMT	z	101	-	32,32,36	0.69	1 (3%)	42,42,47	1.01	3 (7%)

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	OEX	A	401	1,3,41	-	0/0/68/68	0/0/6/6
23	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	406	41	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	A	407	41	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	A	408	-	-	0/53/103/103	0/1/6/6
24	PHO	A	409	-	-	0/53/103/103	0/1/6/6
23	CLA	A	410	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	A	411	-	-	0/29/63/63	0/2/2/2
26	SQD	A	412	-	-	0/49/69/69	0/1/1/1
27	LMG	A	413	-	-	0/46/66/70	0/1/1/1
28	PL9	A	414	-	-	0/53/73/73	0/1/1/1
26	SQD	A	418	-	-	0/49/69/69	0/1/1/1
30	LMT	A	419	-	-	0/21/61/61	0/2/2/2
31	GOL	A	421	-	-	0/4/4/4	0/0/0/0
31	GOL	A	422	-	-	0/4/4/4	0/0/0/0
31	GOL	A	423	32	-	0/4/4/4	0/0/0/0
23	CLA	B	602	41	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	B	621	-	-	0/49/69/69	0/1/1/1
27	LMG	B	622	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
33	HTG	B	624	-	-	0/10/30/30	0/1/1/1
33	HTG	B	625	-	-	0/10/30/30	0/1/1/1
33	HTG	B	626	-	-	0/10/30/30	0/1/1/1
33	HTG	B	630	-	-	0/10/30/30	0/1/1/1
33	HTG	B	631	-	-	0/10/30/30	0/1/1/1
31	GOL	B	633	-	-	0/4/4/4	0/0/0/0
31	GOL	B	634	-	-	0/4/4/4	0/0/0/0
31	GOL	B	635	-	-	0/4/4/4	0/0/0/0
31	GOL	B	636	-	-	0/4/4/4	0/0/0/0
31	GOL	B	637	-	-	0/4/4/4	0/0/0/0
31	GOL	B	638	-	-	0/4/4/4	0/0/0/0
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
34	DGD	C	516	-	-	0/51/91/95	0/2/2/2
34	DGD	C	517	-	-	0/51/91/95	0/2/2/2
34	DGD	C	518	-	-	0/51/91/95	0/2/2/2
27	LMG	C	519	-	-	0/46/66/70	0/1/1/1
30	LMT	C	520	-	-	0/21/61/61	0/2/2/2
33	HTG	C	521	-	-	0/10/30/30	0/1/1/1
33	HTG	C	522	-	-	0/10/30/30	0/1/1/1
31	GOL	C	524	-	-	0/4/4/4	0/0/0/0
31	GOL	C	525	-	-	0/4/4/4	0/0/0/0
31	GOL	C	526	-	-	0/4/4/4	0/0/0/0
35	BCT	D	401	21	-	0/0/0/0	0/0/0/0
23	CLA	D	402	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	D	404	-	-	0/29/63/63	0/2/2/2
28	PL9	D	405	-	-	0/53/73/73	0/1/1/1
34	DGD	D	406	-	-	0/47/68/95	0/1/1/2
26	SQD	D	407	-	-	0/40/60/69	0/1/1/1
36	LHG	D	408	-	-	0/53/53/53	0/0/0/0
36	LHG	D	409	-	-	0/53/53/53	0/0/0/0
36	LHG	D	410	-	-	0/50/50/53	0/0/0/0
27	LMG	D	411	39	-	0/46/66/70	0/1/1/1
33	HTG	D	414	-	-	0/10/30/30	0/1/1/1
31	GOL	D	415	-	-	0/4/4/4	0/0/0/0
36	LHG	E	101	-	-	0/53/53/53	0/0/0/0
37	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
30	LMT	F	102	-	-	0/21/61/61	0/2/2/2
38	RRX	H	101	-	-	0/29/65/65	0/2/2/2
34	DGD	H	102	-	-	0/51/91/95	0/2/2/2
30	LMT	J	102	-	-	0/15/35/61	0/1/1/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
36	LHG	L	101	-	-	0/53/53/53	0/0/0/0
26	SQD	L	103	-	-	0/49/69/69	0/1/1/1
31	GOL	L	104	-	-	0/4/4/4	0/0/0/0
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
40	SO4	O	302	-	-	0/0/0/0	0/0/0/0
33	HTG	O	303	-	-	0/10/30/30	0/1/1/1
31	GOL	O	304	-	-	0/4/4/4	0/0/0/0
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
33	HTG	U	201	-	-	0/6/6/30	0/0/0/1
37	HEM	V	201	16	-	0/10/54/54	0/0/8/8
33	HTG	V	202	-	-	0/3/24/30	0/1/1/1
31	GOL	V	203	-	-	0/4/4/4	0/0/0/0
31	GOL	V	204	-	-	0/4/4/4	0/0/0/0
31	GOL	V	205	-	-	0/4/4/4	0/0/0/0
27	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
30	LMT	Z	102	-	-	0/21/61/61	0/2/2/2
26	SQD	a	401	-	-	0/49/69/69	0/1/1/1
30	LMT	a	402	-	-	0/21/61/61	0/2/2/2
20	OEX	a	404	1,3,41	-	0/0/68/68	0/0/6/6
35	BCT	a	408	21	-	0/0/0/0	0/0/0/0
23	CLA	a	409	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	410	41	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	411	41	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	a	412	-	-	0/53/103/103	0/1/6/6
24	PHO	a	413	-	-	0/53/103/103	0/1/6/6
23	CLA	a	414	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	a	415	-	-	0/29/63/63	0/2/2/2
26	SQD	a	416	-	-	0/49/69/69	0/1/1/1
36	LHG	a	417	-	-	0/44/44/53	0/0/0/0
27	LMG	a	418	-	-	0/46/66/70	0/1/1/1
28	PL9	a	419	-	-	0/53/73/73	0/1/1/1
31	GOL	a	422	-	-	0/4/4/4	0/0/0/0
31	GOL	a	423	-	-	0/4/4/4	0/0/0/0
31	GOL	a	424	-	-	0/4/4/4	0/0/0/0
33	HTG	b	601	-	-	0/10/30/30	0/1/1/1
33	HTG	b	602	-	-	0/10/30/30	0/1/1/1
23	CLA	b	604	41	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
27	LMG	b	623	-	-	0/46/66/70	0/1/1/1
30	LMT	b	624	-	-	0/17/37/61	0/1/1/2
30	LMT	b	625	-	-	0/15/35/61	0/1/1/2
33	HTG	b	626	-	-	0/10/30/30	0/1/1/1
33	HTG	b	627	-	-	0/10/30/30	0/1/1/1
31	GOL	b	632	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GOL	b	633	-	-	0/4/4/4	0/0/0/0
31	GOL	b	634	-	-	0/4/4/4	0/0/0/0
31	GOL	b	635	-	-	0/4/4/4	0/0/0/0
31	GOL	b	636	-	-	0/4/4/4	0/0/0/0
23	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	903	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	905	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	906	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	907	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	908	41	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	912	3	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	913	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	914	-	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	c	915	-	-	0/29/63/63	0/2/2/2
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
34	DGD	c	917	-	-	0/51/91/95	0/2/2/2
34	DGD	c	918	-	-	0/51/91/95	0/2/2/2
34	DGD	c	919	-	-	0/51/91/95	0/2/2/2
27	LMG	c	920	-	-	0/46/66/70	0/1/1/1
27	LMG	c	921	-	-	0/46/66/70	0/1/1/1
30	LMT	c	922	-	-	0/21/61/61	0/2/2/2
33	HTG	c	923	-	-	0/10/30/30	0/1/1/1
33	HTG	c	924	-	-	0/10/30/30	0/1/1/1
31	GOL	c	927	-	-	0/4/4/4	0/0/0/0
31	GOL	c	928	-	-	0/4/4/4	0/0/0/0
31	GOL	c	929	-	-	0/4/4/4	0/0/0/0
31	GOL	c	930	-	-	0/4/4/4	0/0/0/0
33	HTG	d	401	-	-	0/10/30/30	0/1/1/1
23	CLA	d	402	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	d	404	-	-	0/29/63/63	0/2/2/2
28	PL9	d	405	-	-	0/53/73/73	0/1/1/1
34	DGD	d	406	-	-	0/44/64/95	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	d	410	39	-	0/46/66/70	0/1/1/1
37	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
26	SQD	f	102	-	-	2/33/33/69	0/0/0/1
31	GOL	f	104	32	-	0/4/4/4	0/0/0/0
38	RRX	h	101	-	-	0/29/65/65	0/2/2/2
34	DGD	h	102	-	-	0/51/91/95	0/2/2/2
31	GOL	h	103	-	-	0/4/4/4	0/0/0/0
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
36	LHG	l	101	-	-	0/53/53/53	0/0/0/0
31	GOL	l	102	-	-	0/4/4/4	0/0/0/0
30	LMT	m	101	-	-	0/21/61/61	0/2/2/2
30	LMT	m	102	-	-	0/21/61/61	0/2/2/2
25	BCR	t	101	-	-	0/29/63/63	0/2/2/2
30	LMT	t	102	-	-	0/15/35/61	0/1/1/2
33	HTG	u	201	-	-	0/12/14/30	0/0/0/1
37	HEM	v	201	16	-	0/10/54/54	0/0/8/8
31	GOL	v	202	-	-	0/4/4/4	0/0/0/0
31	GOL	v	203	-	-	0/4/4/4	0/0/0/0
31	GOL	v	204	-	-	0/4/4/4	0/0/0/0
30	LMT	z	101	-	-	0/15/55/61	0/2/2/2

All (1061) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	v	201	HEM	C3B-C4B	-8.05	1.44	1.51
26	A	412	SQD	C6-S	-7.78	1.66	1.77
37	F	101	HEM	C3B-C4B	-7.41	1.45	1.51
26	a	416	SQD	C6-S	-7.37	1.67	1.77
37	V	201	HEM	C3B-C4B	-7.27	1.45	1.51
26	a	401	SQD	C6-S	-7.17	1.67	1.77
26	A	418	SQD	C6-S	-6.22	1.68	1.77
37	v	201	HEM	C3D-C4D	-5.73	1.44	1.51
37	V	201	HEM	C3D-C4D	-5.53	1.44	1.51
26	B	621	SQD	C6-S	-5.46	1.69	1.77
26	L	103	SQD	C6-S	-5.08	1.70	1.77
37	f	101	HEM	C3D-C4D	-5.04	1.45	1.51
37	f	101	HEM	C3B-C4B	-4.98	1.47	1.51
23	B	615	CLA	C1C-NC	-4.83	1.29	1.37
26	D	407	SQD	C6-S	-4.28	1.71	1.77
37	V	201	HEM	C2C-C1C	-3.93	1.45	1.52
37	F	101	HEM	C2C-C1C	-3.92	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	413	PHO	C1A-NA	-3.80	1.28	1.37
33	B	624	HTG	C1'-S1	-3.71	1.76	1.81
33	D	414	HTG	C1'-S1	-3.49	1.76	1.81
23	c	902	CLA	C4C-NC	-3.46	1.32	1.37
33	b	627	HTG	C1'-S1	-3.38	1.76	1.81
33	d	401	HTG	C1'-S1	-3.24	1.77	1.81
23	c	909	CLA	C1C-NC	-3.15	1.32	1.37
37	F	101	HEM	C3D-C4D	-3.15	1.47	1.51
24	A	408	PHO	C1A-NA	-3.08	1.30	1.37
24	A	409	PHO	C1A-NA	-3.07	1.30	1.37
23	B	616	CLA	C4C-NC	-3.04	1.32	1.37
23	C	509	CLA	C4C-NC	-3.00	1.32	1.37
37	v	201	HEM	C2C-C1C	-2.99	1.46	1.52
23	c	905	CLA	C1C-NC	-2.94	1.32	1.37
34	c	919	DGD	O2G-C2G	-2.92	1.39	1.46
24	a	413	PHO	C3D-C4D	-2.89	1.34	1.43
23	B	604	CLA	C1C-NC	-2.89	1.32	1.37
23	D	403	CLA	C1C-NC	-2.86	1.33	1.37
33	B	626	HTG	C1'-S1	-2.85	1.77	1.81
37	f	101	HEM	C2C-C1C	-2.83	1.47	1.52
23	c	911	CLA	C4C-NC	-2.83	1.33	1.37
33	c	924	HTG	C1'-S1	-2.82	1.77	1.81
23	B	611	CLA	C1C-NC	-2.81	1.33	1.37
33	c	923	HTG	C1-S1	-2.81	1.76	1.80
33	B	630	HTG	C1-S1	-2.80	1.76	1.80
23	D	403	CLA	C4C-NC	-2.80	1.33	1.37
23	a	411	CLA	C4C-NC	-2.72	1.33	1.37
23	c	909	CLA	C4C-NC	-2.72	1.33	1.37
33	b	601	HTG	C1'-S1	-2.71	1.77	1.81
24	a	412	PHO	C1A-NA	-2.65	1.31	1.37
33	C	522	HTG	C1'-S1	-2.64	1.77	1.81
33	c	923	HTG	C1'-S1	-2.62	1.77	1.81
23	C	510	CLA	C1C-NC	-2.62	1.33	1.37
23	C	508	CLA	C4C-NC	-2.60	1.33	1.37
23	B	605	CLA	C4C-NC	-2.60	1.33	1.37
24	a	413	PHO	CHB-C4A	-2.55	1.35	1.40
23	B	614	CLA	C1C-NC	-2.55	1.33	1.37
23	C	504	CLA	C1C-NC	-2.55	1.33	1.37
27	d	410	LMG	O7-C8	-2.54	1.40	1.46
34	c	918	DGD	O2G-C2G	-2.53	1.40	1.46
33	B	630	HTG	C1'-S1	-2.51	1.78	1.81
23	c	903	CLA	C4C-NC	-2.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	PHO	C3D-C4D	-2.51	1.35	1.43
33	C	521	HTG	C1'-S1	-2.50	1.78	1.81
23	C	511	CLA	C4C-NC	-2.48	1.33	1.37
23	C	508	CLA	C1C-NC	-2.44	1.33	1.37
23	b	619	CLA	C1C-NC	-2.43	1.33	1.37
23	A	407	CLA	C4C-NC	-2.42	1.33	1.37
37	v	201	HEM	C2D-C1D	-2.42	1.43	1.51
33	O	303	HTG	C1'-S1	-2.41	1.78	1.81
23	C	502	CLA	C1C-NC	-2.39	1.33	1.37
25	D	404	BCR	C30-C25	-2.39	1.50	1.53
33	b	626	HTG	C1'-S1	-2.37	1.78	1.81
24	A	408	PHO	CHB-C4A	-2.36	1.36	1.40
33	b	601	HTG	C1-S1	-2.35	1.76	1.80
33	b	627	HTG	C1-S1	-2.34	1.76	1.80
37	v	201	HEM	C2B-C1B	-2.34	1.44	1.51
33	B	625	HTG	C1'-S1	-2.32	1.78	1.81
23	c	903	CLA	C1C-NC	-2.31	1.33	1.37
25	C	515	BCR	C1-C6	-2.30	1.50	1.53
23	b	609	CLA	C1C-NC	-2.29	1.33	1.37
23	c	910	CLA	C1C-NC	-2.28	1.33	1.37
23	C	513	CLA	C4C-NC	-2.27	1.34	1.37
23	c	907	CLA	C1C-NC	-2.27	1.33	1.37
24	A	408	PHO	C3D-C4D	-2.26	1.36	1.43
24	A	409	PHO	CHB-C4A	-2.25	1.36	1.40
23	b	618	CLA	C4C-NC	-2.24	1.34	1.37
23	b	611	CLA	C4C-NC	-2.21	1.34	1.37
23	C	504	CLA	C4C-NC	-2.21	1.34	1.37
23	C	511	CLA	C1C-NC	-2.20	1.34	1.37
23	b	607	CLA	C1C-NC	-2.18	1.34	1.37
27	C	519	LMG	O7-C8	-2.18	1.41	1.46
33	B	631	HTG	C1'-S1	-2.17	1.78	1.81
23	b	607	CLA	C4C-NC	-2.15	1.34	1.37
23	c	908	CLA	C1C-NC	-2.10	1.34	1.37
26	f	102	SQD	O47-C45	-2.09	1.44	1.46
23	B	608	CLA	C1C-NC	-2.09	1.34	1.37
24	a	412	PHO	C4B-NB	-2.08	1.32	1.37
28	D	405	PL9	C2-C1	-2.06	1.38	1.44
23	C	505	CLA	C2A-C1A	-2.05	1.48	1.52
23	d	403	CLA	C1C-NC	-2.04	1.34	1.37
33	d	401	HTG	C1-S1	-2.02	1.77	1.80
33	u	201	HTG	C1'-S1	-2.02	1.78	1.81
34	c	917	DGD	O2G-C1B	2.00	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C4C-C3C	2.01	1.48	1.45
26	D	407	SQD	O6-C1	2.01	1.43	1.40
25	t	101	BCR	C12-C13	2.01	1.50	1.45
23	a	410	CLA	C4C-C3C	2.01	1.48	1.45
36	D	410	LHG	C4-C5	2.01	1.56	1.50
23	A	405	CLA	CMC-C2C	2.01	1.55	1.50
37	V	201	HEM	C4C-NC	2.02	1.38	1.36
23	B	612	CLA	C3B-C2B	2.02	1.43	1.40
23	B	605	CLA	C3D-C2D	2.02	1.45	1.40
23	b	608	CLA	C3B-CAB	2.02	1.52	1.47
23	D	402	CLA	C1B-CHB	2.03	1.45	1.39
23	C	509	CLA	CHD-C4C	2.03	1.45	1.41
34	c	919	DGD	O2D-C2D	2.03	1.47	1.43
30	C	520	LMT	O1'-C1'	2.03	1.43	1.40
25	d	404	BCR	C23-C22	2.04	1.50	1.45
23	B	606	CLA	CHD-C4C	2.04	1.45	1.41
23	B	614	CLA	OBD-CAD	2.04	1.25	1.22
37	v	201	HEM	FE-NC	2.04	2.03	1.95
24	a	413	PHO	CHD-C4C	2.04	1.45	1.40
23	b	610	CLA	OBD-CAD	2.05	1.25	1.22
23	C	502	CLA	CHD-C4C	2.05	1.46	1.41
23	C	506	CLA	C1C-C2C	2.05	1.48	1.44
23	A	410	CLA	O2D-CGD	2.06	1.38	1.33
25	b	621	BCR	C24-C25	2.06	1.53	1.45
23	A	407	CLA	CHD-C4C	2.06	1.46	1.41
23	A	406	CLA	CMC-C2C	2.06	1.55	1.50
23	C	511	CLA	C1A-CHA	2.06	1.51	1.43
25	B	619	BCR	C23-C22	2.06	1.50	1.45
23	b	619	CLA	CHD-C4C	2.06	1.46	1.41
23	b	617	CLA	C4C-C3C	2.07	1.48	1.45
23	A	406	CLA	CHD-C4C	2.07	1.46	1.41
28	d	405	PL9	C2-C3	2.07	1.40	1.34
25	k	102	BCR	C12-C13	2.08	1.50	1.45
23	c	904	CLA	C1C-C2C	2.08	1.48	1.44
25	B	619	BCR	C24-C25	2.09	1.53	1.45
25	c	915	BCR	C12-C13	2.09	1.50	1.45
23	B	608	CLA	C2-C3	2.10	1.37	1.33
30	m	102	LMT	O1'-C1'	2.10	1.43	1.40
27	c	920	LMG	O1-C1	2.10	1.43	1.40
23	C	507	CLA	C1A-CHA	2.10	1.51	1.43
23	d	403	CLA	C1C-C2C	2.10	1.48	1.44
23	a	409	CLA	C3D-C2D	2.10	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	620	BCR	C26-C25	2.10	1.37	1.34
23	C	501	CLA	C4C-C3C	2.11	1.48	1.45
23	A	405	CLA	C4C-C3C	2.11	1.48	1.45
28	D	405	PL9	C12-C13	2.11	1.56	1.50
25	K	102	BCR	C12-C13	2.12	1.50	1.45
27	c	921	LMG	O1-C1	2.12	1.44	1.40
23	b	619	CLA	C2-C3	2.12	1.37	1.33
24	a	413	PHO	C4D-ND	2.13	1.41	1.36
23	C	511	CLA	C4C-C3C	2.13	1.48	1.45
37	F	101	HEM	CMA-C3A	2.13	1.56	1.51
34	C	516	DGD	O5D-C1E	2.14	1.44	1.40
23	b	607	CLA	OBD-CAD	2.14	1.25	1.22
23	b	610	CLA	CHD-C4C	2.14	1.46	1.41
28	D	405	PL9	C13-C14	2.14	1.37	1.33
23	C	501	CLA	C1C-C2C	2.14	1.48	1.44
23	B	605	CLA	C4B-CHC	2.14	1.45	1.39
23	B	611	CLA	CHD-C4C	2.14	1.46	1.41
23	c	912	CLA	C4C-C3C	2.15	1.48	1.45
24	a	412	PHO	C2-C3	2.15	1.37	1.33
23	A	406	CLA	C1-C2	2.15	1.56	1.49
23	b	607	CLA	O2A-CGA	2.15	1.39	1.33
23	c	908	CLA	C1A-CHA	2.15	1.52	1.43
25	B	618	BCR	C30-C25	2.15	1.56	1.53
23	C	512	CLA	C1C-C2C	2.15	1.48	1.44
27	Z	101	LMG	O1-C1	2.15	1.44	1.40
37	v	201	HEM	CAA-C2A	2.16	1.55	1.52
28	D	405	PL9	C23-C24	2.16	1.37	1.33
23	B	617	CLA	CHD-C4C	2.16	1.46	1.41
23	B	610	CLA	O2D-CGD	2.16	1.38	1.33
23	c	910	CLA	C1C-C2C	2.17	1.48	1.44
23	B	616	CLA	C4B-CHC	2.17	1.45	1.39
23	B	613	CLA	C4C-C3C	2.17	1.48	1.45
25	c	916	BCR	C12-C13	2.17	1.50	1.45
23	b	608	CLA	C1B-CHB	2.17	1.45	1.39
23	C	508	CLA	C1C-C2C	2.17	1.48	1.44
23	b	615	CLA	C3B-C2B	2.17	1.43	1.40
25	k	102	BCR	C26-C25	2.18	1.37	1.34
23	A	407	CLA	C3B-C2B	2.18	1.43	1.40
23	b	605	CLA	C4B-CHC	2.19	1.45	1.39
23	C	508	CLA	OBD-CAD	2.19	1.25	1.22
23	c	910	CLA	C4C-C3C	2.19	1.49	1.45
23	c	908	CLA	C4C-C3C	2.19	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	903	CLA	CHD-C4C	2.20	1.46	1.41
23	d	402	CLA	O2D-CGD	2.20	1.38	1.33
23	c	907	CLA	C4B-CHC	2.20	1.45	1.39
23	a	410	CLA	C4B-CHC	2.20	1.45	1.39
23	A	406	CLA	C3D-C2D	2.21	1.45	1.40
23	a	409	CLA	C1B-CHB	2.21	1.45	1.39
25	k	101	BCR	C26-C25	2.21	1.37	1.34
25	b	621	BCR	C26-C25	2.22	1.37	1.34
23	C	511	CLA	C4B-CHC	2.22	1.46	1.39
23	b	618	CLA	C4C-C3C	2.22	1.49	1.45
28	d	405	PL9	C21-C19	2.22	1.56	1.51
23	B	602	CLA	C2-C3	2.23	1.37	1.33
27	c	920	LMG	O3-C3	2.23	1.48	1.43
25	d	404	BCR	C33-C5	2.23	1.54	1.51
23	b	607	CLA	CHD-C4C	2.24	1.46	1.41
23	C	510	CLA	C4B-CHC	2.24	1.46	1.39
23	B	612	CLA	O2A-CGA	2.24	1.40	1.33
23	c	902	CLA	C3D-C2D	2.24	1.45	1.40
23	a	411	CLA	CHD-C4C	2.25	1.46	1.41
23	B	602	CLA	C1C-C2C	2.25	1.49	1.44
23	A	406	CLA	C4C-C3C	2.26	1.49	1.45
25	b	620	BCR	C23-C22	2.26	1.50	1.45
34	d	406	DGD	O3G-C1D	2.27	1.44	1.40
24	a	413	PHO	C3B-C4B	2.27	1.48	1.43
23	B	613	CLA	O2A-CGA	2.28	1.40	1.33
25	d	404	BCR	C12-C13	2.28	1.51	1.45
23	c	903	CLA	C3D-C2D	2.28	1.45	1.40
23	c	903	CLA	C4C-C3C	2.29	1.49	1.45
23	b	612	CLA	CHD-C4C	2.29	1.46	1.41
36	d	409	LHG	C4-C5	2.30	1.57	1.50
34	c	919	DGD	O5D-C1E	2.30	1.44	1.40
34	c	918	DGD	O5D-C1E	2.31	1.44	1.40
23	D	403	CLA	C4B-CHC	2.31	1.46	1.39
36	d	407	LHG	O7-C7	2.31	1.41	1.34
23	C	503	CLA	C1B-CHB	2.31	1.46	1.39
23	B	611	CLA	C4C-C3C	2.32	1.49	1.45
25	D	404	BCR	C12-C13	2.32	1.51	1.45
23	A	406	CLA	O2D-CGD	2.32	1.39	1.33
23	B	602	CLA	C4C-C3C	2.32	1.49	1.45
23	b	606	CLA	CHD-C4C	2.33	1.46	1.41
34	c	919	DGD	O4D-C4D	2.33	1.48	1.43
34	C	518	DGD	O2G-C1B	2.33	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	405	PL9	C17-C18	2.33	1.57	1.50
23	B	608	CLA	C4C-C3C	2.34	1.49	1.45
25	B	618	BCR	C5-C6	2.34	1.38	1.34
24	a	412	PHO	CMA-C3A	2.34	1.58	1.53
23	B	612	CLA	C4C-C3C	2.34	1.49	1.45
23	a	411	CLA	C4B-CHC	2.34	1.46	1.39
28	D	405	PL9	C41-C39	2.35	1.56	1.51
23	B	609	CLA	OBD-CAD	2.35	1.25	1.22
23	c	914	CLA	C4C-C3C	2.35	1.49	1.45
23	A	410	CLA	CHD-C4C	2.35	1.46	1.41
23	B	603	CLA	C3B-CAB	2.35	1.52	1.47
23	B	607	CLA	CHD-C4C	2.35	1.46	1.41
23	B	617	CLA	C4C-C3C	2.36	1.49	1.45
23	B	612	CLA	CHD-C4C	2.36	1.46	1.41
23	c	910	CLA	C4B-CHC	2.36	1.46	1.39
37	V	201	HEM	CMB-C2B	2.37	1.58	1.53
37	V	201	HEM	C3C-CAC	2.37	1.55	1.51
23	a	410	CLA	C1-C2	2.37	1.56	1.49
23	a	410	CLA	O2D-CGD	2.37	1.39	1.33
23	B	607	CLA	C4B-CHC	2.37	1.46	1.39
23	b	613	CLA	C3D-C2D	2.37	1.45	1.40
23	b	609	CLA	C1C-C2C	2.38	1.49	1.44
23	b	618	CLA	C1B-CHB	2.38	1.46	1.39
25	B	620	BCR	C23-C22	2.38	1.51	1.45
37	f	101	HEM	C3B-CAB	2.38	1.55	1.51
25	a	415	BCR	C27-C26	2.39	1.56	1.51
23	a	409	CLA	CHD-C4C	2.39	1.46	1.41
23	C	512	CLA	C4B-CHC	2.39	1.46	1.39
23	b	613	CLA	O2A-CGA	2.40	1.40	1.33
23	C	510	CLA	C4C-C3C	2.40	1.49	1.45
23	B	604	CLA	C2-C3	2.40	1.37	1.33
23	B	613	CLA	C3D-C2D	2.40	1.45	1.40
23	b	616	CLA	C4C-C3C	2.40	1.49	1.45
28	a	419	PL9	C2-C3	2.41	1.41	1.34
23	c	905	CLA	C4B-CHC	2.41	1.46	1.39
23	C	503	CLA	C3D-C2D	2.41	1.45	1.40
23	c	907	CLA	C3D-C2D	2.41	1.45	1.40
23	c	903	CLA	C4B-CHC	2.42	1.46	1.39
24	a	413	PHO	C4C-C3C	2.42	1.49	1.45
37	V	201	HEM	FE-ND	2.42	2.10	1.97
23	B	604	CLA	CHD-C4C	2.42	1.46	1.41
33	O	303	HTG	O5-C1	2.42	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	z	101	LMT	O1'-C1'	2.43	1.44	1.40
23	b	605	CLA	C3D-C2D	2.43	1.46	1.40
23	B	610	CLA	C2-C3	2.43	1.37	1.33
23	C	510	CLA	CHD-C4C	2.44	1.46	1.41
28	D	405	PL9	C28-C29	2.44	1.37	1.33
23	A	410	CLA	C3D-C2D	2.44	1.46	1.40
23	B	606	CLA	C3D-C2D	2.44	1.46	1.40
30	c	922	LMT	O1'-C1'	2.44	1.44	1.40
23	B	614	CLA	CHD-C4C	2.44	1.46	1.41
23	a	411	CLA	C4C-C3C	2.45	1.49	1.45
23	a	410	CLA	C1B-CHB	2.46	1.46	1.39
23	b	606	CLA	C1B-CHB	2.46	1.46	1.39
28	d	405	PL9	C13-C14	2.46	1.37	1.33
23	C	503	CLA	C4C-C3C	2.46	1.49	1.45
23	c	909	CLA	OBD-CAD	2.46	1.26	1.22
28	D	405	PL9	C6-C5	2.47	1.49	1.35
23	b	611	CLA	C3D-C2D	2.47	1.46	1.40
30	b	624	LMT	O1'-C1'	2.47	1.44	1.40
25	B	619	BCR	C5-C6	2.47	1.38	1.34
36	l	101	LHG	O7-C7	2.47	1.41	1.34
36	d	408	LHG	O8-C23	2.47	1.40	1.33
38	H	101	RRX	C1-C6	2.47	1.57	1.53
25	t	101	BCR	C23-C22	2.48	1.51	1.45
23	C	503	CLA	C1C-C2C	2.48	1.49	1.44
23	B	612	CLA	C4B-CHC	2.48	1.46	1.39
23	B	602	CLA	C3D-C2D	2.48	1.46	1.40
36	d	408	LHG	O7-C7	2.49	1.41	1.34
37	f	101	HEM	FE-NB	2.49	2.10	1.97
23	b	615	CLA	C4B-CHC	2.49	1.46	1.39
24	A	408	PHO	CHD-C1D	2.49	1.43	1.38
23	b	612	CLA	C4B-CHC	2.50	1.46	1.39
25	b	622	BCR	C26-C25	2.51	1.38	1.34
23	A	407	CLA	O2A-CGA	2.51	1.40	1.33
23	b	610	CLA	C4B-CHC	2.52	1.46	1.39
23	c	909	CLA	C1C-C2C	2.52	1.49	1.44
23	a	411	CLA	C1B-CHB	2.52	1.46	1.39
28	A	414	PL9	C6-C5	2.52	1.50	1.35
23	B	614	CLA	O2D-CGD	2.52	1.39	1.33
24	a	413	PHO	CHC-C4B	2.53	1.46	1.40
23	b	617	CLA	OBD-CAD	2.53	1.26	1.22
23	C	502	CLA	C4B-CHC	2.53	1.46	1.39
23	B	610	CLA	C1B-CHB	2.53	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4C-C3C	2.54	1.49	1.45
23	C	507	CLA	C4C-C3C	2.54	1.49	1.45
23	c	904	CLA	OBD-CAD	2.54	1.26	1.22
23	B	607	CLA	C3D-C2D	2.54	1.46	1.40
23	a	414	CLA	CHD-C4C	2.54	1.47	1.41
30	Z	102	LMT	O1'-C1'	2.55	1.44	1.40
23	C	501	CLA	C1B-CHB	2.55	1.46	1.39
23	c	914	CLA	C1C-C2C	2.55	1.49	1.44
23	C	509	CLA	C4B-CHC	2.55	1.46	1.39
23	B	609	CLA	C3D-C2D	2.55	1.46	1.40
23	B	617	CLA	C1B-CHB	2.56	1.46	1.39
23	b	605	CLA	C4C-C3C	2.56	1.49	1.45
23	B	617	CLA	C2-C3	2.56	1.38	1.33
30	B	623	LMT	O1'-C1'	2.56	1.44	1.40
23	C	509	CLA	C1B-CHB	2.57	1.46	1.39
23	D	402	CLA	CHD-C4C	2.57	1.47	1.41
23	b	618	CLA	O2A-CGA	2.57	1.41	1.33
34	c	919	DGD	O2G-C1B	2.57	1.42	1.34
23	b	611	CLA	O2A-CGA	2.58	1.41	1.33
28	d	405	PL9	C6-C5	2.59	1.50	1.35
24	a	412	PHO	OBD-CAD	2.59	1.27	1.22
23	d	403	CLA	CHD-C4C	2.59	1.47	1.41
23	C	504	CLA	OBD-CAD	2.59	1.26	1.22
23	b	610	CLA	O2A-CGA	2.59	1.41	1.33
23	B	614	CLA	O2A-CGA	2.59	1.41	1.33
23	c	907	CLA	C1B-CHB	2.59	1.47	1.39
23	c	902	CLA	CHD-C4C	2.60	1.47	1.41
23	A	410	CLA	C4C-C3C	2.60	1.49	1.45
23	b	612	CLA	C4C-C3C	2.61	1.49	1.45
23	B	615	CLA	C3D-C2D	2.61	1.46	1.40
36	D	409	LHG	O7-C7	2.61	1.42	1.34
28	a	419	PL9	C6-C5	2.62	1.50	1.35
23	b	604	CLA	C4C-C3C	2.62	1.49	1.45
23	c	911	CLA	C3D-C2D	2.63	1.46	1.40
23	B	617	CLA	C4B-CHC	2.63	1.47	1.39
23	A	405	CLA	C3D-C2D	2.64	1.46	1.40
28	A	414	PL9	C2-C3	2.64	1.41	1.34
28	D	405	PL9	C22-C23	2.64	1.58	1.50
23	b	609	CLA	O2A-CGA	2.65	1.41	1.33
23	c	902	CLA	C4B-CHC	2.65	1.47	1.39
23	b	606	CLA	O2A-CGA	2.65	1.41	1.33
23	B	602	CLA	CHD-C4C	2.66	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	CHD-C4C	2.66	1.47	1.41
23	B	609	CLA	C1B-CHB	2.67	1.47	1.39
26	B	621	SQD	O6-C1	2.67	1.45	1.40
36	L	101	LHG	O7-C7	2.67	1.42	1.34
23	b	615	CLA	C1B-CHB	2.67	1.47	1.39
23	b	613	CLA	C1B-CHB	2.67	1.47	1.39
23	b	614	CLA	CHD-C4C	2.67	1.47	1.41
23	B	605	CLA	CHD-C4C	2.67	1.47	1.41
37	F	101	HEM	C3B-CAB	2.67	1.56	1.51
27	D	411	LMG	O8-C28	2.67	1.41	1.33
34	H	102	DGD	O2G-C1B	2.68	1.42	1.34
37	f	101	HEM	C1C-NC	2.68	1.39	1.36
23	C	504	CLA	C3D-C2D	2.69	1.46	1.40
23	B	616	CLA	C1B-CHB	2.70	1.47	1.39
23	c	906	CLA	C4C-C3C	2.70	1.49	1.45
23	b	604	CLA	C1C-C2C	2.71	1.50	1.44
23	C	505	CLA	CHD-C4C	2.71	1.47	1.41
23	b	616	CLA	C4B-CHC	2.71	1.47	1.39
23	c	908	CLA	C1C-C2C	2.71	1.50	1.44
23	c	906	CLA	C4B-CHC	2.72	1.47	1.39
23	B	612	CLA	O2D-CGD	2.72	1.40	1.33
23	c	907	CLA	C1C-C2C	2.72	1.50	1.44
23	B	608	CLA	C4B-CHC	2.72	1.47	1.39
23	B	603	CLA	C4B-CHC	2.73	1.47	1.39
28	d	405	PL9	C18-C19	2.73	1.38	1.33
23	c	913	CLA	CHD-C4C	2.73	1.47	1.41
23	b	607	CLA	C3D-C2D	2.73	1.46	1.40
37	v	201	HEM	C3C-CAC	2.73	1.56	1.51
23	D	403	CLA	C4C-C3C	2.73	1.50	1.45
28	d	405	PL9	C41-C39	2.73	1.57	1.51
24	A	408	PHO	O2D-CGD	2.73	1.40	1.33
23	B	602	CLA	C1B-CHB	2.73	1.47	1.39
23	C	506	CLA	CHD-C4C	2.74	1.47	1.41
23	B	614	CLA	C4B-CHC	2.75	1.47	1.39
23	c	910	CLA	C1B-CHB	2.75	1.47	1.39
23	B	613	CLA	C4B-CHC	2.75	1.47	1.39
23	b	616	CLA	C3D-C2D	2.75	1.46	1.40
23	C	504	CLA	O2A-CGA	2.76	1.41	1.33
23	C	506	CLA	C3D-C2D	2.76	1.46	1.40
24	A	408	PHO	CHD-C4C	2.76	1.47	1.40
23	D	402	CLA	C4B-CHC	2.77	1.47	1.39
23	c	904	CLA	CHD-C4C	2.77	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402	CLA	C3B-CAB	2.77	1.53	1.47
23	c	904	CLA	C4C-C3C	2.78	1.50	1.45
23	d	403	CLA	C1B-CHB	2.78	1.47	1.39
23	a	411	CLA	O2A-CGA	2.79	1.41	1.33
28	d	405	PL9	C43-C44	2.79	1.38	1.33
24	A	409	PHO	O2A-CGA	2.79	1.41	1.33
23	b	611	CLA	CHD-C4C	2.80	1.47	1.41
23	c	906	CLA	C3D-C2D	2.81	1.46	1.40
23	a	409	CLA	O2A-CGA	2.81	1.41	1.33
23	B	611	CLA	C1B-CHB	2.81	1.47	1.39
23	b	611	CLA	C4B-CHC	2.81	1.47	1.39
23	b	609	CLA	C4B-CHC	2.82	1.47	1.39
23	B	605	CLA	O2A-CGA	2.82	1.41	1.33
23	b	613	CLA	C4B-CHC	2.82	1.47	1.39
23	c	909	CLA	C4B-CHC	2.82	1.47	1.39
23	B	614	CLA	C4C-C3C	2.82	1.50	1.45
24	A	409	PHO	C3D-C2D	2.82	1.46	1.38
34	c	918	DGD	O2G-C1B	2.83	1.42	1.34
37	V	201	HEM	C1C-NC	2.83	1.39	1.36
23	C	510	CLA	CHC-C1C	2.83	1.44	1.35
36	L	101	LHG	O8-C23	2.83	1.41	1.33
23	B	609	CLA	CHC-C1C	2.84	1.44	1.35
23	c	911	CLA	C4B-CHC	2.84	1.47	1.39
23	b	610	CLA	C1B-CHB	2.84	1.47	1.39
23	B	610	CLA	OBD-CAD	2.84	1.26	1.22
23	b	608	CLA	O2A-CGA	2.84	1.41	1.33
23	C	502	CLA	C3D-C2D	2.85	1.47	1.40
23	B	603	CLA	CHD-C4C	2.85	1.47	1.41
23	B	607	CLA	C1B-CHB	2.85	1.47	1.39
23	a	409	CLA	CHC-C1C	2.85	1.44	1.35
23	C	510	CLA	C3D-C2D	2.85	1.47	1.40
23	B	614	CLA	C3B-C2B	2.85	1.44	1.40
23	A	406	CLA	O2A-CGA	2.85	1.41	1.33
23	B	607	CLA	O2A-CGA	2.85	1.41	1.33
23	b	609	CLA	CHD-C4C	2.86	1.47	1.41
23	c	906	CLA	O2D-CGD	2.86	1.40	1.33
23	b	606	CLA	C3D-C2D	2.86	1.47	1.40
23	B	610	CLA	C3D-C2D	2.87	1.47	1.40
23	b	613	CLA	CHD-C4C	2.87	1.47	1.41
23	C	507	CLA	CHD-C4C	2.87	1.47	1.41
23	C	512	CLA	OBD-CAD	2.87	1.26	1.22
23	B	608	CLA	C3D-C2D	2.87	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1B-CHB	2.88	1.47	1.39
23	B	606	CLA	OBD-CAD	2.88	1.26	1.22
23	B	609	CLA	CHD-C4C	2.88	1.48	1.41
23	B	612	CLA	C3D-C2D	2.89	1.47	1.40
23	C	505	CLA	O2A-CGA	2.89	1.42	1.33
23	C	513	CLA	C4B-CHC	2.89	1.47	1.39
23	C	505	CLA	C1B-CHB	2.90	1.47	1.39
23	b	619	CLA	C1C-C2C	2.90	1.50	1.44
23	C	508	CLA	C4B-CHC	2.90	1.47	1.39
24	a	412	PHO	CHC-C4B	2.90	1.47	1.40
23	b	609	CLA	C3D-C2D	2.90	1.47	1.40
23	C	508	CLA	CHD-C4C	2.91	1.48	1.41
23	c	914	CLA	C4B-CHC	2.91	1.47	1.39
23	c	909	CLA	C1B-CHB	2.92	1.47	1.39
23	C	502	CLA	O2A-CGA	2.92	1.42	1.33
36	d	409	LHG	O8-C23	2.92	1.42	1.33
23	B	613	CLA	C1B-CHB	2.93	1.47	1.39
23	B	608	CLA	OBD-CAD	2.93	1.26	1.22
23	C	503	CLA	CHD-C4C	2.93	1.48	1.41
23	b	607	CLA	C1B-CHB	2.93	1.47	1.39
30	a	402	LMT	O1'-C1'	2.94	1.45	1.40
23	C	512	CLA	C4C-C3C	2.94	1.50	1.45
36	d	409	LHG	O7-C7	2.95	1.43	1.34
23	b	612	CLA	C1B-CHB	2.95	1.48	1.39
23	c	907	CLA	OBD-CAD	2.95	1.26	1.22
37	v	201	HEM	FE-ND	2.95	2.13	1.97
23	b	615	CLA	OBD-CAD	2.95	1.26	1.22
23	c	904	CLA	C4B-CHC	2.95	1.48	1.39
30	M	101	LMT	O1'-C1'	2.95	1.45	1.40
23	C	508	CLA	O2A-CGA	2.95	1.42	1.33
27	B	622	LMG	O7-C10	2.96	1.43	1.34
23	C	502	CLA	C1B-CHB	2.96	1.48	1.39
23	b	615	CLA	C3D-C2D	2.96	1.47	1.40
23	b	610	CLA	C3B-C2B	2.96	1.44	1.40
36	d	407	LHG	O8-C23	2.97	1.42	1.33
25	D	404	BCR	C5-C6	2.97	1.39	1.34
23	b	617	CLA	CHD-C4C	2.97	1.48	1.41
23	b	617	CLA	C4B-CHC	2.97	1.48	1.39
23	c	908	CLA	CHD-C4C	2.97	1.48	1.41
23	c	911	CLA	CHD-C4C	2.98	1.48	1.41
23	B	607	CLA	C4C-C3C	2.98	1.50	1.45
23	C	513	CLA	CHD-C4C	2.99	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1C-C2C	2.99	1.50	1.44
23	C	506	CLA	C4B-CHC	2.99	1.48	1.39
23	a	410	CLA	CHD-C4C	2.99	1.48	1.41
36	l	101	LHG	O8-C23	2.99	1.42	1.33
23	B	603	CLA	O2D-CGD	2.99	1.40	1.33
38	H	101	RRX	C33-C5	2.99	1.56	1.51
23	a	411	CLA	OBD-CAD	3.01	1.26	1.22
23	C	507	CLA	OBD-CAD	3.01	1.26	1.22
23	d	403	CLA	OBD-CAD	3.01	1.27	1.22
23	B	616	CLA	C4C-C3C	3.02	1.50	1.45
23	d	403	CLA	C4B-CHC	3.02	1.48	1.39
23	C	507	CLA	C4B-CHC	3.02	1.48	1.39
23	B	608	CLA	O2D-CGD	3.02	1.40	1.33
28	D	405	PL9	C18-C19	3.02	1.38	1.33
23	C	509	CLA	C3B-C2B	3.02	1.44	1.40
23	C	505	CLA	C4C-C3C	3.02	1.50	1.45
23	c	904	CLA	C3D-C2D	3.03	1.47	1.40
23	b	611	CLA	C1B-CHB	3.03	1.48	1.39
23	b	612	CLA	C3D-C2D	3.03	1.47	1.40
23	B	603	CLA	C3D-C2D	3.03	1.47	1.40
23	A	410	CLA	O2A-CGA	3.03	1.42	1.33
23	C	503	CLA	C4B-CHC	3.03	1.48	1.39
25	a	415	BCR	C8-C9	3.03	1.52	1.45
23	B	606	CLA	O2A-CGA	3.04	1.42	1.33
23	C	501	CLA	O2A-CGA	3.04	1.42	1.33
23	b	619	CLA	C4B-CHC	3.04	1.48	1.39
23	b	614	CLA	C3D-C2D	3.05	1.47	1.40
23	b	609	CLA	OBD-CAD	3.05	1.27	1.22
34	c	917	DGD	O1G-C1A	3.05	1.42	1.33
23	a	410	CLA	O2A-CGA	3.05	1.42	1.33
23	b	619	CLA	C1B-CHB	3.05	1.48	1.39
23	c	905	CLA	C4C-C3C	3.06	1.50	1.45
38	H	101	RRX	C5-C6	3.07	1.39	1.34
34	C	517	DGD	O2G-C1B	3.07	1.43	1.34
23	b	604	CLA	CHD-C4C	3.07	1.48	1.41
23	b	615	CLA	O2A-CGA	3.07	1.42	1.33
23	B	611	CLA	OBD-CAD	3.08	1.27	1.22
23	C	510	CLA	C1B-CHB	3.08	1.48	1.39
23	b	613	CLA	C3B-C2B	3.08	1.44	1.40
23	C	505	CLA	C4B-CHC	3.08	1.48	1.39
23	b	605	CLA	C1B-CHB	3.09	1.48	1.39
23	c	910	CLA	C3D-C2D	3.09	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C3B-C2B	3.09	1.44	1.40
23	c	909	CLA	O2A-CGA	3.09	1.42	1.33
23	c	911	CLA	C1B-CHB	3.09	1.48	1.39
23	D	403	CLA	C3D-C2D	3.10	1.47	1.40
23	b	609	CLA	C1B-CHB	3.10	1.48	1.39
30	J	102	LMT	O1'-C1'	3.10	1.45	1.40
23	C	509	CLA	C3D-C2D	3.10	1.47	1.40
23	C	513	CLA	OBD-CAD	3.11	1.27	1.22
23	c	904	CLA	O2A-CGA	3.11	1.42	1.33
23	c	912	CLA	C3D-C2D	3.11	1.47	1.40
34	h	102	DGD	O2G-C1B	3.12	1.43	1.34
34	D	406	DGD	O3G-C1D	3.12	1.45	1.40
23	C	506	CLA	OBD-CAD	3.12	1.27	1.22
23	C	505	CLA	C3D-C2D	3.12	1.47	1.40
23	c	905	CLA	O2A-CGA	3.13	1.42	1.33
23	B	611	CLA	O2A-CGA	3.13	1.42	1.33
23	A	405	CLA	C1B-CHB	3.13	1.48	1.39
23	c	912	CLA	CHD-C4C	3.13	1.48	1.41
23	B	616	CLA	C3D-C2D	3.13	1.47	1.40
23	c	906	CLA	OBD-CAD	3.14	1.27	1.22
25	a	415	BCR	C26-C25	3.14	1.39	1.34
23	D	402	CLA	CHC-C1C	3.15	1.45	1.35
23	c	914	CLA	CHD-C4C	3.15	1.48	1.41
23	B	605	CLA	C3B-C2B	3.16	1.44	1.40
23	b	619	CLA	C3D-C2D	3.16	1.47	1.40
23	C	501	CLA	CHD-C4C	3.16	1.48	1.41
23	d	402	CLA	C4B-CHC	3.16	1.48	1.39
27	b	623	LMG	O7-C10	3.16	1.43	1.34
23	c	907	CLA	CHD-C4C	3.16	1.48	1.41
23	C	511	CLA	CHD-C4C	3.16	1.48	1.41
23	C	512	CLA	CHD-C4C	3.17	1.48	1.41
23	c	906	CLA	C1B-CHB	3.17	1.48	1.39
23	B	608	CLA	CHD-C4C	3.18	1.48	1.41
23	B	613	CLA	C3B-C2B	3.18	1.44	1.40
23	B	614	CLA	C1B-CHB	3.19	1.48	1.39
23	d	403	CLA	C3D-C2D	3.19	1.47	1.40
34	h	102	DGD	O1G-C1A	3.19	1.42	1.33
23	C	504	CLA	C1B-CHB	3.20	1.48	1.39
23	D	403	CLA	O2D-CGD	3.20	1.41	1.33
36	D	410	LHG	O7-C7	3.21	1.43	1.34
23	b	608	CLA	OBD-CAD	3.21	1.27	1.22
23	B	610	CLA	O2A-CGA	3.22	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	CHD-C4C	3.22	1.48	1.41
23	B	610	CLA	C4B-CHC	3.23	1.48	1.39
34	c	917	DGD	O5D-C1E	3.23	1.46	1.40
23	C	501	CLA	O2D-CGD	3.23	1.41	1.33
23	c	902	CLA	C4C-C3C	3.23	1.50	1.45
23	C	501	CLA	C3D-C2D	3.24	1.47	1.40
23	c	913	CLA	C4C-C3C	3.25	1.50	1.45
23	c	913	CLA	C1B-CHB	3.25	1.48	1.39
23	B	615	CLA	O2A-CGA	3.25	1.43	1.33
23	B	605	CLA	C1B-CHB	3.25	1.48	1.39
23	c	903	CLA	O2A-CGA	3.25	1.43	1.33
23	c	907	CLA	CHC-C1C	3.25	1.45	1.35
23	C	507	CLA	C3D-C2D	3.25	1.47	1.40
23	c	908	CLA	C1B-CHB	3.25	1.48	1.39
23	c	908	CLA	C4B-CHC	3.26	1.48	1.39
23	B	617	CLA	C3D-C2D	3.27	1.48	1.40
23	b	605	CLA	O2A-CGA	3.27	1.43	1.33
34	C	516	DGD	O2G-C1B	3.28	1.44	1.34
23	b	604	CLA	C1B-CHB	3.28	1.48	1.39
23	A	407	CLA	C3D-C2D	3.28	1.48	1.40
23	B	611	CLA	C4B-CHC	3.29	1.48	1.39
23	C	513	CLA	O2A-CGA	3.29	1.43	1.33
23	C	501	CLA	C4B-CHC	3.30	1.48	1.39
23	B	611	CLA	O2D-CGD	3.30	1.41	1.33
23	A	406	CLA	C4B-CHC	3.30	1.48	1.39
34	C	516	DGD	O1G-C1A	3.30	1.43	1.33
23	B	603	CLA	OBD-CAD	3.30	1.27	1.22
23	B	602	CLA	C4B-CHC	3.30	1.48	1.39
26	A	412	SQD	O48-C23	3.31	1.43	1.33
23	b	611	CLA	O2D-CGD	3.31	1.41	1.33
23	C	508	CLA	C3D-C2D	3.31	1.48	1.40
23	B	604	CLA	C3D-C2D	3.31	1.48	1.40
23	A	405	CLA	CHD-C4C	3.32	1.49	1.41
23	b	617	CLA	C1B-CHB	3.32	1.49	1.39
23	C	511	CLA	OBD-CAD	3.32	1.27	1.22
36	D	409	LHG	O8-C23	3.32	1.43	1.33
24	a	412	PHO	C3D-C2D	3.32	1.47	1.38
23	B	603	CLA	C4C-C3C	3.32	1.51	1.45
23	c	913	CLA	C3D-C2D	3.33	1.48	1.40
36	D	408	LHG	O8-C23	3.33	1.43	1.33
23	B	616	CLA	CHD-C4C	3.33	1.49	1.41
24	a	413	PHO	C3D-C2D	3.34	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	913	CLA	C4B-CHC	3.34	1.49	1.39
23	A	407	CLA	O2D-CGD	3.35	1.41	1.33
24	A	409	PHO	CHC-C4B	3.35	1.48	1.40
23	a	411	CLA	C3D-C2D	3.35	1.48	1.40
23	a	411	CLA	C3B-C2B	3.35	1.44	1.40
37	V	201	HEM	C3B-CAB	3.35	1.57	1.51
23	C	507	CLA	O2A-CGA	3.35	1.43	1.33
23	B	612	CLA	OBD-CAD	3.35	1.27	1.22
23	b	617	CLA	CHC-C1C	3.36	1.45	1.35
34	H	102	DGD	O1G-C1A	3.36	1.43	1.33
23	C	505	CLA	OBD-CAD	3.37	1.27	1.22
23	a	414	CLA	O2D-CGD	3.37	1.41	1.33
23	B	617	CLA	O2A-CGA	3.37	1.43	1.33
23	B	608	CLA	C1B-CHB	3.37	1.49	1.39
23	B	605	CLA	CHC-C1C	3.37	1.45	1.35
23	B	609	CLA	O2A-CGA	3.39	1.43	1.33
23	c	905	CLA	C1B-CHB	3.39	1.49	1.39
23	c	905	CLA	C3D-C2D	3.39	1.48	1.40
34	c	919	DGD	O1G-C1A	3.39	1.43	1.33
23	B	604	CLA	O2A-CGA	3.40	1.43	1.33
28	A	414	PL9	C7-C3	3.40	1.54	1.51
23	B	613	CLA	O2D-CGD	3.40	1.41	1.33
23	B	613	CLA	OBD-CAD	3.41	1.27	1.22
23	c	910	CLA	CHC-C1C	3.41	1.46	1.35
34	C	518	DGD	O1G-C1A	3.41	1.43	1.33
23	c	908	CLA	C3D-C2D	3.41	1.48	1.40
23	B	605	CLA	O2D-CGD	3.41	1.41	1.33
23	a	411	CLA	O2D-CGD	3.42	1.41	1.33
25	b	621	BCR	C5-C6	3.42	1.39	1.34
23	d	402	CLA	C3D-C2D	3.42	1.48	1.40
23	C	502	CLA	OBD-CAD	3.43	1.27	1.22
23	c	908	CLA	O2D-CGD	3.43	1.41	1.33
23	C	504	CLA	O2D-CGD	3.44	1.42	1.33
23	B	604	CLA	C1B-CHB	3.45	1.49	1.39
23	c	903	CLA	CHC-C1C	3.45	1.46	1.35
23	b	614	CLA	O2A-CGA	3.46	1.43	1.33
23	c	914	CLA	C1B-CHB	3.46	1.49	1.39
23	D	403	CLA	OBD-CAD	3.46	1.27	1.22
23	C	513	CLA	C3D-C2D	3.46	1.48	1.40
23	c	906	CLA	O2A-CGA	3.46	1.43	1.33
24	a	413	PHO	O2A-CGA	3.47	1.43	1.33
23	b	618	CLA	CHC-C1C	3.47	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	410	LMG	O8-C28	3.48	1.43	1.33
23	c	903	CLA	C1B-CHB	3.48	1.49	1.39
23	B	611	CLA	C3D-C2D	3.48	1.48	1.40
30	A	419	LMT	O1'-C1'	3.48	1.46	1.40
23	a	410	CLA	C3B-C2B	3.48	1.44	1.40
23	A	405	CLA	C3B-C2B	3.48	1.44	1.40
23	B	606	CLA	C1B-CHB	3.48	1.49	1.39
23	c	914	CLA	C3D-C2D	3.49	1.48	1.40
23	B	617	CLA	O2D-CGD	3.49	1.42	1.33
23	c	903	CLA	C3C-C2C	3.49	1.44	1.36
23	a	410	CLA	OBD-CAD	3.50	1.27	1.22
23	c	902	CLA	C1B-CHB	3.51	1.49	1.39
23	C	512	CLA	C1B-CHB	3.52	1.49	1.39
23	c	913	CLA	OBD-CAD	3.52	1.27	1.22
23	c	908	CLA	O2A-CGA	3.52	1.43	1.33
23	C	508	CLA	C4C-C3C	3.53	1.51	1.45
23	b	618	CLA	CHD-C4C	3.53	1.49	1.41
23	d	403	CLA	C4C-C3C	3.53	1.51	1.45
23	B	612	CLA	CHC-C1C	3.53	1.46	1.35
23	D	402	CLA	C3C-C2C	3.53	1.44	1.36
23	b	606	CLA	C3B-C2B	3.53	1.45	1.40
24	A	408	PHO	O2A-CGA	3.54	1.44	1.33
23	b	608	CLA	C3B-C2B	3.54	1.45	1.40
23	c	909	CLA	C3D-C2D	3.54	1.48	1.40
23	b	617	CLA	C3C-C2C	3.54	1.44	1.36
24	a	412	PHO	CHC-C1C	3.55	1.45	1.38
23	C	513	CLA	C1B-CHB	3.55	1.49	1.39
26	a	416	SQD	O48-C23	3.55	1.44	1.33
37	V	201	HEM	CMA-C3A	3.55	1.58	1.51
23	B	615	CLA	C1B-CHB	3.55	1.49	1.39
23	B	614	CLA	C3D-C2D	3.55	1.48	1.40
36	D	410	LHG	O8-C23	3.55	1.44	1.33
23	b	612	CLA	O2A-CGA	3.56	1.44	1.33
23	A	405	CLA	C4B-CHC	3.56	1.49	1.39
23	C	511	CLA	CHC-C1C	3.56	1.46	1.35
23	b	604	CLA	OBD-CAD	3.57	1.27	1.22
23	d	403	CLA	O2D-CGD	3.57	1.42	1.33
24	A	409	PHO	OBD-CAD	3.57	1.28	1.22
23	b	607	CLA	C3B-C2B	3.57	1.45	1.40
23	C	512	CLA	C3D-C2D	3.57	1.48	1.40
28	D	405	PL9	C21-C19	3.57	1.59	1.51
23	c	904	CLA	C1B-CHB	3.58	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	O2D-CGD	3.58	1.42	1.33
23	A	406	CLA	C3B-C2B	3.58	1.45	1.40
23	c	912	CLA	CHC-C1C	3.58	1.46	1.35
27	D	411	LMG	O7-C10	3.58	1.45	1.34
23	C	510	CLA	O2A-CGA	3.58	1.44	1.33
23	c	905	CLA	CHC-C1C	3.58	1.46	1.35
23	a	414	CLA	O2A-CGA	3.59	1.44	1.33
23	c	902	CLA	OBD-CAD	3.59	1.27	1.22
23	c	910	CLA	O2A-CGA	3.59	1.44	1.33
26	a	416	SQD	O47-C7	3.59	1.45	1.34
23	b	613	CLA	CHC-C1C	3.59	1.46	1.35
23	c	906	CLA	CHD-C4C	3.60	1.49	1.41
23	b	609	CLA	CHC-C1C	3.61	1.46	1.35
23	B	615	CLA	O2D-CGD	3.61	1.42	1.33
27	d	410	LMG	O7-C10	3.61	1.45	1.34
23	A	410	CLA	C4B-CHC	3.61	1.49	1.39
23	c	905	CLA	OBD-CAD	3.62	1.27	1.22
27	C	519	LMG	O7-C10	3.63	1.45	1.34
23	b	619	CLA	OBD-CAD	3.63	1.27	1.22
24	A	409	PHO	CHC-C1C	3.64	1.45	1.38
23	B	607	CLA	OBD-CAD	3.64	1.27	1.22
23	B	603	CLA	C1B-CHB	3.64	1.49	1.39
23	B	604	CLA	OBD-CAD	3.64	1.27	1.22
23	c	908	CLA	C3B-C2B	3.64	1.45	1.40
23	a	414	CLA	C1B-CHB	3.65	1.49	1.39
23	c	909	CLA	C4C-C3C	3.65	1.51	1.45
23	c	902	CLA	CHC-C1C	3.65	1.46	1.35
23	C	511	CLA	C3D-C2D	3.65	1.48	1.40
23	C	503	CLA	O2D-CGD	3.65	1.42	1.33
23	B	602	CLA	OBD-CAD	3.65	1.27	1.22
23	B	604	CLA	CHC-C1C	3.66	1.46	1.35
23	A	410	CLA	C1B-CHB	3.66	1.49	1.39
23	b	617	CLA	C3B-C2B	3.66	1.45	1.40
23	d	403	CLA	CHC-C1C	3.67	1.46	1.35
23	C	505	CLA	CHC-C1C	3.67	1.46	1.35
24	A	409	PHO	O2D-CGD	3.67	1.42	1.33
26	B	621	SQD	O48-C23	3.67	1.44	1.33
23	b	605	CLA	CHD-C4C	3.69	1.49	1.41
23	c	902	CLA	O2D-CGD	3.69	1.42	1.33
24	A	408	PHO	CHC-C1C	3.69	1.45	1.38
23	A	405	CLA	OBD-CAD	3.70	1.28	1.22
34	C	517	DGD	O1G-C1A	3.70	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	O2A-CGA	3.70	1.44	1.33
26	A	412	SQD	O47-C7	3.70	1.45	1.34
23	b	615	CLA	CHC-C1C	3.70	1.46	1.35
23	b	618	CLA	C3D-C2D	3.70	1.49	1.40
23	C	512	CLA	O2A-CGA	3.71	1.44	1.33
26	L	103	SQD	O48-C23	3.71	1.44	1.33
23	b	604	CLA	C3D-C2D	3.71	1.49	1.40
23	b	604	CLA	C4B-CHC	3.71	1.50	1.39
23	c	912	CLA	C1B-CHB	3.72	1.50	1.39
23	a	409	CLA	O2D-CGD	3.72	1.42	1.33
23	C	508	CLA	C1B-CHB	3.72	1.50	1.39
23	C	504	CLA	CHC-C1C	3.72	1.47	1.35
23	b	613	CLA	C4C-C3C	3.73	1.51	1.45
23	c	902	CLA	O2A-CGA	3.73	1.44	1.33
23	B	612	CLA	C3C-C2C	3.73	1.44	1.36
24	A	408	PHO	C3C-C2C	3.74	1.44	1.36
23	B	609	CLA	C3B-C2B	3.74	1.45	1.40
23	b	611	CLA	CHC-C1C	3.74	1.47	1.35
23	B	602	CLA	CHC-C1C	3.75	1.47	1.35
28	a	419	PL9	C7-C3	3.76	1.54	1.51
23	b	614	CLA	C1B-CHB	3.76	1.50	1.39
23	B	617	CLA	OBD-CAD	3.76	1.28	1.22
23	c	911	CLA	CHC-C1C	3.76	1.47	1.35
23	b	614	CLA	CHC-C1C	3.78	1.47	1.35
23	B	616	CLA	C3B-C2B	3.79	1.45	1.40
23	c	912	CLA	O2A-CGA	3.79	1.44	1.33
23	C	506	CLA	C1B-CHB	3.79	1.50	1.39
23	D	402	CLA	OBD-CAD	3.80	1.28	1.22
34	h	102	DGD	O5D-C1E	3.80	1.47	1.40
23	C	507	CLA	O2D-CGD	3.80	1.42	1.33
23	b	615	CLA	O2D-CGD	3.81	1.42	1.33
23	b	617	CLA	O2D-CGD	3.81	1.42	1.33
23	A	410	CLA	C3B-C2B	3.81	1.45	1.40
23	B	616	CLA	CHC-C1C	3.82	1.47	1.35
37	f	101	HEM	FE-NC	3.84	2.10	1.95
24	A	409	PHO	C3C-C2C	3.84	1.45	1.36
23	B	606	CLA	C3B-C2B	3.84	1.45	1.40
23	c	911	CLA	O2A-CGA	3.84	1.44	1.33
30	B	623	LMT	O6B-C6B	3.85	1.59	1.42
23	A	406	CLA	CHC-C1C	3.85	1.47	1.35
23	B	615	CLA	C3C-C2C	3.85	1.45	1.36
23	B	604	CLA	C3B-C2B	3.85	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	908	CLA	OBD-CAD	3.85	1.28	1.22
23	C	511	CLA	O2A-CGA	3.86	1.44	1.33
23	a	411	CLA	CHC-C1C	3.86	1.47	1.35
23	C	506	CLA	CHC-C1C	3.86	1.47	1.35
23	b	610	CLA	C3D-C2D	3.87	1.49	1.40
23	b	607	CLA	O2D-CGD	3.87	1.43	1.33
23	c	907	CLA	O2A-CGA	3.87	1.45	1.33
23	c	909	CLA	CHC-C1C	3.88	1.47	1.35
27	b	623	LMG	O8-C28	3.89	1.45	1.33
23	D	402	CLA	O2D-CGD	3.90	1.43	1.33
23	B	611	CLA	C3B-C2B	3.90	1.45	1.40
27	a	418	LMG	O8-C28	3.90	1.45	1.33
23	b	610	CLA	O2D-CGD	3.91	1.43	1.33
23	B	616	CLA	OBD-CAD	3.91	1.28	1.22
23	C	501	CLA	OBD-CAD	3.91	1.28	1.22
23	D	403	CLA	O2A-CGA	3.91	1.45	1.33
23	C	509	CLA	CHC-C1C	3.92	1.47	1.35
23	b	612	CLA	OBD-CAD	3.93	1.28	1.22
23	a	414	CLA	OBD-CAD	3.93	1.28	1.22
23	C	504	CLA	CHD-C4C	3.95	1.50	1.41
23	b	614	CLA	C3C-C2C	3.95	1.45	1.36
23	B	608	CLA	CHC-C1C	3.96	1.47	1.35
23	D	402	CLA	C4C-C3C	3.97	1.52	1.45
23	c	906	CLA	CHC-C1C	3.98	1.47	1.35
23	C	511	CLA	C1B-CHB	3.98	1.50	1.39
23	C	513	CLA	CHC-C1C	3.98	1.47	1.35
34	c	918	DGD	O1G-C1A	3.98	1.45	1.33
23	C	509	CLA	O2A-CGA	3.98	1.45	1.33
23	A	407	CLA	CHC-C1C	3.98	1.47	1.35
23	c	911	CLA	OBD-CAD	3.98	1.28	1.22
23	C	507	CLA	CHC-C1C	4.00	1.47	1.35
26	A	418	SQD	O47-C7	4.01	1.46	1.34
23	d	403	CLA	O2A-CGA	4.02	1.45	1.33
23	D	403	CLA	C1B-CHB	4.02	1.50	1.39
37	v	201	HEM	C3B-CAB	4.06	1.58	1.51
36	E	101	LHG	O7-C7	4.06	1.46	1.34
23	b	604	CLA	CHC-C1C	4.07	1.48	1.35
23	C	506	CLA	C3C-C2C	4.08	1.45	1.36
23	c	906	CLA	C3C-C2C	4.08	1.45	1.36
23	B	610	CLA	C3B-C2B	4.08	1.45	1.40
23	C	501	CLA	C3C-C2C	4.09	1.45	1.36
24	a	413	PHO	O2D-CGD	4.09	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHC-C1C	4.09	1.48	1.35
23	b	616	CLA	O2A-CGA	4.10	1.45	1.33
27	a	418	LMG	O7-C10	4.10	1.46	1.34
23	a	414	CLA	CHC-C1C	4.10	1.48	1.35
27	A	413	LMG	O8-C28	4.10	1.45	1.33
23	A	405	CLA	O2D-CGD	4.10	1.43	1.33
23	B	604	CLA	C3C-C2C	4.11	1.45	1.36
23	c	908	CLA	CHC-C1C	4.11	1.48	1.35
23	c	904	CLA	O2D-CGD	4.12	1.43	1.33
34	d	406	DGD	O2G-C1B	4.14	1.46	1.34
23	B	617	CLA	CHC-C1C	4.14	1.48	1.35
23	D	402	CLA	O2A-CGA	4.14	1.45	1.33
23	b	619	CLA	O2A-CGA	4.14	1.45	1.33
23	D	403	CLA	CHC-C1C	4.14	1.48	1.35
23	B	616	CLA	O2D-CGD	4.16	1.43	1.33
24	a	412	PHO	CHD-C4C	4.17	1.50	1.40
23	C	502	CLA	C3B-C2B	4.17	1.45	1.40
23	b	616	CLA	C3B-C2B	4.17	1.45	1.40
23	C	503	CLA	O2A-CGA	4.17	1.45	1.33
23	b	608	CLA	CHC-C1C	4.17	1.48	1.35
23	b	616	CLA	OBD-CAD	4.18	1.28	1.22
23	B	614	CLA	CHC-C1C	4.18	1.48	1.35
23	B	611	CLA	C3C-C2C	4.19	1.45	1.36
23	c	904	CLA	CHC-C1C	4.19	1.48	1.35
23	b	606	CLA	OBD-CAD	4.20	1.28	1.22
23	C	503	CLA	CHC-C1C	4.20	1.48	1.35
23	b	612	CLA	C3B-C2B	4.20	1.45	1.40
23	B	610	CLA	CHC-C1C	4.20	1.48	1.35
23	c	910	CLA	C3C-C2C	4.20	1.45	1.36
23	A	410	CLA	CHC-C1C	4.20	1.48	1.35
23	D	403	CLA	C3B-C2B	4.20	1.45	1.40
23	C	510	CLA	O2D-CGD	4.21	1.43	1.33
23	A	410	CLA	OBD-CAD	4.21	1.28	1.22
23	b	609	CLA	O2D-CGD	4.21	1.43	1.33
27	c	920	LMG	O7-C10	4.21	1.46	1.34
23	b	611	CLA	C3C-C2C	4.23	1.45	1.36
23	b	605	CLA	CHC-C1C	4.24	1.48	1.35
27	A	413	LMG	O7-C10	4.24	1.47	1.34
23	c	913	CLA	O2A-CGA	4.24	1.46	1.33
23	c	905	CLA	C3B-C2B	4.25	1.45	1.40
23	C	506	CLA	O2A-CGA	4.25	1.46	1.33
23	C	511	CLA	C3C-C2C	4.25	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C3C-C2C	4.25	1.45	1.36
23	C	512	CLA	CHC-C1C	4.25	1.48	1.35
23	C	502	CLA	C3C-C2C	4.26	1.45	1.36
23	b	617	CLA	O2A-CGA	4.26	1.46	1.33
23	a	411	CLA	C3C-C2C	4.26	1.45	1.36
23	c	913	CLA	CHC-C1C	4.27	1.48	1.35
27	Z	101	LMG	O8-C28	4.27	1.46	1.33
23	B	611	CLA	CHC-C1C	4.27	1.48	1.35
23	B	613	CLA	C3C-C2C	4.27	1.45	1.36
23	C	505	CLA	C3B-C2B	4.28	1.46	1.40
23	B	605	CLA	C3C-C2C	4.28	1.46	1.36
34	H	102	DGD	O5D-C1E	4.29	1.47	1.40
27	C	519	LMG	O8-C28	4.29	1.46	1.33
23	C	508	CLA	CHC-C1C	4.29	1.48	1.35
23	b	614	CLA	O2D-CGD	4.30	1.44	1.33
23	B	609	CLA	O2D-CGD	4.30	1.44	1.33
23	c	902	CLA	C3C-C2C	4.30	1.46	1.36
23	C	501	CLA	CHC-C1C	4.31	1.48	1.35
24	a	412	PHO	CHB-C1B	4.31	1.47	1.38
26	D	407	SQD	O48-C23	4.31	1.46	1.33
23	d	402	CLA	CHC-C1C	4.32	1.48	1.35
24	a	412	PHO	C3B-C2B	4.32	1.45	1.36
23	b	614	CLA	C3B-C2B	4.32	1.46	1.40
23	C	511	CLA	C3B-C2B	4.32	1.46	1.40
23	c	914	CLA	O2A-CGA	4.33	1.46	1.33
24	a	412	PHO	CHD-C1D	4.33	1.47	1.38
37	v	201	HEM	C1C-NC	4.33	1.41	1.36
23	C	504	CLA	C3C-C2C	4.34	1.46	1.36
23	B	606	CLA	CHC-C1C	4.34	1.48	1.35
23	C	510	CLA	OBD-CAD	4.34	1.29	1.22
23	B	609	CLA	C3C-C2C	4.34	1.46	1.36
23	c	905	CLA	O2D-CGD	4.35	1.44	1.33
23	b	607	CLA	CHC-C1C	4.36	1.49	1.35
27	c	921	LMG	O8-C28	4.36	1.46	1.33
23	b	616	CLA	C3C-C2C	4.36	1.46	1.36
24	a	413	PHO	C3C-C2C	4.37	1.46	1.36
23	d	402	CLA	C3C-C2C	4.37	1.46	1.36
23	b	606	CLA	O2D-CGD	4.38	1.44	1.33
36	a	417	LHG	O7-C7	4.39	1.47	1.34
23	b	606	CLA	CHC-C1C	4.39	1.49	1.35
23	a	410	CLA	CHC-C1C	4.39	1.49	1.35
23	A	407	CLA	OBD-CAD	4.40	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	CLA	C3C-C2C	4.41	1.46	1.36
23	b	618	CLA	O2D-CGD	4.41	1.44	1.33
23	B	608	CLA	C3C-C2C	4.41	1.46	1.36
36	E	101	LHG	O8-C23	4.42	1.46	1.33
24	a	413	PHO	C3B-C2B	4.42	1.46	1.36
23	c	914	CLA	OBD-CAD	4.44	1.29	1.22
23	C	506	CLA	O2D-CGD	4.45	1.44	1.33
23	C	509	CLA	C3C-C2C	4.46	1.46	1.36
23	A	405	CLA	CHC-C1C	4.46	1.49	1.35
23	C	510	CLA	C3B-C2B	4.46	1.46	1.40
23	d	402	CLA	O2A-CGA	4.46	1.46	1.33
23	C	513	CLA	O2D-CGD	4.47	1.44	1.33
23	c	912	CLA	C3C-C2C	4.47	1.46	1.36
27	c	920	LMG	O8-C28	4.47	1.46	1.33
23	B	607	CLA	CHC-C1C	4.48	1.49	1.35
26	a	401	SQD	O48-C23	4.49	1.46	1.33
34	D	406	DGD	O1G-C1A	4.50	1.46	1.33
23	c	914	CLA	CHC-C1C	4.50	1.49	1.35
23	C	512	CLA	O2D-CGD	4.51	1.44	1.33
27	B	622	LMG	O8-C28	4.52	1.46	1.33
23	b	613	CLA	OBD-CAD	4.52	1.29	1.22
23	b	604	CLA	C3C-C2C	4.55	1.46	1.36
23	b	619	CLA	O2D-CGD	4.55	1.44	1.33
23	d	402	CLA	C3B-C2B	4.56	1.46	1.40
24	a	412	PHO	O2D-CGD	4.56	1.44	1.33
23	a	414	CLA	C3C-C2C	4.57	1.46	1.36
26	B	621	SQD	O47-C7	4.57	1.48	1.34
26	L	103	SQD	O47-C7	4.58	1.48	1.34
23	A	405	CLA	C3C-C2C	4.58	1.46	1.36
23	c	911	CLA	C3B-C2B	4.58	1.46	1.40
23	B	606	CLA	O2D-CGD	4.58	1.44	1.33
36	a	417	LHG	O8-C23	4.59	1.47	1.33
23	B	615	CLA	CHC-C1C	4.59	1.49	1.35
23	a	409	CLA	C3B-C2B	4.59	1.46	1.40
26	f	102	SQD	O48-C23	4.60	1.47	1.33
23	B	608	CLA	C3B-C2B	4.63	1.46	1.40
23	a	409	CLA	C3C-C2C	4.64	1.46	1.36
23	C	509	CLA	O2D-CGD	4.65	1.45	1.33
23	C	505	CLA	O2D-CGD	4.65	1.45	1.33
23	D	403	CLA	C3C-C2C	4.66	1.46	1.36
23	b	609	CLA	C3C-C2C	4.67	1.46	1.36
24	A	409	PHO	CHB-C1B	4.68	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	921	LMG	O7-C10	4.68	1.48	1.34
23	B	607	CLA	O2D-CGD	4.69	1.45	1.33
24	a	413	PHO	CHD-C1D	4.69	1.47	1.38
23	c	910	CLA	O2D-CGD	4.69	1.45	1.33
23	c	911	CLA	C3C-C2C	4.71	1.46	1.36
28	d	405	PL9	C7-C3	4.72	1.55	1.51
23	B	602	CLA	C3C-C2C	4.72	1.46	1.36
23	C	512	CLA	C3B-C2B	4.73	1.46	1.40
23	C	509	CLA	OBD-CAD	4.74	1.29	1.22
26	a	401	SQD	O47-C7	4.74	1.48	1.34
23	b	619	CLA	C3C-C2C	4.74	1.47	1.36
23	C	502	CLA	CHC-C1C	4.74	1.50	1.35
23	b	611	CLA	OBD-CAD	4.76	1.29	1.22
23	B	617	CLA	C3B-C2B	4.76	1.46	1.40
23	B	610	CLA	C3C-C2C	4.76	1.47	1.36
23	a	410	CLA	C3C-C2C	4.76	1.47	1.36
23	b	619	CLA	CHC-C1C	4.77	1.50	1.35
23	b	608	CLA	O2D-CGD	4.78	1.45	1.33
23	b	608	CLA	C3C-C2C	4.78	1.47	1.36
24	A	409	PHO	CHD-C1D	4.79	1.48	1.38
23	A	410	CLA	C3C-C2C	4.79	1.47	1.36
23	b	618	CLA	C3B-C2B	4.79	1.46	1.40
23	C	501	CLA	C3B-C2B	4.79	1.46	1.40
23	b	610	CLA	CHC-C1C	4.80	1.50	1.35
23	c	907	CLA	C3C-C2C	4.80	1.47	1.36
23	C	511	CLA	O2D-CGD	4.80	1.45	1.33
23	B	613	CLA	CHC-C1C	4.81	1.50	1.35
23	B	614	CLA	C3C-C2C	4.82	1.47	1.36
23	b	616	CLA	O2D-CGD	4.82	1.45	1.33
23	c	903	CLA	O2D-CGD	4.82	1.45	1.33
23	B	602	CLA	O2D-CGD	4.82	1.45	1.33
23	B	603	CLA	CHC-C1C	4.82	1.50	1.35
23	C	502	CLA	O2D-CGD	4.82	1.45	1.33
26	D	407	SQD	O47-C7	4.83	1.48	1.34
27	Z	101	LMG	O7-C10	4.83	1.48	1.34
23	c	912	CLA	O2D-CGD	4.83	1.45	1.33
23	C	508	CLA	O2D-CGD	4.85	1.45	1.33
23	B	616	CLA	C3C-C2C	4.85	1.47	1.36
23	c	911	CLA	O2D-CGD	4.85	1.45	1.33
34	D	406	DGD	O2G-C1B	4.87	1.48	1.34
23	b	619	CLA	C3B-C2B	4.87	1.46	1.40
26	A	418	SQD	O48-C23	4.88	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	101	HEM	FE-NC	4.89	2.15	1.95
23	b	611	CLA	C3B-C2B	4.90	1.46	1.40
23	a	414	CLA	C3B-C2B	4.91	1.46	1.40
23	b	613	CLA	O2D-CGD	4.92	1.45	1.33
23	D	402	CLA	C3B-C2B	4.92	1.46	1.40
23	c	914	CLA	O2D-CGD	4.92	1.45	1.33
23	b	618	CLA	C3C-C2C	4.93	1.47	1.36
23	b	604	CLA	O2A-CGA	4.94	1.48	1.33
34	d	406	DGD	O1G-C1A	4.96	1.48	1.33
23	B	607	CLA	C3C-C2C	4.98	1.47	1.36
23	c	912	CLA	OBD-CAD	4.98	1.30	1.22
23	b	607	CLA	C3C-C2C	5.00	1.47	1.36
23	B	602	CLA	C3B-C2B	5.02	1.46	1.40
23	C	505	CLA	C3C-C2C	5.03	1.47	1.36
23	c	906	CLA	C3B-C2B	5.04	1.47	1.40
23	b	604	CLA	O2D-CGD	5.05	1.46	1.33
23	b	612	CLA	CHC-C1C	5.09	1.51	1.35
23	c	909	CLA	C3B-C2B	5.10	1.47	1.40
23	B	617	CLA	C3C-C2C	5.10	1.47	1.36
23	c	909	CLA	C3C-C2C	5.10	1.47	1.36
24	A	408	PHO	C3B-C2B	5.11	1.47	1.36
23	C	510	CLA	C3C-C2C	5.12	1.47	1.36
23	c	914	CLA	C3C-C2C	5.19	1.47	1.36
23	c	913	CLA	O2D-CGD	5.20	1.46	1.33
23	B	606	CLA	C3C-C2C	5.20	1.48	1.36
23	b	606	CLA	C3C-C2C	5.21	1.48	1.36
23	C	503	CLA	C3C-C2C	5.21	1.48	1.36
23	c	907	CLA	O2D-CGD	5.22	1.46	1.33
23	C	507	CLA	C3C-C2C	5.24	1.48	1.36
23	b	605	CLA	C3B-C2B	5.25	1.47	1.40
23	b	618	CLA	OBD-CAD	5.25	1.30	1.22
24	a	412	PHO	C3C-C2C	5.27	1.48	1.36
23	c	910	CLA	C3B-C2B	5.27	1.47	1.40
23	C	512	CLA	C3C-C2C	5.29	1.48	1.36
23	c	907	CLA	C3B-C2B	5.29	1.47	1.40
23	b	604	CLA	C3B-C2B	5.30	1.47	1.40
23	d	403	CLA	C3C-C2C	5.31	1.48	1.36
23	c	903	CLA	OBD-CAD	5.31	1.30	1.22
24	a	413	PHO	CHC-C1C	5.32	1.49	1.38
23	B	602	CLA	O2A-CGA	5.32	1.49	1.33
23	b	612	CLA	C3C-C2C	5.33	1.48	1.36
23	c	904	CLA	C3B-C2B	5.33	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	909	CLA	O2D-CGD	5.36	1.46	1.33
23	b	612	CLA	O2D-CGD	5.40	1.47	1.33
23	c	904	CLA	C3C-C2C	5.41	1.48	1.36
23	C	504	CLA	C3B-C2B	5.42	1.47	1.40
23	c	908	CLA	C3C-C2C	5.45	1.48	1.36
23	b	615	CLA	C3C-C2C	5.46	1.48	1.36
24	A	409	PHO	C3B-C2B	5.49	1.48	1.36
23	c	913	CLA	C3B-C2B	5.49	1.47	1.40
23	C	513	CLA	C3C-C2C	5.53	1.48	1.36
23	a	409	CLA	OBD-CAD	5.54	1.30	1.22
23	b	613	CLA	C3C-C2C	5.57	1.48	1.36
24	A	408	PHO	CHB-C1B	5.67	1.49	1.38
23	B	607	CLA	C3B-C2B	5.67	1.47	1.40
23	C	506	CLA	C3B-C2B	5.70	1.47	1.40
26	f	102	SQD	O47-C7	5.71	1.46	1.33
23	c	912	CLA	C3B-C2B	5.72	1.47	1.40
23	b	605	CLA	OBD-CAD	5.72	1.31	1.22
23	A	406	CLA	OBD-CAD	5.73	1.31	1.22
23	C	503	CLA	C3B-C2B	5.74	1.47	1.40
23	c	913	CLA	C3C-C2C	5.75	1.49	1.36
23	d	403	CLA	C3B-C2B	5.81	1.48	1.40
23	c	903	CLA	C3B-C2B	5.82	1.48	1.40
23	B	603	CLA	C3C-C2C	5.85	1.49	1.36
23	b	605	CLA	C3C-C2C	5.86	1.49	1.36
23	c	905	CLA	C3C-C2C	5.89	1.49	1.36
23	B	603	CLA	C3B-C2B	5.97	1.48	1.40
23	b	610	CLA	C3C-C2C	5.99	1.49	1.36
23	b	609	CLA	C3B-C2B	6.01	1.48	1.40
23	C	508	CLA	C3C-C2C	6.04	1.49	1.36
23	C	508	CLA	C3B-C2B	6.23	1.48	1.40
23	c	902	CLA	C3B-C2B	6.23	1.48	1.40
23	c	914	CLA	C3B-C2B	6.25	1.48	1.40
24	a	413	PHO	CHB-C1B	6.28	1.50	1.38
23	C	513	CLA	C3B-C2B	6.57	1.49	1.40
23	C	507	CLA	C3B-C2B	7.24	1.49	1.40
23	c	910	CLA	OBD-CAD	7.84	1.34	1.22

All (2018) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	501	CLA	O2D-CGD-O1D	-9.91	103.33	123.79
23	c	907	CLA	CHD-C4C-C3C	-6.86	114.33	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	412	SQD	O7-S-C6	-6.60	101.37	106.94
23	b	619	CLA	CHD-C4C-C3C	-6.57	114.78	124.94
23	C	502	CLA	CHD-C4C-C3C	-6.54	114.83	124.94
23	B	604	CLA	CHD-C4C-C3C	-6.34	115.14	124.94
23	B	612	CLA	CHD-C4C-C3C	-6.17	115.40	124.94
37	f	101	HEM	CBA-CAA-C2A	-6.16	101.48	112.53
25	B	620	BCR	C38-C26-C25	-6.11	118.61	124.61
33	V	202	HTG	O5-C1-C2	-6.07	101.94	110.19
23	C	510	CLA	CHD-C4C-C3C	-6.04	115.60	124.94
26	A	412	SQD	C1-C2-C3	-6.03	98.09	109.97
23	C	506	CLA	CHD-C4C-C3C	-6.02	115.64	124.94
24	A	408	PHO	C3D-C2D-C1D	-5.92	96.27	105.77
38	H	101	RRX	C24-C23-C22	-5.91	117.21	126.22
23	B	607	CLA	CHD-C4C-C3C	-5.81	115.96	124.94
23	b	615	CLA	CHD-C4C-C3C	-5.81	115.97	124.94
23	a	414	CLA	CHD-C4C-C3C	-5.77	116.03	124.94
25	b	620	BCR	C33-C5-C6	-5.74	118.97	124.61
26	B	621	SQD	C1-O5-C5	-5.71	102.66	113.75
23	c	908	CLA	CHD-C4C-C3C	-5.70	116.14	124.94
23	B	602	CLA	CHD-C4C-C3C	-5.62	116.25	124.94
33	V	202	HTG	C1-O5-C5	-5.62	102.03	112.74
26	a	416	SQD	C1-O5-C5	-5.61	102.85	113.75
23	a	410	CLA	CHD-C4C-C3C	-5.61	116.27	124.94
26	a	416	SQD	C1-C2-C3	-5.60	98.93	109.97
23	B	617	CLA	CHD-C4C-C3C	-5.53	116.39	124.94
25	C	515	BCR	C7-C8-C9	-5.51	117.81	126.22
24	A	409	PHO	C4C-C3C-C2C	-5.50	100.67	106.81
26	A	412	SQD	C1-O5-C5	-5.48	103.12	113.75
26	a	401	SQD	C1-O5-C5	-5.46	103.15	113.75
23	b	606	CLA	CHD-C4C-C3C	-5.43	116.55	124.94
23	B	604	CLA	C1C-C2C-C3C	-5.38	100.48	106.91
25	D	404	BCR	C7-C8-C9	-5.37	118.03	126.22
24	A	408	PHO	C4C-C3C-C2C	-5.35	100.84	106.81
23	c	903	CLA	CHD-C4C-C3C	-5.29	116.76	124.94
23	b	604	CLA	CHD-C4C-C3C	-5.29	116.77	124.94
24	A	409	PHO	C3D-C2D-C1D	-5.26	97.32	105.77
23	B	605	CLA	C1C-C2C-C3C	-5.23	100.65	106.91
37	F	101	HEM	CBD-CAD-C3D	-5.18	98.46	113.55
36	D	408	LHG	O8-C23-O10	-5.18	110.13	123.49
23	A	406	CLA	C1C-C2C-C3C	-5.15	100.75	106.91
23	D	402	CLA	CHD-C4C-C3C	-5.13	117.01	124.94
23	C	504	CLA	C1C-C2C-C3C	-5.13	100.78	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402	CLA	CHD-C4C-C3C	-5.10	117.05	124.94
23	b	619	CLA	O1D-CGD-CBD	-5.10	117.31	124.62
27	C	519	LMG	O1-C7-C8	-5.08	98.89	110.99
26	f	102	SQD	O47-C7-O49	-5.06	118.78	125.50
23	d	403	CLA	O1D-CGD-CBD	-5.03	117.42	124.62
33	V	202	HTG	C1-C2-C3	-5.01	99.60	110.69
23	D	402	CLA	C4B-CHC-C1C	-4.99	118.54	129.26
23	c	912	CLA	CHD-C4C-C3C	-4.99	117.23	124.94
23	C	506	CLA	C3B-CAB-CBB	-4.95	116.19	126.32
23	c	908	CLA	O2D-CGD-O1D	-4.92	113.64	123.79
37	v	201	HEM	C3B-CAB-CBB	-4.92	116.92	124.46
37	V	201	HEM	C3B-CAB-CBB	-4.90	116.94	124.46
23	c	906	CLA	CHD-C4C-C3C	-4.86	117.43	124.94
25	K	101	BCR	C38-C26-C25	-4.82	119.88	124.61
25	d	404	BCR	C38-C26-C25	-4.81	119.88	124.61
23	A	410	CLA	CHD-C4C-C3C	-4.81	117.51	124.94
25	c	915	BCR	C33-C5-C6	-4.81	119.88	124.61
37	F	101	HEM	CAA-C2A-C1A	-4.80	121.79	127.01
23	B	616	CLA	CHD-C4C-C3C	-4.78	117.55	124.94
23	C	505	CLA	CHD-C4C-C3C	-4.77	117.57	124.94
23	B	607	CLA	C4B-CHC-C1C	-4.74	119.08	129.26
25	K	102	BCR	C11-C10-C9	-4.74	120.35	127.20
23	B	611	CLA	CHD-C4C-C3C	-4.73	117.64	124.94
23	b	606	CLA	O2D-CGD-O1D	-4.73	114.03	123.79
23	d	402	CLA	C4B-CHC-C1C	-4.72	119.12	129.26
23	b	610	CLA	CHD-C4C-C3C	-4.69	117.70	124.94
23	b	616	CLA	CHD-C4C-C3C	-4.68	117.71	124.94
23	B	614	CLA	CHD-C4C-C3C	-4.67	117.73	124.94
23	C	503	CLA	CHD-C4C-C3C	-4.65	117.76	124.94
23	b	608	CLA	CHD-C4C-C3C	-4.65	117.76	124.94
23	B	609	CLA	CHD-C4C-C3C	-4.62	117.80	124.94
23	b	618	CLA	C3B-CAB-CBB	-4.62	116.87	126.32
23	c	910	CLA	CHD-C4C-C3C	-4.61	117.81	124.94
24	a	413	PHO	C3D-C2D-C1D	-4.59	98.40	105.77
25	B	620	BCR	C24-C23-C22	-4.58	119.23	126.22
23	B	610	CLA	O2D-CGD-O1D	-4.58	114.33	123.79
23	B	610	CLA	CHD-C4C-C3C	-4.57	117.88	124.94
23	c	906	CLA	O2D-CGD-O1D	-4.56	114.38	123.79
23	c	902	CLA	C1C-C2C-C3C	-4.55	101.46	106.91
23	C	503	CLA	C3B-CAB-CBB	-4.55	117.01	126.32
24	a	413	PHO	O2D-CGD-O1D	-4.55	114.40	123.79
23	b	617	CLA	O2D-CGD-O1D	-4.53	114.43	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	618	BCR	C33-C5-C6	-4.53	120.16	124.61
23	C	501	CLA	CHD-C4C-C3C	-4.51	117.97	124.94
23	B	603	CLA	CHD-C4C-C3C	-4.50	117.98	124.94
23	B	602	CLA	O1D-CGD-CBD	-4.50	118.17	124.62
23	B	609	CLA	C1C-C2C-C3C	-4.50	101.52	106.91
23	C	504	CLA	C3B-CAB-CBB	-4.50	117.11	126.32
25	D	404	BCR	C40-C30-C25	-4.49	103.27	110.30
23	C	507	CLA	CHD-C4C-C3C	-4.48	118.02	124.94
24	a	412	PHO	O2D-CGD-O1D	-4.47	114.55	123.79
23	A	410	CLA	C4B-CHC-C1C	-4.47	119.65	129.26
23	b	606	CLA	C1C-C2C-C3C	-4.47	101.56	106.91
23	b	609	CLA	CHD-C4C-C3C	-4.46	118.05	124.94
23	b	618	CLA	C1C-C2C-C3C	-4.46	101.58	106.91
23	b	612	CLA	C3B-CAB-CBB	-4.45	117.21	126.32
23	d	402	CLA	C1C-C2C-C3C	-4.45	101.59	106.91
34	h	102	DGD	C3E-C4E-C5E	-4.45	102.44	110.20
24	a	412	PHO	C3D-C2D-C1D	-4.45	98.63	105.77
25	k	102	BCR	C7-C8-C9	-4.44	119.44	126.22
23	b	611	CLA	CHD-C4C-C3C	-4.44	118.08	124.94
23	c	902	CLA	O2D-CGD-O1D	-4.43	114.64	123.79
23	a	411	CLA	CHD-C4C-C3C	-4.43	118.10	124.94
23	b	607	CLA	CHD-C4C-C3C	-4.42	118.11	124.94
26	D	407	SQD	C1-C2-C3	-4.41	101.28	109.97
23	c	914	CLA	CHD-C4C-C3C	-4.41	118.13	124.94
23	d	403	CLA	C3B-CAB-CBB	-4.41	117.30	126.32
25	D	404	BCR	C38-C26-C25	-4.38	120.31	124.61
23	c	913	CLA	C3B-CAB-CBB	-4.37	117.37	126.32
23	b	606	CLA	C3B-CAB-CBB	-4.36	117.39	126.32
23	B	615	CLA	CHD-C4C-C3C	-4.35	118.22	124.94
23	b	617	CLA	C4B-CHC-C1C	-4.35	119.93	129.26
23	C	509	CLA	C1C-C2C-C3C	-4.34	101.72	106.91
23	b	615	CLA	C4C-C3C-C2C	-4.34	99.90	106.94
23	b	607	CLA	C3B-CAB-CBB	-4.32	117.48	126.32
23	c	904	CLA	C3B-CAB-CBB	-4.31	117.51	126.32
26	D	407	SQD	C1-O5-C5	-4.31	105.39	113.75
23	b	617	CLA	C4-C3-C2	-4.30	115.05	123.50
23	B	617	CLA	O2D-CGD-O1D	-4.30	114.91	123.79
23	B	604	CLA	O2D-CGD-O1D	-4.30	114.91	123.79
23	C	512	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
23	A	406	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
23	a	409	CLA	CHD-C4C-C3C	-4.30	118.30	124.94
23	b	607	CLA	C1C-C2C-C3C	-4.29	101.77	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	917	DGD	O3G-C3G-C2G	-4.29	100.77	110.99
23	d	402	CLA	O2D-CGD-O1D	-4.29	114.93	123.79
25	b	620	BCR	C7-C8-C9	-4.28	119.69	126.22
23	C	501	CLA	O1D-CGD-CBD	-4.27	118.50	124.62
25	d	404	BCR	C15-C14-C13	-4.27	121.03	127.20
23	c	902	CLA	CHD-C4C-C3C	-4.26	118.36	124.94
37	F	101	HEM	CBA-CAA-C2A	-4.26	104.89	112.53
36	d	407	LHG	O8-C23-O10	-4.25	112.52	123.49
23	C	502	CLA	C3B-CAB-CBB	-4.25	117.63	126.32
23	A	405	CLA	C1D-CHD-C4C	-4.23	116.20	122.60
25	t	101	BCR	C11-C10-C9	-4.23	121.09	127.20
23	b	611	CLA	C1C-C2C-C3C	-4.21	101.88	106.91
23	a	410	CLA	C3B-CAB-CBB	-4.20	117.72	126.32
23	c	912	CLA	C3B-CAB-CBB	-4.20	117.73	126.32
23	a	411	CLA	C1C-C2C-C3C	-4.19	101.89	106.91
23	b	617	CLA	CHD-C4C-C3C	-4.19	118.47	124.94
23	B	606	CLA	CHD-C4C-C3C	-4.19	118.47	124.94
23	A	406	CLA	C3B-CAB-CBB	-4.18	117.77	126.32
23	c	914	CLA	C3B-CAB-CBB	-4.16	117.81	126.32
34	C	518	DGD	O3G-C3G-C2G	-4.16	101.10	110.99
23	b	614	CLA	CHD-C4C-C3C	-4.15	118.53	124.94
23	B	607	CLA	O2D-CGD-O1D	-4.13	115.26	123.79
23	b	618	CLA	C1D-CHD-C4C	-4.12	116.37	122.60
23	b	615	CLA	C4B-CHC-C1C	-4.12	120.42	129.26
23	c	912	CLA	C1C-C2C-C3C	-4.11	101.99	106.91
34	H	102	DGD	O1G-C1A-O1A	-4.10	112.90	123.49
23	b	605	CLA	O2D-CGD-O1D	-4.10	115.32	123.79
23	C	502	CLA	C4B-CHC-C1C	-4.10	120.46	129.26
23	A	407	CLA	C1C-C2C-C3C	-4.10	102.01	106.91
23	a	410	CLA	C1D-CHD-C4C	-4.10	116.40	122.60
25	K	102	BCR	C7-C8-C9	-4.10	119.97	126.22
23	D	402	CLA	C3B-CAB-CBB	-4.09	117.95	126.32
27	B	622	LMG	O7-C10-O9	-4.09	112.70	123.67
34	C	516	DGD	O3G-C3G-C2G	-4.08	101.29	110.99
24	A	408	PHO	C4D-ND-C1D	-4.07	99.58	107.05
25	t	101	BCR	C38-C26-C25	-4.06	120.62	124.61
28	a	419	PL9	C37-C38-C39	-4.06	118.94	127.76
37	f	101	HEM	CBD-CAD-C3D	-4.06	101.75	113.55
23	b	613	CLA	C1C-C2C-C3C	-4.05	102.06	106.91
23	B	612	CLA	O2D-CGD-O1D	-4.05	115.42	123.79
25	d	404	BCR	C24-C23-C22	-4.04	120.05	126.22
25	t	101	BCR	C28-C27-C26	-4.03	107.48	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	CAA-CBA-CGA	-4.03	101.53	113.32
23	c	903	CLA	C1D-CHD-C4C	-4.02	116.52	122.60
23	d	403	CLA	C1C-C2C-C3C	-4.01	102.11	106.91
27	b	623	LMG	O8-C28-O10	-4.00	113.17	123.49
23	C	507	CLA	CBC-CAC-C3C	-3.99	100.21	112.39
25	a	415	BCR	C38-C26-C25	-3.98	120.69	124.61
37	V	201	HEM	CBD-CAD-C3D	-3.98	101.97	113.55
23	a	414	CLA	C3B-CAB-CBB	-3.98	118.18	126.32
23	B	605	CLA	C1C-NC-C4C	-3.97	101.44	106.27
24	a	412	PHO	C4C-C3C-C2C	-3.97	102.38	106.81
23	C	501	CLA	C3B-CAB-CBB	-3.97	118.20	126.32
36	L	101	LHG	O7-C7-O9	-3.97	113.03	123.67
23	b	605	CLA	C3B-CAB-CBB	-3.96	118.21	126.32
23	C	511	CLA	CHD-C4C-C3C	-3.95	118.83	124.94
23	b	618	CLA	CHD-C4C-C3C	-3.95	118.84	124.94
26	A	412	SQD	C45-O47-C7	-3.95	108.42	117.89
23	B	612	CLA	C1D-CHD-C4C	-3.94	116.63	122.60
23	B	608	CLA	C3B-CAB-CBB	-3.94	118.25	126.32
23	a	414	CLA	C4B-CHC-C1C	-3.93	120.82	129.26
23	c	912	CLA	O2D-CGD-O1D	-3.92	115.69	123.79
23	B	612	CLA	C3B-CAB-CBB	-3.92	118.31	126.32
28	d	405	PL9	C36-C37-C38	-3.90	101.47	111.69
23	B	609	CLA	C4B-CHC-C1C	-3.89	120.91	129.26
37	f	101	HEM	CAA-C2A-C1A	-3.88	122.79	127.01
23	B	613	CLA	C4B-CHC-C1C	-3.87	120.95	129.26
23	b	614	CLA	C1C-C2C-C3C	-3.87	102.28	106.91
23	B	616	CLA	C3B-CAB-CBB	-3.86	118.41	126.32
25	c	916	BCR	C38-C26-C25	-3.86	120.81	124.61
23	C	508	CLA	C1C-C2C-C3C	-3.86	102.29	106.91
23	D	403	CLA	C1C-C2C-C3C	-3.86	102.29	106.91
25	T	101	BCR	C20-C21-C22	-3.85	121.63	127.20
25	D	404	BCR	C24-C23-C22	-3.85	120.34	126.22
23	B	612	CLA	C4B-CHC-C1C	-3.85	121.00	129.26
25	K	102	BCR	C38-C26-C25	-3.83	120.84	124.61
23	a	411	CLA	C4B-CHC-C1C	-3.83	121.03	129.26
23	C	506	CLA	C1C-C2C-C3C	-3.82	102.34	106.91
23	d	403	CLA	CHD-C4C-C3C	-3.81	119.05	124.94
23	B	607	CLA	C3B-CAB-CBB	-3.81	118.52	126.32
23	b	618	CLA	O2D-CGD-O1D	-3.81	115.93	123.79
25	a	415	BCR	C28-C27-C26	-3.81	107.83	113.87
23	C	501	CLA	C1C-C2C-C3C	-3.80	102.36	106.91
25	D	404	BCR	C28-C27-C26	-3.79	107.85	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	t	101	BCR	C33-C5-C6	-3.78	120.89	124.61
28	d	405	PL9	C40-C39-C38	-3.78	116.08	123.50
37	v	201	HEM	CBD-CAD-C3D	-3.78	102.56	113.55
23	C	503	CLA	C1C-C2C-C3C	-3.77	102.40	106.91
23	b	607	CLA	C6-C5-C3	-3.77	104.21	112.48
25	K	102	BCR	C33-C5-C6	-3.77	120.91	124.61
23	c	908	CLA	C1C-C2C-C3C	-3.76	102.41	106.91
34	c	919	DGD	C6B-C5B-C4B	-3.75	95.15	114.53
23	b	607	CLA	O2D-CGD-O1D	-3.75	116.05	123.79
23	C	507	CLA	C3B-CAB-CBB	-3.75	118.65	126.32
23	C	513	CLA	CHD-C4C-C3C	-3.75	119.15	124.94
23	C	507	CLA	C1C-C2C-C3C	-3.74	102.43	106.91
23	b	604	CLA	C1C-C2C-C3C	-3.73	102.45	106.91
23	b	611	CLA	O2D-CGD-O1D	-3.72	116.11	123.79
38	H	101	RRX	C7-C8-C9	-3.72	120.55	126.22
23	B	602	CLA	C1C-C2C-C3C	-3.72	102.46	106.91
27	Z	101	LMG	C9-C8-C7	-3.71	103.38	112.07
30	m	101	LMT	C3'-C4'-C5'	-3.71	102.44	110.84
26	D	407	SQD	C44-O6-C1	-3.71	106.02	113.82
23	b	617	CLA	C3B-CAB-CBB	-3.71	118.73	126.32
23	B	602	CLA	C3B-CAB-CBB	-3.71	118.73	126.32
23	b	606	CLA	C5-C3-C2	-3.70	114.03	121.05
23	B	615	CLA	O2D-CGD-O1D	-3.69	116.16	123.79
23	B	610	CLA	C4B-CHC-C1C	-3.69	121.34	129.26
23	A	405	CLA	C3B-CAB-CBB	-3.68	118.78	126.32
24	a	413	PHO	C4D-ND-C1D	-3.68	100.29	107.05
27	D	411	LMG	O8-C28-O10	-3.68	113.99	123.49
23	B	607	CLA	C1C-C2C-C3C	-3.68	102.51	106.91
28	D	405	PL9	C40-C39-C38	-3.67	116.29	123.50
23	B	609	CLA	O1D-CGD-CBD	-3.67	119.37	124.62
25	B	618	BCR	C15-C14-C13	-3.67	121.90	127.20
25	d	404	BCR	C16-C15-C14	-3.66	115.30	123.39
28	D	405	PL9	C27-C28-C29	-3.66	119.81	127.76
25	k	101	BCR	C38-C26-C25	-3.65	121.02	124.61
23	d	402	CLA	OBD-CAD-C3D	-3.65	120.90	128.35
24	A	409	PHO	C4D-ND-C1D	-3.65	100.35	107.05
23	a	414	CLA	C1C-C2C-C3C	-3.64	102.55	106.91
23	b	605	CLA	CHD-C4C-C3C	-3.64	119.32	124.94
23	b	609	CLA	C4B-CHC-C1C	-3.63	121.46	129.26
23	c	906	CLA	C3B-CAB-CBB	-3.63	118.89	126.32
30	M	102	LMT	C1'-O5'-C5'	-3.63	106.69	113.75
23	B	611	CLA	O2A-CGA-O1A	-3.63	114.12	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C1C-C2C-C3C	-3.63	102.57	106.91
24	a	413	PHO	C4C-C3C-C2C	-3.62	102.77	106.81
23	C	513	CLA	C1C-C2C-C3C	-3.62	102.57	106.91
23	b	613	CLA	CHD-C4C-C3C	-3.62	119.34	124.94
23	B	616	CLA	C1C-C2C-C3C	-3.62	102.58	106.91
23	b	608	CLA	C1C-C2C-C3C	-3.62	102.58	106.91
23	c	910	CLA	O1D-CGD-CBD	-3.61	119.45	124.62
23	C	505	CLA	C3B-CAB-CBB	-3.59	118.96	126.32
23	b	617	CLA	O2A-CGA-O1A	-3.59	114.22	123.49
25	b	622	BCR	C24-C23-C22	-3.58	120.75	126.22
23	b	615	CLA	O2D-CGD-O1D	-3.58	116.39	123.79
36	L	101	LHG	C6-C5-C4	-3.58	103.70	112.07
23	c	904	CLA	CHD-C4C-C3C	-3.58	119.41	124.94
23	A	410	CLA	C1C-C2C-C3C	-3.58	102.63	106.91
23	b	605	CLA	C1C-C2C-C3C	-3.57	102.64	106.91
23	B	612	CLA	C1C-C2C-C3C	-3.56	102.65	106.91
23	B	609	CLA	O2D-CGD-O1D	-3.56	116.44	123.79
23	c	905	CLA	C1C-C2C-C3C	-3.55	102.66	106.91
23	B	611	CLA	O2D-CGD-O1D	-3.54	116.47	123.79
23	B	608	CLA	CBC-CAC-C3C	-3.54	101.58	112.39
23	c	902	CLA	C4B-CHC-C1C	-3.53	121.68	129.26
23	C	509	CLA	CHD-C4C-C3C	-3.53	119.49	124.94
23	B	604	CLA	C3B-CAB-CBB	-3.53	119.10	126.32
23	B	606	CLA	O2A-CGA-O1A	-3.52	114.41	123.49
23	c	912	CLA	C1D-CHD-C4C	-3.52	117.28	122.60
23	B	602	CLA	O2D-CGD-O1D	-3.51	116.54	123.79
23	D	402	CLA	O2D-CGD-O1D	-3.51	116.55	123.79
27	b	623	LMG	O7-C10-O9	-3.50	114.28	123.67
23	A	405	CLA	CHD-C4C-C3C	-3.50	119.53	124.94
23	c	906	CLA	CBC-CAC-C3C	-3.49	101.73	112.39
23	B	613	CLA	CHD-C4C-C3C	-3.49	119.54	124.94
23	C	512	CLA	O2D-CGD-O1D	-3.49	116.58	123.79
23	b	619	CLA	C3B-CAB-CBB	-3.48	119.19	126.32
23	c	904	CLA	OBD-CAD-C3D	-3.47	121.26	128.35
23	C	505	CLA	C1C-C2C-C3C	-3.47	102.76	106.91
25	C	515	BCR	C33-C5-C6	-3.46	121.20	124.61
28	d	405	PL9	C22-C23-C24	-3.46	120.23	127.76
23	c	904	CLA	C1C-C2C-C3C	-3.46	102.77	106.91
23	c	905	CLA	CHD-C4C-C3C	-3.46	119.59	124.94
23	b	612	CLA	CHD-C4C-C3C	-3.46	119.60	124.94
23	a	409	CLA	C1C-C2C-C3C	-3.46	102.78	106.91
23	c	911	CLA	CHD-C4C-C3C	-3.46	119.60	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	O2D-CGD-O1D	-3.46	116.66	123.79
23	C	511	CLA	O2D-CGD-O1D	-3.45	116.67	123.79
23	c	903	CLA	O2D-CGD-O1D	-3.44	116.68	123.79
23	c	914	CLA	C1C-C2C-C3C	-3.44	102.79	106.91
28	D	405	PL9	C36-C37-C38	-3.44	102.68	111.69
23	C	510	CLA	C4B-CHC-C1C	-3.44	121.88	129.26
23	c	910	CLA	C1C-C2C-C3C	-3.44	102.80	106.91
23	b	616	CLA	C4B-CHC-C1C	-3.44	121.88	129.26
23	b	609	CLA	C1C-C2C-C3C	-3.43	102.80	106.91
23	a	414	CLA	C1C-NC-C4C	-3.42	102.11	106.27
23	B	608	CLA	C1C-C2C-C3C	-3.42	102.82	106.91
23	B	608	CLA	CHD-C4C-C3C	-3.41	119.67	124.94
30	C	520	LMT	C2'-C3'-C4'	-3.41	102.11	109.60
25	b	620	BCR	C11-C10-C9	-3.39	122.29	127.20
28	A	414	PL9	C22-C23-C24	-3.39	120.39	127.76
23	B	607	CLA	O1D-CGD-CBD	-3.39	119.77	124.62
23	C	513	CLA	O2D-CGD-O1D	-3.38	116.80	123.79
24	a	412	PHO	C1C-C2C-C3C	-3.37	102.47	106.50
25	B	620	BCR	C15-C14-C13	-3.37	122.33	127.20
25	K	102	BCR	C24-C23-C22	-3.37	121.08	126.22
23	c	909	CLA	CHD-C4C-C3C	-3.37	119.74	124.94
23	B	605	CLA	CHD-C4C-C3C	-3.37	119.74	124.94
23	C	509	CLA	C4B-CHC-C1C	-3.36	122.04	129.26
23	A	407	CLA	O2D-CGD-O1D	-3.35	116.87	123.79
24	A	408	PHO	C1C-NC-C4C	-3.34	99.91	106.51
23	a	410	CLA	C4B-CHC-C1C	-3.34	122.09	129.26
23	c	913	CLA	C1C-C2C-C3C	-3.33	102.92	106.91
28	d	405	PL9	C31-C32-C33	-3.33	102.97	111.69
23	D	402	CLA	CHC-C1C-C2C	-3.32	117.61	126.35
25	B	618	BCR	C7-C8-C9	-3.32	121.15	126.22
28	a	419	PL9	C42-C43-C44	-3.32	120.54	127.76
28	A	414	PL9	C37-C38-C39	-3.32	120.55	127.76
26	A	418	SQD	C1-O5-C5	-3.32	107.31	113.75
34	h	102	DGD	O1G-C1A-O1A	-3.31	114.94	123.49
27	C	519	LMG	O5-C6-C5	-3.31	100.38	111.33
23	c	914	CLA	O2D-CGD-O1D	-3.31	116.95	123.79
23	a	410	CLA	C1C-C2C-C3C	-3.31	102.95	106.91
23	C	504	CLA	C5-C3-C2	-3.31	114.78	121.05
23	c	913	CLA	CHD-C4C-C3C	-3.31	119.83	124.94
23	b	614	CLA	O2D-CGD-O1D	-3.30	116.97	123.79
23	B	616	CLA	C1D-CHD-C4C	-3.30	117.60	122.60
24	a	412	PHO	CBA-CAA-C2A	-3.30	104.42	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	402	LMT	O5'-C1'-O1'	-3.30	102.11	110.05
23	B	614	CLA	C3B-CAB-CBB	-3.29	119.59	126.32
23	d	403	CLA	C4B-CHC-C1C	-3.28	122.21	129.26
23	B	616	CLA	C11-C10-C8	-3.28	104.60	115.49
23	b	614	CLA	CBC-CAC-C3C	-3.28	102.37	112.39
23	B	603	CLA	O2D-CGD-O1D	-3.28	117.02	123.79
23	a	411	CLA	C2A-C1A-CHA	-3.28	117.85	123.89
34	C	517	DGD	O2G-C1B-O1B	-3.27	114.89	123.67
25	K	102	BCR	C20-C21-C22	-3.27	122.48	127.20
23	A	407	CLA	CHD-C4C-C3C	-3.26	119.91	124.94
25	A	411	BCR	C11-C10-C9	-3.25	122.50	127.20
23	B	613	CLA	C3B-CAB-CBB	-3.25	119.66	126.32
37	V	201	HEM	C3C-CAC-CBC	-3.25	119.47	124.46
23	A	406	CLA	C4B-CHC-C1C	-3.24	122.29	129.26
23	C	506	CLA	O1D-CGD-CBD	-3.24	119.97	124.62
27	c	920	LMG	O5-C6-C5	-3.24	100.62	111.33
23	b	604	CLA	O2D-CGD-O1D	-3.24	117.10	123.79
26	a	416	SQD	C45-O47-C7	-3.23	110.13	117.89
23	c	911	CLA	C1C-C2C-C3C	-3.23	103.04	106.91
23	c	907	CLA	C1C-C2C-C3C	-3.23	103.05	106.91
23	D	403	CLA	C4B-CHC-C1C	-3.23	122.32	129.26
23	b	610	CLA	C4B-CHC-C1C	-3.22	122.34	129.26
23	A	406	CLA	C1C-NC-C4C	-3.22	102.35	106.27
23	B	605	CLA	O2D-CGD-O1D	-3.22	117.13	123.79
23	D	402	CLA	C1D-CHD-C4C	-3.22	117.73	122.60
34	c	919	DGD	O3G-C3G-C2G	-3.22	103.34	110.99
23	A	405	CLA	CAA-CBA-CGA	-3.21	103.91	113.32
25	C	514	BCR	C7-C8-C9	-3.21	121.33	126.22
30	b	625	LMT	C3'-C4'-C5'	-3.21	104.61	110.20
23	A	406	CLA	C1D-CHD-C4C	-3.20	117.75	122.60
38	H	101	RRX	C16-C15-C14	-3.19	116.33	123.39
23	C	512	CLA	C1C-C2C-C3C	-3.19	103.09	106.91
27	A	413	LMG	O6-C1-C2	-3.19	103.73	110.28
23	c	908	CLA	O1D-CGD-CBD	-3.19	120.05	124.62
34	c	917	DGD	O5D-C6D-C5D	-3.19	103.31	109.08
25	A	411	BCR	C8-C7-C6	-3.19	117.75	127.32
25	A	411	BCR	C15-C16-C17	-3.18	116.35	123.39
23	B	615	CLA	CBC-CAC-C3C	-3.18	102.69	112.39
23	b	608	CLA	C1C-NC-C4C	-3.18	102.41	106.27
25	D	404	BCR	C10-C11-C12	-3.17	113.45	123.13
36	d	408	LHG	C34-C33-C32	-3.17	98.17	114.53
23	C	501	CLA	C2A-C1A-CHA	-3.17	118.05	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	403	CLA	CHD-C4C-C3C	-3.17	120.05	124.94
24	A	408	PHO	CHC-C1C-C2C	-3.16	118.46	125.61
28	a	419	PL9	C7-C3-C2	-3.16	120.80	123.42
25	B	618	BCR	C24-C23-C22	-3.16	121.41	126.22
27	B	622	LMG	C31-C30-C29	-3.15	101.72	113.29
25	c	915	BCR	C38-C26-C25	-3.15	121.51	124.61
23	C	509	CLA	C3B-CAB-CBB	-3.15	119.87	126.32
23	B	603	CLA	C3B-CAB-CBB	-3.15	119.87	126.32
25	T	101	BCR	C7-C8-C9	-3.15	121.42	126.22
23	B	604	CLA	O2A-CGA-O1A	-3.14	115.38	123.49
27	C	519	LMG	O8-C28-O10	-3.14	115.38	123.49
26	A	418	SQD	C1-C2-C3	-3.13	103.81	109.97
23	b	613	CLA	CAA-CBA-CGA	-3.13	104.16	113.32
23	a	410	CLA	CBC-CAC-C3C	-3.12	102.87	112.39
25	d	404	BCR	C40-C30-C25	-3.12	105.42	110.30
23	b	617	CLA	C1C-C2C-C3C	-3.12	103.18	106.91
23	B	611	CLA	C1C-C2C-C3C	-3.11	103.18	106.91
26	D	407	SQD	O9-S-O7	-3.11	102.13	113.48
23	d	402	CLA	C5-C3-C2	-3.11	115.15	121.05
25	B	618	BCR	C10-C11-C12	-3.11	113.64	123.13
23	b	609	CLA	O2D-CGD-O1D	-3.11	117.37	123.79
23	A	406	CLA	OBD-CAD-C3D	-3.11	122.01	128.35
25	A	411	BCR	C33-C5-C6	-3.11	121.55	124.61
25	t	101	BCR	C12-C13-C14	-3.11	113.98	118.98
23	c	908	CLA	C4B-CHC-C1C	-3.10	122.61	129.26
23	b	611	CLA	O2A-CGA-O1A	-3.09	115.50	123.49
23	C	510	CLA	O2D-CGD-O1D	-3.09	117.41	123.79
23	a	411	CLA	C1C-NC-C4C	-3.08	102.53	106.27
24	A	409	PHO	CAA-C2A-C1A	-3.08	104.76	112.86
34	C	516	DGD	C3G-C2G-C1G	-3.07	104.88	112.07
23	b	616	CLA	C3B-CAB-CBB	-3.07	120.03	126.32
23	B	610	CLA	C1C-C2C-C3C	-3.07	103.24	106.91
28	D	405	PL9	C22-C23-C24	-3.07	121.09	127.76
25	a	415	BCR	C7-C8-C9	-3.06	121.54	126.22
24	A	409	PHO	O2D-CGD-O1D	-3.06	117.46	123.79
23	b	612	CLA	C4C-C3C-C2C	-3.06	101.97	106.94
30	J	102	LMT	C3'-C4'-C5'	-3.06	104.87	110.20
23	c	907	CLA	O2A-CGA-O1A	-3.05	115.61	123.49
25	K	102	BCR	C16-C17-C18	-3.05	122.79	127.20
23	B	605	CLA	C3B-CAB-CBB	-3.05	120.07	126.32
25	t	101	BCR	C7-C6-C5	-3.05	114.39	121.37
23	c	909	CLA	C1C-C2C-C3C	-3.05	103.27	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	O2D-CGD-O1D	-3.04	117.50	123.79
38	h	101	RRX	C38-C26-C25	-3.04	121.62	124.61
23	a	411	CLA	C3B-CAB-CBB	-3.03	120.11	126.32
23	B	610	CLA	CBC-CAC-C3C	-3.03	103.15	112.39
23	C	505	CLA	C4B-CHC-C1C	-3.03	122.76	129.26
25	b	620	BCR	C24-C23-C22	-3.02	121.61	126.22
23	A	406	CLA	CBC-CAC-C3C	-3.02	103.17	112.39
23	B	617	CLA	C4B-CHC-C1C	-3.02	122.78	129.26
23	B	615	CLA	C4B-CHC-C1C	-3.02	122.78	129.26
23	a	409	CLA	C7-C6-C5	-3.02	104.15	113.06
23	B	606	CLA	C2A-C1A-CHA	-3.02	118.33	123.89
25	T	101	BCR	C15-C16-C17	-3.01	116.73	123.39
30	M	102	LMT	C3'-C4'-C5'	-3.01	104.03	110.84
23	C	509	CLA	O2A-CGA-O1A	-3.01	115.73	123.49
23	a	409	CLA	C4B-CHC-C1C	-3.01	122.81	129.26
23	C	508	CLA	CHD-C4C-C3C	-3.00	120.30	124.94
25	K	101	BCR	C40-C30-C25	-3.00	105.60	110.30
23	a	409	CLA	CAC-C3C-C2C	-3.00	122.25	127.51
23	c	911	CLA	C4-C3-C2	-3.00	117.62	123.50
24	a	412	PHO	CHD-C1D-ND	-3.00	119.06	124.66
23	C	512	CLA	C3B-CAB-CBB	-3.00	120.19	126.32
28	D	405	PL9	C31-C32-C33	-2.99	103.84	111.69
25	A	411	BCR	C28-C27-C26	-2.99	109.12	113.87
34	c	918	DGD	O6E-C5E-C4E	-2.99	104.07	109.68
23	b	619	CLA	C4B-CHC-C1C	-2.99	122.84	129.26
24	a	412	PHO	C1C-NC-C4C	-2.99	100.60	106.51
23	B	614	CLA	C1C-C2C-C3C	-2.99	103.33	106.91
23	B	614	CLA	C2A-C1A-CHA	-2.99	118.38	123.89
25	a	415	BCR	C16-C15-C14	-2.99	116.79	123.39
23	c	908	CLA	C3B-CAB-CBB	-2.98	120.21	126.32
23	b	619	CLA	C4C-C3C-C2C	-2.98	102.10	106.94
27	B	622	LMG	O5-C6-C5	-2.98	101.49	111.33
23	C	502	CLA	O2D-CGD-O1D	-2.97	117.65	123.79
23	B	604	CLA	C2A-C1A-CHA	-2.97	118.41	123.89
23	c	903	CLA	C1C-C2C-C3C	-2.97	103.36	106.91
25	k	101	BCR	C24-C23-C22	-2.97	121.69	126.22
24	a	412	PHO	CHD-C4C-C3C	-2.97	118.68	124.58
23	C	502	CLA	C1C-C2C-C3C	-2.97	103.36	106.91
23	C	511	CLA	C3B-CAB-CBB	-2.97	120.25	126.32
23	B	605	CLA	CAA-C2A-C3A	-2.96	104.70	113.22
23	B	604	CLA	C1D-CHD-C4C	-2.96	118.13	122.60
25	C	514	BCR	C11-C10-C9	-2.94	122.95	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	919	DGD	C3E-C4E-C5E	-2.94	105.08	110.20
23	C	504	CLA	CHD-C4C-C3C	-2.93	120.41	124.94
23	C	508	CLA	O2A-CGA-O1A	-2.93	115.93	123.49
33	B	624	HTG	C3'-C2'-C1'	-2.93	101.08	113.18
25	b	622	BCR	C3-C4-C5	-2.93	109.22	113.87
23	b	615	CLA	C1C-NC-C4C	-2.93	102.71	106.27
23	b	616	CLA	C1C-C2C-C3C	-2.92	103.41	106.91
23	B	606	CLA	C1C-C2C-C3C	-2.92	103.41	106.91
23	b	609	CLA	O2A-CGA-O1A	-2.92	115.95	123.49
23	b	605	CLA	CMB-C2B-C1B	-2.92	123.54	128.36
23	c	913	CLA	O2D-CGD-O1D	-2.92	117.77	123.79
23	C	501	CLA	CBC-CAC-C3C	-2.92	103.49	112.39
34	c	919	DGD	O1G-C1A-O1A	-2.91	115.98	123.49
23	A	406	CLA	CAC-C3C-C2C	-2.91	122.41	127.51
23	D	402	CLA	CAA-CBA-CGA	-2.91	104.81	113.32
23	C	506	CLA	C1C-NC-C4C	-2.90	102.74	106.27
26	D	407	SQD	C46-C45-C44	-2.90	105.28	112.07
23	B	615	CLA	C4-C3-C2	-2.90	117.81	123.50
25	B	620	BCR	C32-C1-C6	-2.90	105.75	110.30
23	B	609	CLA	C2A-C1A-CHA	-2.90	118.55	123.89
38	h	101	RRX	C16-C17-C18	-2.90	123.01	127.20
23	C	506	CLA	O2D-CGD-O1D	-2.90	117.81	123.79
23	B	615	CLA	O2A-CGA-O1A	-2.89	116.03	123.49
34	C	516	DGD	O1G-C1G-C2G	-2.89	100.91	108.69
23	B	603	CLA	C1C-C2C-C3C	-2.89	103.46	106.91
26	B	621	SQD	O48-C23-O10	-2.89	116.04	123.49
26	f	102	SQD	C1-O6-C44	-2.88	109.39	113.58
23	b	612	CLA	O2D-CGD-O1D	-2.88	117.83	123.79
25	A	411	BCR	C7-C8-C9	-2.88	121.82	126.22
27	d	410	LMG	O8-C28-O10	-2.88	116.05	123.49
23	b	606	CLA	C4B-CHC-C1C	-2.88	123.07	129.26
24	a	413	PHO	CHD-C1D-ND	-2.88	119.28	124.66
25	b	621	BCR	C8-C7-C6	-2.88	118.68	127.32
23	B	612	CLA	C1C-NC-C4C	-2.87	102.77	106.27
36	d	408	LHG	O8-C23-O10	-2.87	116.08	123.49
23	b	616	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
23	D	402	CLA	O2A-CGA-O1A	-2.87	116.09	123.49
23	C	512	CLA	O1D-CGD-CBD	-2.86	120.52	124.62
23	b	607	CLA	O2A-CGA-O1A	-2.86	116.11	123.49
23	A	410	CLA	C5-C3-C2	-2.85	115.64	121.05
27	B	622	LMG	O8-C28-O10	-2.85	116.13	123.49
23	B	605	CLA	CGD-CBD-CAD	-2.85	100.97	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	416	SQD	O5-C1-C2	-2.85	104.44	110.28
34	c	917	DGD	C6D-O5D-C1E	-2.85	107.84	113.82
25	B	618	BCR	C16-C15-C14	-2.85	117.10	123.39
25	T	101	BCR	C12-C13-C14	-2.84	114.40	118.98
25	t	101	BCR	C20-C21-C22	-2.84	123.09	127.20
23	c	905	CLA	C3B-CAB-CBB	-2.83	120.52	126.32
23	B	617	CLA	C4C-C3C-C2C	-2.83	102.35	106.94
24	A	408	PHO	CHD-C1D-ND	-2.83	119.38	124.66
34	c	919	DGD	C4A-C3A-C2A	-2.83	102.93	113.29
28	D	405	PL9	C42-C41-C39	-2.82	103.51	112.71
25	D	404	BCR	C29-C28-C27	-2.82	104.42	111.53
23	b	616	CLA	C2A-C1A-CHA	-2.82	118.69	123.89
23	c	903	CLA	C3B-CAB-CBB	-2.82	120.55	126.32
23	b	608	CLA	C3A-C2A-C1A	-2.82	96.72	101.50
23	B	606	CLA	C4C-C3C-C2C	-2.81	102.38	106.94
23	a	411	CLA	CBC-CAC-C3C	-2.81	103.80	112.39
36	l	101	LHG	O7-C7-O9	-2.81	116.12	123.67
23	C	502	CLA	C5-C3-C2	-2.81	115.72	121.05
23	C	509	CLA	O2D-CGD-O1D	-2.80	118.00	123.79
23	b	608	CLA	C4C-C3C-C2C	-2.80	102.40	106.94
23	B	617	CLA	C1C-NC-C4C	-2.80	102.86	106.27
25	B	620	BCR	C7-C8-C9	-2.79	121.95	126.22
26	L	103	SQD	O5-C1-C2	-2.79	104.54	110.28
23	a	411	CLA	CBA-CAA-C2A	-2.79	105.85	113.73
25	t	101	BCR	C29-C28-C27	-2.79	104.49	111.53
24	A	409	PHO	C3B-C2B-C1B	-2.79	100.28	106.33
23	b	614	CLA	C4B-CHC-C1C	-2.79	123.27	129.26
23	D	403	CLA	C3B-CAB-CBB	-2.78	120.62	126.32
23	b	604	CLA	C3B-CAB-CBB	-2.78	120.62	126.32
23	C	512	CLA	CBA-CAA-C2A	-2.78	105.89	113.73
23	A	407	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
23	B	605	CLA	C2A-C1A-CHA	-2.77	118.78	123.89
34	D	406	DGD	O2D-C2D-C3D	-2.77	104.10	110.34
24	a	412	PHO	CAA-CBA-CGA	-2.76	105.24	113.32
38	H	101	RRX	C10-C11-C12	-2.76	114.72	123.13
23	B	617	CLA	C2A-C1A-CHA	-2.76	118.80	123.89
25	T	101	BCR	C23-C24-C25	-2.76	119.03	127.32
23	c	909	CLA	C4C-C3C-C2C	-2.76	102.47	106.94
23	C	508	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
23	C	503	CLA	O2D-CGD-O1D	-2.75	118.10	123.79
23	C	511	CLA	CBC-CAC-C3C	-2.75	103.98	112.39
28	d	405	PL9	C37-C36-C34	-2.75	103.75	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	411	BCR	C24-C23-C22	-2.75	122.02	126.22
23	c	905	CLA	C7-C6-C5	-2.74	104.95	113.06
28	D	405	PL9	C3-C2-C1	-2.74	121.30	122.97
26	A	418	SQD	O48-C23-O10	-2.73	116.44	123.49
31	C	524	GOL	O3-C3-C2	-2.73	96.94	110.18
26	A	412	SQD	O48-C23-O10	-2.73	116.44	123.49
23	c	907	CLA	C1D-CHD-C4C	-2.73	118.47	122.60
23	B	602	CLA	C1D-CHD-C4C	-2.73	118.47	122.60
23	B	614	CLA	CBC-CAC-C3C	-2.73	104.07	112.39
23	b	604	CLA	C1D-CHD-C4C	-2.73	118.48	122.60
34	c	918	DGD	O1G-C1A-O1A	-2.73	116.46	123.49
23	B	612	CLA	C2A-C1A-CHA	-2.73	118.87	123.89
23	A	405	CLA	O2D-CGD-O1D	-2.72	118.16	123.79
23	A	407	CLA	CAC-C3C-C2C	-2.72	122.73	127.51
23	D	402	CLA	C2A-C1A-CHA	-2.72	118.87	123.89
23	c	902	CLA	C3B-CAB-CBB	-2.72	120.75	126.32
24	A	409	PHO	CBA-CAA-C2A	-2.72	106.06	113.73
34	c	919	DGD	O3G-C1D-C2D	-2.72	104.61	108.04
28	A	414	PL9	C25-C24-C23	-2.72	118.16	123.50
23	b	608	CLA	O2D-CGD-O1D	-2.72	118.18	123.79
23	D	403	CLA	O2D-CGD-O1D	-2.72	118.18	123.79
23	c	910	CLA	O2D-CGD-O1D	-2.71	118.19	123.79
23	B	616	CLA	C4C-C3C-C2C	-2.71	102.54	106.94
23	B	605	CLA	C5-C3-C2	-2.71	115.92	121.05
23	C	507	CLA	O1D-CGD-CBD	-2.70	120.75	124.62
23	C	511	CLA	C4B-CHC-C1C	-2.70	123.46	129.26
23	b	605	CLA	O2A-CGA-O1A	-2.70	116.53	123.49
34	H	102	DGD	O3G-C3G-C2G	-2.70	104.57	110.99
25	D	404	BCR	C30-C25-C26	-2.70	118.70	122.66
23	b	608	CLA	C2A-C1A-CHA	-2.69	118.92	123.89
25	b	620	BCR	C15-C14-C13	-2.69	123.31	127.20
23	b	610	CLA	C4C-C3C-C2C	-2.69	102.58	106.94
26	A	418	SQD	O5-C1-C2	-2.69	104.76	110.28
23	b	614	CLA	C3B-CAB-CBB	-2.69	120.82	126.32
25	c	915	BCR	C15-C14-C13	-2.68	123.33	127.20
23	B	606	CLA	C4B-CHC-C1C	-2.68	123.51	129.26
23	b	610	CLA	C3B-CAB-CBB	-2.68	120.84	126.32
34	H	102	DGD	O5D-C6D-C5D	-2.68	104.23	109.08
23	b	619	CLA	O2D-CGD-O1D	-2.67	118.27	123.79
23	B	603	CLA	CAA-CBA-CGA	-2.67	105.49	113.32
23	D	402	CLA	OBD-CAD-C3D	-2.67	122.91	128.35
23	C	513	CLA	C3B-CAB-CBB	-2.67	120.86	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	412	SQD	O47-C7-O49	-2.67	116.51	123.67
36	d	408	LHG	C32-C31-C30	-2.66	100.78	114.53
25	d	404	BCR	C7-C8-C9	-2.66	122.16	126.22
23	b	614	CLA	C1D-CHD-C4C	-2.66	118.58	122.60
34	H	102	DGD	O4D-C4D-C3D	-2.66	104.36	110.34
23	A	406	CLA	CHC-C1C-C2C	-2.65	119.37	126.35
23	b	606	CLA	C2A-C1A-CHA	-2.65	119.00	123.89
28	A	414	PL9	C7-C8-C9	-2.65	122.21	126.70
23	c	905	CLA	C4C-C3C-C2C	-2.65	102.64	106.94
24	A	409	PHO	CHD-C1D-ND	-2.65	119.71	124.66
26	a	416	SQD	O47-C7-O49	-2.65	116.57	123.67
24	a	413	PHO	O2A-CGA-O1A	-2.65	116.66	123.49
23	C	512	CLA	OBD-CAD-C3D	-2.64	122.96	128.35
37	F	101	HEM	CMA-C3A-C4A	-2.64	123.99	128.36
23	a	411	CLA	CHC-C1C-C2C	-2.64	119.42	126.35
27	a	418	LMG	O7-C10-O9	-2.64	116.60	123.67
34	c	917	DGD	C1E-C2E-C3E	-2.63	104.78	109.97
23	B	616	CLA	O2D-CGD-O1D	-2.63	118.35	123.79
23	b	613	CLA	O2A-CGA-O1A	-2.63	116.71	123.49
24	a	413	PHO	CHD-C4C-C3C	-2.63	119.36	124.58
34	c	918	DGD	O3D-C3D-C2D	-2.63	104.43	110.34
23	a	414	CLA	O2D-CGD-O1D	-2.62	118.37	123.79
38	h	101	RRX	C33-C5-C6	-2.62	122.03	124.61
30	A	419	LMT	O5'-C1'-C2'	-2.62	104.89	110.28
23	B	614	CLA	C4B-CHC-C1C	-2.62	123.64	129.26
28	D	405	PL9	C12-C13-C14	-2.62	122.07	127.76
23	c	913	CLA	O1D-CGD-CBD	-2.62	120.87	124.62
23	B	605	CLA	O2A-CGA-O1A	-2.62	116.74	123.49
25	k	101	BCR	C33-C5-C6	-2.61	122.04	124.61
25	d	404	BCR	C21-C20-C19	-2.61	115.17	123.13
36	L	101	LHG	O8-C23-O10	-2.61	116.76	123.49
28	A	414	PL9	C17-C18-C19	-2.61	122.09	127.76
23	a	409	CLA	O2A-CGA-O1A	-2.60	116.78	123.49
23	c	902	CLA	CBC-CAC-C3C	-2.60	104.45	112.39
25	c	916	BCR	C15-C16-C17	-2.60	117.64	123.39
23	b	605	CLA	C1D-CHD-C4C	-2.60	118.67	122.60
23	b	619	CLA	C2A-C1A-CHA	-2.60	119.10	123.89
23	B	611	CLA	C1D-CHD-C4C	-2.58	118.70	122.60
26	a	416	SQD	O9-S-O7	-2.58	104.08	113.48
23	b	610	CLA	C1C-C2C-C3C	-2.58	103.82	106.91
28	a	419	PL9	C17-C18-C19	-2.58	122.16	127.76
23	d	402	CLA	C1C-NC-C4C	-2.58	103.14	106.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	O2A-CGA-O1A	-2.57	116.85	123.49
25	c	916	BCR	C11-C10-C9	-2.57	123.48	127.20
23	C	510	CLA	C1C-C2C-C3C	-2.57	103.83	106.91
25	k	102	BCR	C3-C4-C5	-2.57	109.79	113.87
23	c	907	CLA	C2A-C1A-CHA	-2.57	119.15	123.89
23	c	910	CLA	C3B-CAB-CBB	-2.57	121.06	126.32
24	A	408	PHO	C1C-C2C-C3C	-2.57	103.43	106.50
34	c	917	DGD	O2G-C1B-O1B	-2.56	116.80	123.67
30	m	101	LMT	C1'-O5'-C5'	-2.56	108.78	113.75
34	h	102	DGD	O3G-C3G-C2G	-2.56	104.90	110.99
26	a	416	SQD	C44-O6-C1	-2.56	108.44	113.82
25	A	411	BCR	C35-C13-C14	-2.56	119.12	122.90
23	b	610	CLA	O2D-CGD-O1D	-2.56	118.51	123.79
24	A	408	PHO	CBA-CAA-C2A	-2.55	106.53	113.73
30	B	623	LMT	C1B-C2B-C3B	-2.55	104.94	109.97
37	f	101	HEM	CMA-C3A-C4A	-2.55	124.15	128.36
27	B	622	LMG	C9-C8-C7	-2.55	106.11	112.07
23	a	409	CLA	O2D-CGD-O1D	-2.55	118.53	123.79
23	A	410	CLA	C3B-CAB-CBB	-2.54	121.11	126.32
30	M	102	LMT	O1'-C1-C2	-2.54	99.77	109.88
23	D	402	CLA	CHB-C4A-NA	-2.54	121.00	124.51
23	b	612	CLA	C4B-CHC-C1C	-2.54	123.81	129.26
23	B	615	CLA	C4C-C3C-C2C	-2.54	102.82	106.94
23	b	608	CLA	C4B-CHC-C1C	-2.54	123.81	129.26
27	B	622	LMG	C35-C34-C33	-2.53	101.46	114.53
28	d	405	PL9	C16-C14-C13	-2.53	116.26	121.05
25	k	102	BCR	C24-C23-C22	-2.52	122.37	126.22
25	K	101	BCR	C15-C16-C17	-2.52	117.83	123.39
23	C	504	CLA	C4B-CHC-C1C	-2.52	123.86	129.26
34	c	917	DGD	C1D-O6D-C5D	-2.52	108.86	113.75
23	A	410	CLA	O2A-CGA-O1A	-2.51	117.00	123.49
23	B	607	CLA	O2A-CGA-O1A	-2.51	117.01	123.49
23	d	403	CLA	C5-C3-C2	-2.51	116.29	121.05
24	a	413	PHO	CHC-C1C-C2C	-2.51	119.94	125.61
34	C	518	DGD	C4B-C3B-C2B	-2.51	104.10	113.29
36	d	408	LHG	C13-C12-C11	-2.51	101.59	114.53
23	D	403	CLA	C6-C7-C8	-2.50	107.18	115.49
33	B	624	HTG	O3-C3-C4	-2.50	104.70	110.34
23	B	613	CLA	CAA-CBA-CGA	-2.50	105.99	113.32
23	B	604	CLA	C1C-NC-C4C	-2.50	103.23	106.27
25	c	915	BCR	C11-C10-C9	-2.49	123.60	127.20
23	b	619	CLA	C1C-C2C-C3C	-2.49	103.93	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	514	BCR	C38-C26-C25	-2.49	122.16	124.61
23	D	403	CLA	C2A-C1A-CHA	-2.49	119.30	123.89
34	c	918	DGD	O5D-C1E-C2E	-2.49	104.90	108.04
23	c	913	CLA	C6-C5-C3	-2.49	107.03	112.48
28	a	419	PL9	C11-C9-C8	-2.49	116.34	121.05
25	b	620	BCR	C39-C30-C29	-2.48	99.90	108.79
23	b	614	CLA	C14-C13-C15	-2.48	101.53	111.08
23	c	908	CLA	CBC-CAC-C3C	-2.48	104.82	112.39
25	b	622	BCR	C8-C7-C6	-2.48	119.87	127.32
23	a	411	CLA	C4C-C3C-C2C	-2.48	102.92	106.94
23	B	609	CLA	C3B-CAB-CBB	-2.47	121.25	126.32
34	C	516	DGD	C3D-C4D-C5D	-2.47	105.89	110.20
23	a	409	CLA	C1D-CHD-C4C	-2.47	118.86	122.60
30	M	102	LMT	O6'-C6'-C5'	-2.47	103.16	111.33
36	D	409	LHG	C34-C33-C32	-2.47	101.76	114.53
23	B	614	CLA	C14-C13-C15	-2.47	101.57	111.08
25	t	101	BCR	C2-C3-C4	-2.47	105.30	111.53
25	D	404	BCR	C21-C20-C19	-2.47	115.61	123.13
24	a	413	PHO	C1C-C2C-C3C	-2.47	103.55	106.50
34	H	102	DGD	O3G-C1D-C2D	-2.47	104.93	108.04
27	C	519	LMG	C8-O7-C10	-2.47	111.97	117.89
23	B	609	CLA	CHC-C1C-C2C	-2.46	119.87	126.35
30	B	623	LMT	O4'-C4B-C3B	-2.46	104.79	110.34
23	C	510	CLA	C3B-CAB-CBB	-2.46	121.28	126.32
25	K	101	BCR	C39-C30-C25	-2.46	106.44	110.30
24	A	408	PHO	CHD-C4C-C3C	-2.46	119.69	124.58
23	c	907	CLA	C6-C5-C3	-2.46	107.08	112.48
25	T	101	BCR	C23-C22-C21	-2.46	115.02	118.98
26	B	621	SQD	O5-C5-C4	-2.46	105.06	109.68
25	d	404	BCR	C34-C9-C10	-2.46	119.27	122.90
23	d	403	CLA	CBC-CAC-C3C	-2.46	104.88	112.39
25	k	101	BCR	C23-C24-C25	-2.46	119.93	127.32
24	A	409	PHO	CHD-C4C-C3C	-2.46	119.70	124.58
23	b	611	CLA	C3B-CAB-CBB	-2.46	121.29	126.32
27	C	519	LMG	O7-C10-O9	-2.45	117.08	123.67
23	a	410	CLA	OBD-CAD-C3D	-2.45	123.36	128.35
25	T	101	BCR	C28-C27-C26	-2.44	109.99	113.87
23	A	407	CLA	C4B-CHC-C1C	-2.44	124.02	129.26
23	c	910	CLA	C4B-CHC-C1C	-2.44	124.02	129.26
23	a	414	CLA	CHC-C1C-C2C	-2.44	119.94	126.35
25	b	620	BCR	C21-C20-C19	-2.44	115.70	123.13
23	B	608	CLA	C2A-C1A-CHA	-2.44	119.40	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	920	LMG	O8-C28-O10	-2.44	117.21	123.49
23	B	613	CLA	C1C-C2C-C3C	-2.43	104.00	106.91
23	c	906	CLA	C1C-C2C-C3C	-2.43	104.00	106.91
38	H	101	RRX	C38-C26-C25	-2.43	122.22	124.61
23	a	411	CLA	OBD-CAD-C3D	-2.43	123.39	128.35
23	C	502	CLA	C6-C5-C3	-2.43	107.15	112.48
23	C	512	CLA	C2A-C1A-CHA	-2.43	119.41	123.89
23	b	616	CLA	C4C-C3C-C2C	-2.43	103.00	106.94
36	d	408	LHG	O7-C7-O9	-2.43	117.16	123.67
25	k	101	BCR	C8-C9-C10	-2.43	115.07	118.98
23	c	904	CLA	C1D-CHD-C4C	-2.43	118.93	122.60
30	m	101	LMT	C3B-C4B-C5B	-2.43	105.97	110.20
23	b	613	CLA	O2D-CGD-O1D	-2.43	118.78	123.79
24	a	413	PHO	CAA-C2A-C1A	-2.43	106.48	112.86
23	b	612	CLA	C1C-C2C-C3C	-2.43	104.01	106.91
25	K	101	BCR	C10-C11-C12	-2.43	115.74	123.13
23	c	903	CLA	C4B-CHC-C1C	-2.42	124.06	129.26
34	h	102	DGD	O6E-C1E-C2E	-2.42	105.31	110.28
23	b	604	CLA	O1D-CGD-CBD	-2.42	121.15	124.62
23	B	608	CLA	CGD-CBD-CAD	-2.42	102.42	110.62
36	d	407	LHG	C11-C10-C9	-2.42	102.03	114.53
23	C	507	CLA	O2A-CGA-O1A	-2.42	117.25	123.49
25	K	101	BCR	C23-C22-C21	-2.42	115.09	118.98
23	B	617	CLA	CBC-CAC-C3C	-2.41	105.03	112.39
23	A	406	CLA	C16-C17-C18	-2.41	103.71	115.87
27	Z	101	LMG	O8-C28-O10	-2.41	117.27	123.49
23	b	604	CLA	C2A-C1A-CHA	-2.41	119.45	123.89
23	b	616	CLA	C11-C10-C8	-2.41	107.50	115.49
34	H	102	DGD	C3E-C4E-C5E	-2.41	106.00	110.20
30	a	402	LMT	O4'-C4B-C3B	-2.41	104.92	110.34
23	C	510	CLA	O2A-CGA-O1A	-2.41	117.28	123.49
36	D	408	LHG	O7-C7-O9	-2.41	117.21	123.67
23	c	906	CLA	C4-C3-C2	-2.41	118.78	123.50
23	A	405	CLA	C4B-CHC-C1C	-2.41	124.09	129.26
25	c	916	BCR	C8-C7-C6	-2.41	120.09	127.32
25	t	101	BCR	C23-C24-C25	-2.41	120.09	127.32
34	D	406	DGD	O2G-C1B-O1B	-2.40	117.22	123.67
23	B	612	CLA	CAA-CBA-CGA	-2.40	106.29	113.32
23	b	607	CLA	C4C-C3C-C2C	-2.40	103.05	106.94
23	a	411	CLA	C3A-C2A-C1A	-2.40	97.43	101.50
25	B	620	BCR	C23-C24-C25	-2.39	120.12	127.32
23	A	406	CLA	O2D-CGD-O1D	-2.39	118.84	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	516	DGD	CDB-CCB-CBB	-2.39	102.18	114.53
23	c	905	CLA	C4B-CHC-C1C	-2.39	124.12	129.26
23	b	612	CLA	C7-C6-C5	-2.39	106.00	113.06
23	C	510	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
36	l	101	LHG	O8-C23-O10	-2.39	117.32	123.49
23	b	618	CLA	O2A-CGA-O1A	-2.39	117.33	123.49
23	b	607	CLA	C4B-CHC-C1C	-2.39	124.13	129.26
23	d	403	CLA	C2A-C1A-CHA	-2.39	119.49	123.89
34	C	518	DGD	O1G-C1A-O1A	-2.39	117.33	123.49
23	c	909	CLA	O2A-CGA-O1A	-2.39	117.33	123.49
34	c	917	DGD	C3G-C2G-C1G	-2.38	106.49	112.07
23	B	606	CLA	C3B-CAB-CBB	-2.38	121.44	126.32
36	D	409	LHG	O8-C23-O10	-2.38	117.34	123.49
34	H	102	DGD	C2G-O2G-C1B	-2.38	112.17	117.89
23	b	617	CLA	CBC-CAC-C3C	-2.38	105.11	112.39
25	D	404	BCR	C15-C14-C13	-2.38	123.75	127.20
23	B	610	CLA	C4C-C3C-C2C	-2.38	103.08	106.94
27	c	920	LMG	C8-O7-C10	-2.38	112.17	117.89
24	A	408	PHO	O2D-CGD-O1D	-2.38	118.87	123.79
23	B	604	CLA	CHC-C1C-NC	-2.38	119.19	123.67
23	C	510	CLA	C4C-C3C-C2C	-2.38	103.08	106.94
26	A	412	SQD	C44-O6-C1	-2.38	108.83	113.82
34	c	919	DGD	C8B-C7B-C6B	-2.38	102.26	114.53
36	D	408	LHG	C11-C10-C9	-2.38	102.27	114.53
25	C	514	BCR	C40-C30-C25	-2.37	106.58	110.30
25	b	622	BCR	C40-C30-C25	-2.37	106.58	110.30
23	C	508	CLA	C2A-C1A-CHA	-2.37	119.52	123.89
23	C	508	CLA	C4B-CHC-C1C	-2.37	124.17	129.26
34	C	517	DGD	O1G-C1A-O1A	-2.37	117.38	123.49
23	c	912	CLA	CBC-CAC-C3C	-2.37	105.17	112.39
23	B	617	CLA	C1C-C2C-C3C	-2.37	104.08	106.91
23	c	902	CLA	O2A-CGA-O1A	-2.37	117.39	123.49
25	T	101	BCR	C24-C23-C22	-2.36	122.61	126.22
34	d	406	DGD	O2G-C1B-O1B	-2.36	117.33	123.67
23	B	602	CLA	OBD-CAD-C3D	-2.36	123.54	128.35
23	c	907	CLA	C3B-CAB-CBB	-2.36	121.49	126.32
23	B	610	CLA	C2A-C1A-CHA	-2.36	119.54	123.89
23	b	606	CLA	O2A-CGA-O1A	-2.36	117.41	123.49
23	b	612	CLA	C2A-C1A-CHA	-2.36	119.55	123.89
36	l	101	LHG	O3-P-O5	-2.36	100.47	109.62
23	B	604	CLA	C4B-CHC-C1C	-2.35	124.20	129.26
34	c	919	DGD	O5D-C6D-C5D	-2.35	104.82	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	913	CLA	CBA-CAA-C2A	-2.35	107.10	113.73
25	a	415	BCR	C15-C14-C13	-2.35	123.80	127.20
30	t	102	LMT	C1-O1'-C1'	-2.35	109.84	113.94
23	c	908	CLA	C5-C3-C2	-2.35	116.60	121.05
23	C	513	CLA	O2A-CGA-O1A	-2.35	117.44	123.49
23	c	904	CLA	CBC-CAC-C3C	-2.35	105.23	112.39
25	A	411	BCR	C20-C21-C22	-2.35	123.81	127.20
23	c	903	CLA	O2A-CGA-O1A	-2.34	117.44	123.49
25	T	101	BCR	C21-C20-C19	-2.34	115.98	123.13
25	D	404	BCR	C32-C1-C2	-2.34	100.39	108.79
26	a	401	SQD	O48-C23-O10	-2.34	117.45	123.49
25	d	404	BCR	C30-C25-C26	-2.34	119.22	122.66
23	c	910	CLA	C4C-C3C-C2C	-2.34	103.15	106.94
36	D	409	LHG	C13-C12-C11	-2.34	102.46	114.53
23	B	603	CLA	C14-C13-C12	-2.33	102.10	111.08
25	d	404	BCR	C33-C5-C6	-2.33	122.32	124.61
23	B	616	CLA	C2A-C1A-CHA	-2.33	119.59	123.89
26	D	407	SQD	O48-C23-O10	-2.33	117.48	123.49
25	d	404	BCR	C32-C1-C2	-2.33	100.44	108.79
23	a	409	CLA	C3B-CAB-CBB	-2.33	121.56	126.32
23	B	614	CLA	O2A-CGA-O1A	-2.32	117.49	123.49
38	h	101	RRX	C7-C8-C9	-2.32	122.67	126.22
23	b	606	CLA	C7-C6-C5	-2.32	106.20	113.06
25	C	514	BCR	C23-C22-C21	-2.32	115.24	118.98
23	B	611	CLA	C4C-C3C-C2C	-2.32	103.18	106.94
28	d	405	PL9	C11-C9-C8	-2.32	116.65	121.05
28	D	405	PL9	C46-C47-C48	-2.32	105.61	111.69
31	B	633	GOL	O3-C3-C2	-2.32	98.94	110.18
25	b	620	BCR	C20-C21-C22	-2.32	123.85	127.20
23	b	605	CLA	C2A-C1A-CHA	-2.32	119.62	123.89
23	C	506	CLA	C4B-CHC-C1C	-2.31	124.29	129.26
23	b	610	CLA	CGD-CBD-CAD	-2.31	102.78	110.62
36	L	101	LHG	C34-C33-C32	-2.31	102.59	114.53
23	B	614	CLA	C4C-C3C-C2C	-2.31	103.20	106.94
23	c	902	CLA	C2A-C1A-CHA	-2.31	119.64	123.89
23	a	411	CLA	O2D-CGD-O1D	-2.31	119.03	123.79
23	A	406	CLA	C3A-C2A-C1A	-2.30	97.59	101.50
23	a	414	CLA	OBD-CAD-C3D	-2.30	123.65	128.35
23	b	617	CLA	O1D-CGD-CBD	-2.30	121.32	124.62
23	C	505	CLA	OBD-CAD-C3D	-2.30	123.66	128.35
23	c	912	CLA	C5-C3-C2	-2.30	116.69	121.05
23	c	909	CLA	C2A-C1A-CHA	-2.30	119.65	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	515	BCR	C23-C24-C25	-2.30	120.42	127.32
30	b	625	LMT	O1'-C1'-C2'	-2.30	105.14	108.04
34	c	918	DGD	O2G-C1B-O1B	-2.29	117.52	123.67
23	B	603	CLA	C4C-C3C-C2C	-2.29	103.23	106.94
23	c	906	CLA	O2A-CGA-O1A	-2.29	117.58	123.49
25	B	619	BCR	C30-C25-C26	-2.29	119.30	122.66
34	C	518	DGD	O2G-C1B-O1B	-2.29	117.53	123.67
27	c	920	LMG	O1-C7-C8	-2.29	105.55	110.99
26	a	401	SQD	C1-C2-C3	-2.29	105.47	109.97
28	a	419	PL9	C26-C24-C23	-2.28	116.72	121.05
30	M	101	LMT	O2'-C2'-C3'	-2.28	105.20	110.34
25	B	620	BCR	C10-C11-C12	-2.28	116.17	123.13
23	B	608	CLA	C7-C6-C5	-2.28	106.33	113.06
23	C	509	CLA	CHC-C1C-C2C	-2.28	120.36	126.35
23	a	414	CLA	C4C-C3C-C2C	-2.28	103.25	106.94
25	b	620	BCR	C40-C30-C25	-2.28	106.73	110.30
28	a	419	PL9	C11-C12-C13	-2.28	105.73	111.69
23	c	907	CLA	C4B-CHC-C1C	-2.28	124.37	129.26
34	C	518	DGD	C3D-C4D-C5D	-2.28	106.23	110.20
23	A	405	CLA	C4C-C3C-C2C	-2.27	103.25	106.94
28	D	405	PL9	C11-C9-C8	-2.27	116.74	121.05
27	b	623	LMG	C1-O6-C5	-2.27	109.33	113.75
23	b	616	CLA	C1C-NC-C4C	-2.27	103.51	106.27
23	C	505	CLA	C1C-NC-C4C	-2.27	103.51	106.27
27	d	410	LMG	O1-C7-C8	-2.27	105.59	110.99
23	b	610	CLA	CBC-CAC-C3C	-2.27	105.46	112.39
28	a	419	PL9	C45-C44-C43	-2.27	119.05	123.50
23	C	513	CLA	C2A-C1A-CHA	-2.26	119.72	123.89
25	K	101	BCR	C7-C8-C9	-2.26	122.77	126.22
23	c	903	CLA	O1D-CGD-CBD	-2.26	121.38	124.62
24	A	409	PHO	C16-C15-C13	-2.26	107.99	115.49
27	C	519	LMG	C9-C8-C7	-2.26	106.78	112.07
37	f	101	HEM	C2C-C1C-NC	-2.26	106.40	110.21
23	C	504	CLA	C7-C6-C5	-2.26	106.39	113.06
23	C	502	CLA	C16-C17-C18	-2.26	104.48	115.87
25	K	101	BCR	C29-C28-C27	-2.26	105.84	111.53
38	H	101	RRX	C16-C17-C18	-2.26	123.94	127.20
25	B	619	BCR	C15-C16-C17	-2.26	118.40	123.39
27	B	622	LMG	C9-O8-C28	-2.25	110.54	116.85
26	L	103	SQD	O9-S-O7	-2.24	105.30	113.48
23	C	513	CLA	OBD-CAD-C3D	-2.24	123.78	128.35
23	b	619	CLA	CBC-CAC-C3C	-2.24	105.55	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	101	BCR	C37-C22-C21	-2.24	119.59	122.90
23	b	615	CLA	C3B-CAB-CBB	-2.24	121.73	126.32
23	D	403	CLA	CBC-CAC-C3C	-2.24	105.55	112.39
23	C	503	CLA	CHC-C1C-NC	-2.24	119.46	123.67
27	d	410	LMG	O2-C2-C1	-2.24	105.11	110.02
26	D	407	SQD	O4-C4-C3	-2.24	105.30	110.34
23	b	613	CLA	C1D-CHD-C4C	-2.24	119.22	122.60
23	C	503	CLA	C5-C3-C2	-2.23	116.81	121.05
25	C	515	BCR	C40-C30-C25	-2.23	106.80	110.30
23	C	512	CLA	C1D-CHD-C4C	-2.23	119.22	122.60
23	A	405	CLA	CHC-C1C-C2C	-2.23	120.48	126.35
23	B	606	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
34	c	917	DGD	CDB-CCB-CBB	-2.23	103.02	114.53
23	b	616	CLA	C12-C11-C10	-2.23	101.94	112.99
23	b	609	CLA	CBC-CAC-C3C	-2.22	105.61	112.39
24	A	408	PHO	C16-C17-C18	-2.22	104.66	115.87
25	D	404	BCR	C33-C5-C6	-2.22	122.42	124.61
34	H	102	DGD	C3D-C4D-C5D	-2.22	106.33	110.20
23	c	911	CLA	C2A-C1A-CHA	-2.22	119.80	123.89
26	a	416	SQD	O48-C23-O10	-2.22	117.77	123.49
23	c	913	CLA	CBC-CAC-C3C	-2.22	105.62	112.39
23	D	402	CLA	C1C-NC-C4C	-2.22	103.57	106.27
24	A	408	PHO	CAA-C2A-C1A	-2.22	107.03	112.86
38	H	101	RRX	C21-C20-C19	-2.22	116.37	123.13
23	b	619	CLA	O2A-CGA-O1A	-2.22	117.77	123.49
23	B	613	CLA	C4C-C3C-C2C	-2.21	103.35	106.94
25	b	620	BCR	C16-C17-C18	-2.21	124.00	127.20
25	D	404	BCR	C39-C30-C25	-2.21	106.84	110.30
23	c	904	CLA	C7-C6-C5	-2.21	106.53	113.06
24	a	412	PHO	CHC-C1C-C2C	-2.21	120.61	125.61
28	a	419	PL9	C27-C28-C29	-2.21	122.96	127.76
24	A	408	PHO	C3B-C2B-C1B	-2.21	101.55	106.33
23	b	618	CLA	OBD-CAD-C3D	-2.21	123.85	128.35
23	c	908	CLA	C4C-C3C-C2C	-2.21	103.36	106.94
23	c	910	CLA	O2A-CGA-O1A	-2.20	117.80	123.49
23	B	602	CLA	C2A-C1A-CHA	-2.20	119.83	123.89
23	c	911	CLA	C4C-C3C-C2C	-2.20	103.37	106.94
33	B	625	HTG	O2-C2-C3	-2.20	105.38	110.34
23	B	615	CLA	C2A-C1A-CHA	-2.20	119.83	123.89
30	M	102	LMT	O2B-C2B-C1B	-2.20	105.20	110.02
34	C	516	DGD	O6E-C1E-C2E	-2.20	105.76	110.28
23	c	904	CLA	O2D-CGD-O1D	-2.20	119.25	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	621	BCR	C38-C26-C25	-2.20	122.45	124.61
23	b	618	CLA	C5-C3-C2	-2.20	116.88	121.05
23	b	607	CLA	C7-C6-C5	-2.20	106.57	113.06
24	A	408	PHO	C7-C6-C5	-2.20	106.57	113.06
23	c	908	CLA	O2A-CGA-O1A	-2.19	117.83	123.49
23	B	609	CLA	C11-C12-C13	-2.19	108.22	115.49
23	C	506	CLA	O2A-CGA-O1A	-2.19	117.83	123.49
36	d	409	LHG	O8-C23-O10	-2.19	117.84	123.49
25	k	102	BCR	C28-C27-C26	-2.19	110.39	113.87
23	c	914	CLA	CAA-CBA-CGA	-2.19	106.91	113.32
23	C	503	CLA	OBD-CAD-C3D	-2.19	123.89	128.35
23	c	906	CLA	C4C-C3C-C2C	-2.19	103.39	106.94
23	D	402	CLA	C4C-C3C-C2C	-2.19	103.39	106.94
27	c	921	LMG	O6-C1-C2	-2.19	105.79	110.28
34	c	919	DGD	O1G-C1G-C2G	-2.19	102.81	108.69
26	a	416	SQD	O48-C46-C45	-2.18	102.81	108.69
27	d	410	LMG	C9-C8-C7	-2.18	106.96	112.07
23	C	508	CLA	C4C-C3C-C2C	-2.18	103.40	106.94
23	b	617	CLA	C2A-C1A-CHA	-2.18	119.87	123.89
34	C	516	DGD	C6D-O5D-C1E	-2.18	109.23	113.82
25	b	622	BCR	C23-C22-C21	-2.18	115.47	118.98
23	b	608	CLA	C5-C3-C2	-2.18	116.92	121.05
23	C	512	CLA	C4B-CHC-C1C	-2.18	124.59	129.26
23	c	903	CLA	C16-C17-C18	-2.17	104.91	115.87
23	B	612	CLA	O2A-CGA-O1A	-2.17	117.88	123.49
23	c	903	CLA	C4C-C3C-C2C	-2.17	103.42	106.94
23	c	905	CLA	O2D-CGD-O1D	-2.17	119.31	123.79
23	c	912	CLA	O2A-CGA-O1A	-2.17	117.89	123.49
38	h	101	RRX	C11-C10-C9	-2.17	124.06	127.20
26	L	103	SQD	C1-O5-C5	-2.17	109.54	113.75
23	b	608	CLA	CAC-C3C-C2C	-2.17	123.71	127.51
24	A	409	PHO	CHC-C1C-C2C	-2.17	120.71	125.61
24	a	413	PHO	CBA-CAA-C2A	-2.17	107.62	113.73
26	A	412	SQD	C9-C8-C7	-2.16	105.09	113.59
30	M	102	LMT	C3B-C4B-C5B	-2.16	106.43	110.20
36	L	101	LHG	C13-C12-C11	-2.16	103.37	114.53
25	d	404	BCR	C10-C11-C12	-2.16	116.55	123.13
23	C	509	CLA	C1C-NC-C4C	-2.16	103.64	106.27
25	b	621	BCR	C8-C9-C10	-2.16	115.51	118.98
23	B	608	CLA	O1D-CGD-CBD	-2.16	121.53	124.62
38	h	101	RRX	C24-C23-C22	-2.16	122.93	126.22
24	a	413	PHO	C3B-C2B-C1B	-2.15	101.66	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	H	101	RRX	C29-C28-C27	-2.15	106.50	110.32
23	A	407	CLA	CMB-C2B-C1B	-2.15	124.80	128.36
23	b	618	CLA	C11-C10-C8	-2.15	108.35	115.49
23	D	402	CLA	C5-C3-C2	-2.15	116.97	121.05
25	b	621	BCR	C16-C15-C14	-2.15	118.64	123.39
36	d	407	LHG	O7-C7-O9	-2.15	117.91	123.67
23	b	610	CLA	C7-C6-C5	-2.15	106.72	113.06
23	B	616	CLA	C5-C3-C2	-2.14	116.98	121.05
23	A	406	CLA	C2A-C1A-CHA	-2.14	119.94	123.89
23	B	606	CLA	C1C-NC-C4C	-2.14	103.66	106.27
23	B	612	CLA	C3A-C2A-C1A	-2.14	97.87	101.50
25	K	101	BCR	C33-C5-C6	-2.14	122.51	124.61
30	a	402	LMT	C8-C7-C6	-2.14	103.50	114.53
38	h	101	RRX	C20-C21-C22	-2.14	124.11	127.20
30	a	402	LMT	O2'-C2'-C3'	-2.13	105.53	110.34
25	B	619	BCR	C7-C8-C9	-2.13	122.96	126.22
23	b	612	CLA	O1D-CGD-CBD	-2.13	121.57	124.62
25	K	102	BCR	C37-C22-C21	-2.13	119.75	122.90
27	A	413	LMG	O2-C2-C3	-2.13	105.55	110.34
30	C	520	LMT	C3'-C4'-C5'	-2.13	106.03	110.84
23	a	411	CLA	O2A-CGA-O1A	-2.13	118.00	123.49
34	C	518	DGD	C7B-C6B-C5B	-2.13	103.55	114.53
23	d	402	CLA	C2A-C1A-CHA	-2.13	119.97	123.89
28	A	414	PL9	C12-C13-C14	-2.12	123.15	127.76
28	a	419	PL9	C16-C14-C13	-2.12	117.02	121.05
23	b	608	CLA	C14-C13-C12	-2.12	102.91	111.08
23	b	605	CLA	C16-C17-C18	-2.12	105.17	115.87
23	d	402	CLA	CHC-C1C-C2C	-2.12	120.78	126.35
28	D	405	PL9	C27-C26-C24	-2.12	105.81	112.71
27	B	622	LMG	O4-C4-C3	-2.12	105.57	110.34
23	c	905	CLA	C2A-C1A-CHA	-2.12	119.99	123.89
24	a	412	PHO	C7-C6-C5	-2.12	106.81	113.06
25	a	415	BCR	C8-C7-C6	-2.11	120.98	127.32
24	A	409	PHO	C1C-NC-C4C	-2.11	102.35	106.51
36	d	407	LHG	O8-C6-C5	-2.10	103.03	108.69
26	A	418	SQD	O8-S-O9	-2.10	106.71	111.61
26	A	412	SQD	O5-C1-C2	-2.10	105.96	110.28
23	A	405	CLA	OBD-CAD-C3D	-2.10	124.06	128.35
23	C	505	CLA	O2A-CGA-O1A	-2.10	118.07	123.49
24	a	412	PHO	C3B-C2B-C1B	-2.10	101.78	106.33
25	T	101	BCR	C19-C18-C17	-2.10	115.60	118.98
23	c	906	CLA	C11-C12-C13	-2.10	108.52	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	410	CLA	O2D-CGD-O1D	-2.10	119.46	123.79
23	c	911	CLA	O2D-CGD-O1D	-2.10	119.46	123.79
30	C	520	LMT	O3B-C3B-C2B	-2.10	105.61	110.34
25	b	621	BCR	C35-C13-C14	-2.09	119.81	122.90
23	c	906	CLA	OBD-CAD-C3D	-2.09	124.08	128.35
23	B	603	CLA	C1D-CHD-C4C	-2.09	119.44	122.60
23	A	407	CLA	CGD-CBD-CAD	-2.09	103.54	110.62
23	c	912	CLA	O1D-CGD-CBD	-2.09	121.63	124.62
23	b	609	CLA	CHC-C1C-C2C	-2.09	120.87	126.35
23	c	904	CLA	C4C-C3C-C2C	-2.08	103.56	106.94
23	B	611	CLA	C2A-C1A-CHA	-2.08	120.05	123.89
27	d	410	LMG	O8-C9-C8	-2.08	103.08	108.69
26	f	102	SQD	O8-S-O9	-2.08	106.76	111.61
23	B	606	CLA	C4-C3-C2	-2.08	119.41	123.50
23	c	905	CLA	O1D-CGD-CBD	-2.08	121.64	124.62
25	k	101	BCR	C15-C16-C17	-2.08	118.79	123.39
38	H	101	RRX	C23-C24-C25	-2.08	121.07	127.32
28	D	405	PL9	C50-C49-C48	-2.08	115.92	122.61
27	c	921	LMG	C9-C8-C7	-2.08	107.20	112.07
37	f	101	HEM	C3C-CAC-CBC	-2.08	121.27	124.46
23	D	402	CLA	CMB-C2B-C1B	-2.08	124.92	128.36
28	d	405	PL9	C7-C8-C9	-2.08	123.17	126.70
23	c	903	CLA	C6-C5-C3	-2.08	107.92	112.48
34	c	918	DGD	O4E-C4E-C3E	-2.08	105.66	110.34
36	D	409	LHG	O7-C7-O9	-2.08	118.09	123.67
23	b	618	CLA	C4B-CHC-C1C	-2.08	124.80	129.26
23	b	615	CLA	C5-C3-C2	-2.08	117.11	121.05
25	c	916	BCR	C19-C18-C17	-2.08	115.64	118.98
23	c	911	CLA	C4B-CHC-C1C	-2.08	124.80	129.26
23	c	911	CLA	C1D-CHD-C4C	-2.07	119.46	122.60
23	a	414	CLA	C1D-CHD-C4C	-2.07	119.47	122.60
25	b	621	BCR	C11-C12-C13	-2.07	120.23	126.32
28	a	419	PL9	C21-C22-C23	-2.07	106.27	111.69
34	C	516	DGD	O6D-C1D-O3G	-2.07	105.08	110.05
25	d	404	BCR	C37-C22-C21	-2.07	119.85	122.90
23	b	614	CLA	C7-C6-C5	-2.07	106.96	113.06
23	B	607	CLA	C4C-C3C-C2C	-2.07	103.59	106.94
30	t	102	LMT	O2'-C2'-C3'	-2.06	105.69	110.34
25	B	618	BCR	C34-C9-C10	-2.06	119.85	122.90
23	C	507	CLA	OBD-CAD-C3D	-2.06	124.14	128.35
25	B	619	BCR	C32-C1-C6	-2.06	107.07	110.30
23	a	414	CLA	O2A-CGA-O1A	-2.06	118.17	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	C1C-C2C-C3C	-2.06	104.44	106.91
25	T	101	BCR	C29-C28-C27	-2.06	106.33	111.53
23	A	405	CLA	C7-C6-C5	-2.06	106.97	113.06
23	B	617	CLA	C3B-CAB-CBB	-2.06	122.10	126.32
34	C	516	DGD	O2G-C1B-O1B	-2.06	118.14	123.67
23	C	511	CLA	CHC-C1C-C2C	-2.06	120.94	126.35
30	m	101	LMT	C10-C9-C8	-2.06	103.90	114.53
25	b	620	BCR	C15-C16-C17	-2.06	118.84	123.39
23	b	612	CLA	CBC-CAC-C3C	-2.06	106.11	112.39
23	b	612	CLA	C1C-NC-C4C	-2.06	103.77	106.27
26	L	103	SQD	C28-C27-C26	-2.06	103.91	114.53
23	C	506	CLA	C4C-C3C-C2C	-2.06	103.61	106.94
25	t	101	BCR	C21-C20-C19	-2.06	116.86	123.13
23	B	611	CLA	C6-C5-C3	-2.06	107.97	112.48
23	B	614	CLA	CAA-CBA-CGA	-2.06	107.30	113.32
25	K	102	BCR	C34-C9-C10	-2.06	119.86	122.90
25	c	916	BCR	C7-C8-C9	-2.05	123.08	126.22
23	A	406	CLA	C11-C10-C8	-2.05	108.67	115.49
23	B	610	CLA	C3B-CAB-CBB	-2.05	122.12	126.32
27	b	623	LMG	C38-C37-C36	-2.05	103.95	114.53
27	d	410	LMG	O7-C10-O9	-2.05	118.17	123.67
23	b	608	CLA	CHC-C1C-NC	-2.04	119.83	123.67
23	B	608	CLA	CAA-CBA-CGA	-2.04	107.33	113.32
23	C	509	CLA	C4C-C3C-C2C	-2.04	103.63	106.94
23	C	501	CLA	CHC-C1C-C2C	-2.04	120.98	126.35
23	B	608	CLA	C3A-C2A-C1A	-2.04	98.04	101.50
23	b	614	CLA	C2A-C1A-CHA	-2.04	120.13	123.89
23	c	913	CLA	C4C-C3C-C2C	-2.04	103.64	106.94
23	b	617	CLA	C1D-CHD-C4C	-2.04	119.52	122.60
33	u	201	HTG	O3-C3-C2	-2.04	106.67	111.10
23	A	405	CLA	C2A-C1A-CHA	-2.04	120.14	123.89
23	A	407	CLA	CBC-CAC-C3C	-2.04	106.18	112.39
25	B	618	BCR	C15-C16-C17	-2.03	118.89	123.39
23	c	908	CLA	C11-C12-C13	-2.03	108.74	115.49
23	C	502	CLA	C4C-C3C-C2C	-2.03	103.64	106.94
23	a	410	CLA	O2D-CGD-O1D	-2.03	119.59	123.79
23	a	410	CLA	CGD-CBD-CAD	-2.03	103.75	110.62
24	A	409	PHO	O2A-CGA-O1A	-2.03	118.26	123.49
23	B	607	CLA	CBC-CAC-C3C	-2.03	106.20	112.39
33	B	624	HTG	O5-C5-C4	-2.02	105.88	109.68
27	b	623	LMG	C9-C8-C7	-2.02	107.34	112.07
23	C	503	CLA	C4C-C3C-C2C	-2.02	103.66	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406	CLA	C4-C3-C2	-2.02	119.53	123.50
25	k	101	BCR	C2-C3-C4	-2.02	106.43	111.53
25	k	101	BCR	C20-C21-C22	-2.02	124.28	127.20
26	L	103	SQD	O47-C7-O49	-2.02	118.25	123.67
36	d	408	LHG	O2-C2-C1	-2.02	99.39	108.65
37	v	201	HEM	CMA-C3A-C4A	-2.02	125.03	128.36
23	c	904	CLA	C2A-C1A-CHA	-2.02	120.17	123.89
26	A	412	SQD	O9-S-O7	-2.02	106.13	113.48
23	b	611	CLA	C6-C5-C3	-2.01	108.07	112.48
28	d	405	PL9	C50-C49-C48	-2.01	116.14	122.61
30	a	402	LMT	O5'-C1'-C2'	-2.01	106.16	110.28
23	C	504	CLA	C2A-C1A-CHA	-2.01	120.19	123.89
34	C	518	DGD	C3A-C2A-C1A	-2.01	105.71	113.59
23	b	606	CLA	C1C-NC-C4C	-2.01	103.83	106.27
30	t	102	LMT	O5'-C1'-O1'	-2.01	105.22	110.05
23	c	907	CLA	O2D-CGD-O1D	-2.00	119.65	123.79
30	m	101	LMT	O2B-C2B-C1B	-2.00	105.63	110.02
26	B	621	SQD	O8-S-O9	-2.00	106.95	111.61
23	b	608	CLA	C4-C3-C2	-2.00	119.57	123.50
34	C	517	DGD	O3D-C3D-C2D	-2.00	105.83	110.34
25	B	619	BCR	C2-C1-C6	2.00	113.53	110.36
23	C	508	CLA	CHB-C4A-NA	2.01	127.29	124.51
30	m	101	LMT	C1B-O5B-C5B	2.01	117.64	113.75
23	c	903	CLA	CMB-C2B-C3B	2.01	129.02	125.09
25	D	404	BCR	C4-C5-C6	2.01	125.34	122.78
36	E	101	LHG	O8-C23-C24	2.01	118.03	111.90
30	Z	102	LMT	C3B-C4B-C5B	2.01	113.70	110.20
34	h	102	DGD	O5D-C1E-C2E	2.01	110.58	108.04
23	d	403	CLA	CMC-C2C-C3C	2.01	131.79	125.94
23	A	405	CLA	OBD-CAD-CBD	2.01	128.98	125.94
25	K	102	BCR	C37-C22-C23	2.02	121.45	118.10
30	m	102	LMT	C1'-O5'-C5'	2.02	117.66	113.75
34	d	406	DGD	O2D-C2D-C3D	2.02	114.88	110.34
23	b	614	CLA	CAC-C3C-C4C	2.02	127.76	124.83
23	C	503	CLA	CED-O2D-CGD	2.02	120.73	115.99
23	b	611	CLA	CMC-C2C-C1C	2.02	128.15	125.02
30	B	623	LMT	O1B-C1B-O5B	2.02	115.80	110.68
23	c	906	CLA	O2A-CGA-CBA	2.02	118.06	111.90
23	B	614	CLA	O2A-CGA-CBA	2.02	118.07	111.90
30	b	624	LMT	O5'-C5'-C6'	2.03	111.47	106.36
23	A	410	CLA	O2A-CGA-CBA	2.03	118.08	111.90
23	b	607	CLA	O2A-CGA-CBA	2.03	118.08	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	CMC-C2C-C3C	2.03	131.84	125.94
28	d	405	PL9	C3-C4-C5	2.03	121.60	118.62
23	C	512	CLA	CAC-C3C-C4C	2.03	127.78	124.83
24	A	409	PHO	C3D-C4D-ND	2.03	116.19	109.65
25	c	915	BCR	C35-C13-C12	2.03	121.48	118.10
38	h	101	RRX	C34-C9-C8	2.04	121.49	118.10
28	A	414	PL9	C26-C24-C23	2.04	124.92	121.05
30	c	922	LMT	O2'-C2'-C1'	2.04	114.49	110.02
30	C	520	LMT	O1B-C4'-C5'	2.04	114.68	109.32
33	c	924	HTG	O5-C1-C2	2.04	112.96	110.19
23	b	617	CLA	C5-C3-C2	2.04	124.92	121.05
23	A	406	CLA	CMC-C2C-C1C	2.04	128.18	125.02
23	C	507	CLA	O2A-CGA-CBA	2.04	118.13	111.90
33	B	626	HTG	O5-C1-C2	2.05	112.97	110.19
23	C	501	CLA	C4A-NA-C1A	2.05	109.01	106.36
23	D	403	CLA	CMD-C2D-C3D	2.05	129.10	125.09
37	V	201	HEM	C3B-C4B-CHC	2.05	126.05	123.16
34	d	406	DGD	O2G-C2G-C1G	2.06	115.62	108.36
23	b	616	CLA	CMD-C2D-C3D	2.06	129.12	125.09
33	b	626	HTG	O4-C4-C5	2.06	114.71	109.24
23	a	410	CLA	C4-C3-C5	2.07	118.56	115.41
30	z	101	LMT	O1B-C1B-C2B	2.07	113.14	108.10
25	B	619	BCR	C37-C22-C23	2.07	121.55	118.10
23	b	608	CLA	C1D-CHD-C4C	2.08	125.74	122.60
23	A	406	CLA	C3D-CAD-CBD	2.08	110.53	107.60
23	c	911	CLA	CAC-C3C-C4C	2.08	127.84	124.83
23	c	913	CLA	CED-O2D-CGD	2.08	120.86	115.99
23	b	609	CLA	CMD-C2D-C3D	2.08	129.16	125.09
25	K	102	BCR	C34-C9-C8	2.08	121.56	118.10
23	B	605	CLA	O2A-CGA-CBA	2.08	118.24	111.90
23	B	608	CLA	CAC-C3C-C4C	2.09	127.86	124.83
33	d	401	HTG	O5-C1-C2	2.09	113.03	110.19
30	z	101	LMT	O1B-C4'-C3'	2.09	112.57	107.17
26	A	412	SQD	O48-C23-C24	2.10	118.30	111.90
24	a	412	PHO	C4D-C3D-C2D	2.10	109.12	106.74
25	k	101	BCR	C29-C30-C25	2.10	113.69	110.36
23	a	411	CLA	CED-O2D-CGD	2.10	120.93	115.99
23	A	410	CLA	CED-O2D-CGD	2.11	120.93	115.99
23	c	904	CLA	OBD-CAD-CBD	2.11	129.12	125.94
23	D	403	CLA	CMB-C2B-C3B	2.11	129.21	125.09
23	C	506	CLA	O2A-CGA-CBA	2.11	118.32	111.90
23	B	605	CLA	C3B-C4B-NB	2.11	111.94	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	913	CLA	CMD-C2D-C3D	2.12	129.23	125.09
36	D	410	LHG	O7-C5-C4	2.12	115.83	108.36
23	b	619	CLA	C4A-NA-C1A	2.12	109.10	106.36
24	a	413	PHO	C4D-C3D-C2D	2.12	109.14	106.74
34	c	917	DGD	C1G-O1G-C1A	2.12	122.79	116.85
33	B	631	HTG	C1-O5-C5	2.12	116.79	112.74
33	B	624	HTG	O5-C5-C6	2.13	111.73	106.36
23	B	610	CLA	C4A-NA-C1A	2.13	109.11	106.36
23	C	507	CLA	CHB-C4A-NA	2.13	127.45	124.51
23	b	614	CLA	C6-C5-C3	2.13	117.16	112.48
23	c	905	CLA	CMB-C2B-C3B	2.13	129.25	125.09
23	c	910	CLA	CMC-C2C-C1C	2.13	128.32	125.02
23	c	913	CLA	CMB-C2B-C1B	2.13	131.89	128.36
23	C	505	CLA	C3B-C4B-NB	2.13	111.97	109.21
26	A	418	SQD	C44-O6-C1	2.13	118.30	113.82
34	D	406	DGD	C3D-C4D-C5D	2.13	113.92	110.20
30	m	101	LMT	C6'-C5'-C4'	2.14	119.46	113.25
23	c	902	CLA	CMB-C2B-C1B	2.14	131.90	128.36
30	b	624	LMT	C1'-O5'-C5'	2.14	117.89	113.75
23	b	615	CLA	C6-C5-C3	2.14	117.18	112.48
23	b	605	CLA	CED-O2D-CGD	2.14	121.01	115.99
23	B	612	CLA	C4-C3-C5	2.15	118.70	115.41
28	A	414	PL9	C15-C14-C16	2.16	118.70	115.41
23	B	613	CLA	O2A-CGA-CBA	2.16	118.47	111.90
24	A	409	PHO	C4D-C3D-C2D	2.16	109.18	106.74
34	H	102	DGD	O2G-C1B-C2B	2.16	116.23	111.53
23	c	910	CLA	O2A-CGA-CBA	2.16	118.50	111.90
25	C	514	BCR	C29-C30-C25	2.17	113.80	110.36
36	d	409	LHG	O8-C23-C24	2.17	118.51	111.90
23	C	508	CLA	C1D-CHD-C4C	2.17	125.89	122.60
23	A	406	CLA	C3B-C4B-NB	2.17	112.02	109.21
30	c	922	LMT	O3B-C3B-C4B	2.17	115.23	110.34
23	b	618	CLA	OBD-CAD-CBD	2.17	129.22	125.94
28	D	405	PL9	C51-C49-C50	2.18	119.99	114.64
37	v	201	HEM	C4B-CHC-C1C	2.18	129.47	125.82
26	D	407	SQD	O5-C1-O6	2.18	115.31	110.05
23	b	612	CLA	C4-C3-C5	2.18	118.74	115.41
23	d	402	CLA	CMB-C2B-C3B	2.18	129.36	125.09
23	c	907	CLA	O2A-CGA-CBA	2.19	118.56	111.90
23	d	402	CLA	C3D-CAD-CBD	2.19	110.69	107.60
30	J	102	LMT	C1'-C2'-C3'	2.19	114.28	109.97
26	a	416	SQD	O48-C23-C24	2.19	118.57	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	410	CLA	O2D-CGD-CBD	2.19	114.30	111.30
30	M	102	LMT	O4'-C4B-C3B	2.19	115.27	110.34
33	B	625	HTG	O4-C4-C5	2.19	115.05	109.24
36	l	101	LHG	O4-P-O5	2.19	124.41	112.53
25	a	415	BCR	C35-C13-C12	2.19	121.75	118.10
25	C	514	BCR	C37-C22-C23	2.19	121.75	118.10
23	B	603	CLA	C3B-C4B-NB	2.19	112.05	109.21
25	k	101	BCR	C1-C6-C7	2.20	121.97	115.82
28	A	414	PL9	C10-C9-C11	2.20	118.76	115.41
34	c	919	DGD	C4E-C3E-C2E	2.20	114.89	110.79
23	c	902	CLA	O2A-CGA-CBA	2.20	118.60	111.90
23	B	612	CLA	CAC-C3C-C4C	2.21	128.03	124.83
34	d	406	DGD	O6D-C5D-C6D	2.21	111.46	106.64
23	D	403	CLA	C4-C3-C5	2.21	118.78	115.41
23	b	616	CLA	O2D-CGD-CBD	2.21	114.33	111.30
23	B	610	CLA	CED-O2D-CGD	2.21	121.17	115.99
25	K	101	BCR	C38-C26-C27	2.21	117.62	113.43
36	E	101	LHG	C6-O8-C23	2.21	123.04	116.85
30	a	402	LMT	O5B-C5B-C6B	2.22	111.95	106.36
23	b	613	CLA	O2A-CGA-CBA	2.22	118.65	111.90
23	A	405	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	B	621	SQD	O47-C45-C46	2.22	116.19	108.36
27	c	920	LMG	C3-C4-C5	2.22	114.07	110.20
23	b	614	CLA	C16-C15-C13	2.22	122.86	115.49
23	c	908	CLA	CAC-C3C-C4C	2.23	128.06	124.83
23	C	513	CLA	CMC-C2C-C1C	2.23	128.47	125.02
23	b	604	CLA	CED-O2D-CGD	2.23	121.22	115.99
33	B	630	HTG	O2-C2-C3	2.23	115.36	110.34
23	a	409	CLA	CMC-C2C-C3C	2.23	132.42	125.94
23	C	502	CLA	C3B-C4B-NB	2.23	112.09	109.21
23	c	905	CLA	CMD-C2D-C3D	2.23	129.45	125.09
26	L	103	SQD	O48-C23-C24	2.23	118.70	111.90
23	C	504	CLA	CMC-C2C-C1C	2.24	128.48	125.02
25	c	916	BCR	C35-C13-C12	2.24	121.82	118.10
23	b	615	CLA	CMC-C2C-C1C	2.24	128.48	125.02
25	D	404	BCR	C38-C26-C27	2.24	117.68	113.43
25	d	404	BCR	C34-C9-C8	2.24	121.83	118.10
33	B	625	HTG	C1-C2-C3	2.25	115.66	110.69
23	c	905	CLA	C16-C15-C13	2.25	122.94	115.49
23	B	602	CLA	OBD-CAD-CBD	2.25	129.33	125.94
26	D	407	SQD	O6-C44-C45	2.25	116.33	110.99
23	c	912	CLA	CHB-C4A-NA	2.25	127.62	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	514	BCR	C2-C1-C6	2.25	113.93	110.36
23	b	609	CLA	O2A-CGA-CBA	2.25	118.76	111.90
23	c	903	CLA	O2A-CGA-CBA	2.25	118.76	111.90
23	B	614	CLA	C3B-C4B-NB	2.26	112.13	109.21
23	c	909	CLA	CAC-C3C-C2C	2.26	131.47	127.51
23	D	402	CLA	OBD-CAD-CBD	2.27	129.36	125.94
25	D	404	BCR	C31-C1-C2	2.27	116.90	108.79
23	a	414	CLA	O2A-CGA-CBA	2.27	118.81	111.90
36	a	417	LHG	C6-O8-C23	2.27	123.20	116.85
34	h	102	DGD	C6D-C5D-C4D	2.27	117.17	112.03
34	c	917	DGD	O2G-C1B-C2B	2.27	116.47	111.53
38	H	101	RRX	C34-C9-C8	2.27	121.88	118.10
34	D	406	DGD	O6D-C5D-C4D	2.27	113.95	109.68
27	D	411	LMG	O8-C28-C29	2.28	118.83	111.90
30	b	625	LMT	C1-O1'-C1'	2.28	117.92	113.94
30	M	101	LMT	C2'-C3'-C4'	2.28	114.61	109.60
23	B	616	CLA	CMB-C2B-C3B	2.28	129.56	125.09
23	C	501	CLA	CMB-C2B-C1B	2.29	132.15	128.36
23	b	609	CLA	C4-C3-C5	2.29	118.90	115.41
33	b	602	HTG	C1-O5-C5	2.29	117.11	112.74
27	b	623	LMG	O1-C1-C2	2.29	110.93	108.04
23	a	411	CLA	C3D-CAD-CBD	2.29	110.84	107.60
34	h	102	DGD	C6D-O5D-C1E	2.30	118.64	113.82
23	B	604	CLA	C4A-NA-C1A	2.30	109.33	106.36
23	b	615	CLA	CED-O2D-CGD	2.30	121.38	115.99
23	C	504	CLA	C4A-NA-C1A	2.30	109.33	106.36
23	a	409	CLA	O2A-CGA-CBA	2.30	118.92	111.90
23	B	613	CLA	C4A-NA-C1A	2.31	109.34	106.36
23	c	904	CLA	O2A-CGA-CBA	2.31	118.94	111.90
25	K	101	BCR	C4-C5-C6	2.31	125.73	122.78
23	a	411	CLA	CMD-C2D-C3D	2.32	129.62	125.09
36	D	410	LHG	O7-C7-C8	2.32	116.56	111.53
27	A	413	LMG	O8-C28-C29	2.32	118.97	111.90
28	a	419	PL9	C10-C9-C11	2.32	118.95	115.41
23	b	607	CLA	CMD-C2D-C3D	2.33	129.64	125.09
23	a	410	CLA	C3B-C4B-NB	2.33	112.22	109.21
25	D	404	BCR	C40-C30-C39	2.34	115.86	108.37
23	C	506	CLA	C4A-NA-C1A	2.34	109.38	106.36
33	b	626	HTG	C1'-S1-C1	2.34	103.53	100.30
23	c	904	CLA	CED-O2D-CGD	2.35	121.49	115.99
34	D	406	DGD	O1G-C1A-C2A	2.35	119.05	111.90
23	c	909	CLA	CMC-C2C-C3C	2.35	132.76	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	411	CLA	O2A-CGA-CBA	2.35	119.06	111.90
23	B	615	CLA	C4A-NA-C1A	2.35	109.40	106.36
23	c	913	CLA	O2A-CGA-CBA	2.36	119.08	111.90
23	C	510	CLA	CMB-C2B-C3B	2.36	129.70	125.09
23	D	402	CLA	CMC-C2C-C1C	2.36	128.67	125.02
26	A	412	SQD	O3-C3-C4	2.36	115.65	110.34
23	d	403	CLA	CAC-C3C-C4C	2.36	128.26	124.83
25	A	411	BCR	C35-C13-C12	2.36	122.03	118.10
36	d	408	LHG	O8-C23-C24	2.36	119.10	111.90
25	B	618	BCR	C24-C25-C26	2.36	126.79	121.37
23	c	904	CLA	CMB-C2B-C3B	2.37	129.72	125.09
23	B	611	CLA	CAC-C3C-C4C	2.37	128.27	124.83
23	c	908	CLA	C3B-C4B-NB	2.37	112.28	109.21
23	c	914	CLA	CED-O2D-CGD	2.37	121.55	115.99
34	C	516	DGD	C1G-O1G-C1A	2.37	123.48	116.85
23	B	612	CLA	C4A-NA-C1A	2.38	109.44	106.36
23	B	611	CLA	C4A-NA-C1A	2.38	109.44	106.36
27	Z	101	LMG	O6-C5-C4	2.38	114.15	109.68
23	d	403	CLA	CMB-C2B-C1B	2.39	132.31	128.36
23	c	912	CLA	CMC-C2C-C1C	2.39	128.71	125.02
30	b	625	LMT	C1'-C2'-C3'	2.39	114.68	109.97
23	C	504	CLA	C3B-C4B-NB	2.39	112.30	109.21
23	b	614	CLA	CMD-C2D-C3D	2.40	129.77	125.09
23	A	407	CLA	CED-O2D-CGD	2.40	121.61	115.99
23	C	508	CLA	C3B-C4B-NB	2.40	112.31	109.21
24	A	409	PHO	CMB-C2B-C1B	2.40	128.97	125.06
30	B	623	LMT	O2'-C2'-C1'	2.40	115.29	110.02
23	A	410	CLA	C6-C5-C3	2.41	117.77	112.48
23	C	511	CLA	CAC-C3C-C4C	2.41	128.33	124.83
23	C	509	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	b	619	CLA	CED-O2D-CGD	2.42	121.67	115.99
23	b	617	CLA	CED-O2D-CGD	2.42	121.67	115.99
23	c	911	CLA	C3B-C4B-NB	2.42	112.34	109.21
28	a	419	PL9	C53-C6-C1	2.42	120.73	114.94
23	c	909	CLA	C4-C3-C5	2.43	119.12	115.41
27	Z	101	LMG	O1-C7-C8	2.43	116.78	110.99
23	B	604	CLA	CMD-C2D-C3D	2.43	129.85	125.09
30	m	102	LMT	O2'-C2'-C1'	2.43	115.36	110.02
23	C	508	CLA	C4A-NA-C1A	2.44	109.51	106.36
25	b	620	BCR	C33-C5-C4	2.44	118.06	113.43
27	d	410	LMG	O8-C28-C29	2.44	119.34	111.90
23	C	511	CLA	C4-C3-C5	2.45	119.14	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	906	CLA	C4-C3-C5	2.45	119.14	115.41
23	d	402	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	B	606	CLA	CMB-C2B-C3B	2.45	129.88	125.09
37	f	101	HEM	CMD-C2D-C3D	2.46	125.22	114.35
28	d	405	PL9	C25-C24-C26	2.46	119.16	115.41
33	B	631	HTG	O5-C5-C6	2.46	112.57	106.36
30	M	101	LMT	O5'-C5'-C6'	2.47	112.59	106.36
23	C	513	CLA	CMB-C2B-C3B	2.47	129.92	125.09
23	b	605	CLA	O2A-CGA-CBA	2.47	119.43	111.90
23	C	512	CLA	CMB-C2B-C3B	2.47	129.93	125.09
34	d	406	DGD	C4D-C3D-C2D	2.48	115.42	110.79
23	C	502	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	D	406	DGD	O3G-C3G-C2G	2.49	116.90	110.99
26	a	416	SQD	O5-C1-O6	2.49	116.04	110.05
23	B	603	CLA	CMD-C2D-C3D	2.49	129.96	125.09
23	C	511	CLA	C3A-C2A-C1A	2.50	105.73	101.50
33	C	522	HTG	O5-C5-C4	2.50	114.37	109.68
23	c	906	CLA	C4A-NA-C1A	2.50	109.59	106.36
36	d	408	LHG	O7-C7-C8	2.50	116.96	111.53
34	c	918	DGD	O1G-C1A-C2A	2.50	119.52	111.90
26	L	103	SQD	C4-C3-C2	2.50	115.46	110.79
23	b	619	CLA	C3B-C4B-NB	2.51	112.45	109.21
24	A	409	PHO	CED-O2D-CGD	2.51	121.88	115.99
25	b	620	BCR	C39-C30-C25	2.51	114.24	110.30
23	B	602	CLA	C3B-C4B-NB	2.52	112.46	109.21
27	c	921	LMG	O8-C9-C8	2.52	115.46	108.69
30	J	102	LMT	O1'-C1'-C2'	2.53	111.23	108.04
23	b	616	CLA	CMB-C2B-C3B	2.53	130.03	125.09
23	B	604	CLA	C4-C3-C5	2.53	119.27	115.41
23	B	605	CLA	CMC-C2C-C1C	2.53	128.94	125.02
27	a	418	LMG	O8-C28-C29	2.53	119.62	111.90
23	c	910	CLA	OBD-CAD-CBD	2.54	129.76	125.94
25	d	404	BCR	C30-C25-C24	2.54	122.92	115.82
23	C	501	CLA	CMD-C2D-C3D	2.54	130.06	125.09
24	A	408	PHO	C4D-C3D-C2D	2.54	109.61	106.74
36	D	409	LHG	O8-C23-C24	2.54	119.65	111.90
34	C	516	DGD	O6E-C5E-C6E	2.54	112.79	106.36
30	A	419	LMT	C1-O1'-C1'	2.55	118.39	113.94
23	B	614	CLA	C4-C3-C5	2.55	119.30	115.41
23	B	613	CLA	CED-O2D-CGD	2.55	121.96	115.99
28	d	405	PL9	C53-C6-C1	2.55	121.03	114.94
23	b	616	CLA	C4A-NA-C1A	2.55	109.66	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	CMB-C2B-C3B	2.55	130.08	125.09
23	C	512	CLA	C4A-NA-C1A	2.55	109.66	106.36
37	F	101	HEM	C2C-C1C-CHC	2.55	127.56	123.68
23	d	403	CLA	CED-O2D-CGD	2.55	121.98	115.99
23	b	610	CLA	CMD-C2D-C3D	2.56	130.09	125.09
23	b	607	CLA	C3B-C4B-NB	2.56	112.52	109.21
23	b	607	CLA	CED-O2D-CGD	2.56	121.99	115.99
30	c	922	LMT	O5'-C5'-C6'	2.56	112.83	106.36
23	c	912	CLA	O2A-CGA-CBA	2.57	119.72	111.90
24	a	412	PHO	C2B-C1B-NB	2.57	113.58	109.73
23	b	613	CLA	CMD-C2D-C3D	2.58	130.13	125.09
36	l	101	LHG	O7-C7-C8	2.58	117.14	111.53
23	a	409	CLA	O2D-CGD-CBD	2.59	114.84	111.30
34	h	102	DGD	O2G-C1B-C2B	2.59	117.15	111.53
26	B	621	SQD	O47-C7-C8	2.59	117.15	111.53
23	B	605	CLA	CAC-C3C-C4C	2.60	128.60	124.83
23	b	611	CLA	CAC-C3C-C4C	2.60	128.60	124.83
27	c	920	LMG	O8-C9-C8	2.60	115.68	108.69
23	B	603	CLA	CMB-C2B-C3B	2.60	130.17	125.09
34	H	102	DGD	O6E-C5E-C6E	2.60	112.94	106.36
23	a	409	CLA	C3B-C4B-NB	2.61	112.58	109.21
26	A	418	SQD	O48-C46-C45	2.61	115.72	108.69
25	D	404	BCR	C32-C1-C6	2.61	114.40	110.30
23	C	510	CLA	CMC-C2C-C1C	2.61	129.06	125.02
30	b	624	LMT	C3'-C4'-C5'	2.61	116.75	110.84
24	a	413	PHO	CMB-C2B-C1B	2.62	129.32	125.06
23	c	903	CLA	CAC-C3C-C4C	2.62	128.63	124.83
34	C	516	DGD	C1E-O6E-C5E	2.62	118.83	113.75
26	D	407	SQD	C3-C4-C5	2.62	114.77	110.20
23	C	506	CLA	CMB-C2B-C3B	2.63	130.23	125.09
23	c	903	CLA	C4A-NA-C1A	2.63	109.76	106.36
30	C	520	LMT	O1'-C1'-C2'	2.63	111.36	108.04
25	B	620	BCR	C2-C1-C6	2.63	114.53	110.36
23	C	513	CLA	O2A-CGA-CBA	2.63	119.92	111.90
23	C	509	CLA	C3B-C4B-NB	2.63	112.61	109.21
27	b	623	LMG	C13-C12-C11	2.63	122.94	113.29
23	c	912	CLA	C3B-C4B-NB	2.63	112.61	109.21
23	c	906	CLA	CMC-C2C-C1C	2.63	129.10	125.02
23	b	617	CLA	O2A-CGA-CBA	2.64	119.93	111.90
23	c	913	CLA	C4A-NA-C1A	2.64	109.77	106.36
23	B	611	CLA	C4-C3-C5	2.64	119.44	115.41
36	d	409	LHG	O7-C7-C8	2.64	117.27	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CED-O2D-CGD	2.65	122.20	115.99
26	a	401	SQD	O48-C46-C45	2.65	115.82	108.69
23	A	410	CLA	CMD-C2D-C3D	2.65	130.27	125.09
34	D	406	DGD	O6D-C5D-C6D	2.65	112.03	106.61
27	Z	101	LMG	O8-C28-C29	2.65	119.99	111.90
23	b	610	CLA	C3B-C4B-NB	2.66	112.64	109.21
34	d	406	DGD	O1G-C1A-C2A	2.66	120.00	111.90
30	b	624	LMT	C2'-C3'-C4'	2.66	115.44	109.60
23	b	616	CLA	O2A-CGA-CBA	2.67	120.03	111.90
30	z	101	LMT	O5B-C5B-C6B	2.67	113.10	106.36
23	c	904	CLA	O2D-CGD-CBD	2.67	114.96	111.30
25	B	620	BCR	C38-C26-C27	2.68	118.50	113.43
34	d	406	DGD	C1G-O1G-C1A	2.68	124.33	116.85
27	c	921	LMG	O8-C28-C29	2.68	120.06	111.90
23	B	613	CLA	CMB-C2B-C3B	2.68	130.33	125.09
38	H	101	RRX	C36-C18-C17	2.68	126.86	122.90
25	D	404	BCR	C30-C25-C24	2.69	123.34	115.82
23	c	910	CLA	CED-O2D-CGD	2.69	122.29	115.99
23	C	505	CLA	CMB-C2B-C3B	2.69	130.34	125.09
34	c	918	DGD	O5D-C6D-C5D	2.69	113.95	109.08
23	b	607	CLA	CMB-C2B-C3B	2.69	130.35	125.09
23	B	614	CLA	CAC-C3C-C4C	2.69	128.74	124.83
23	C	510	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	D	402	CLA	O2D-CGD-CBD	2.70	115.00	111.30
23	b	615	CLA	O2A-CGA-CBA	2.70	120.14	111.90
33	b	626	HTG	C1-C2-C3	2.70	116.68	110.69
23	b	618	CLA	C4A-NA-C1A	2.71	109.86	106.36
23	c	907	CLA	CED-O2D-CGD	2.71	122.34	115.99
23	B	616	CLA	C3B-C4B-NB	2.71	112.71	109.21
23	B	602	CLA	O2A-CGA-CBA	2.72	120.19	111.90
26	A	412	SQD	O2-C2-C1	2.72	115.99	110.02
23	b	613	CLA	C3B-C4B-NB	2.73	112.73	109.21
23	c	908	CLA	O2A-CGA-CBA	2.73	120.21	111.90
23	b	612	CLA	CMD-C2D-C3D	2.73	130.43	125.09
27	C	519	LMG	O8-C9-C8	2.73	116.04	108.69
23	b	617	CLA	CAC-C3C-C4C	2.74	128.80	124.83
23	B	616	CLA	CAC-C3C-C2C	2.74	132.31	127.51
30	B	623	LMT	O1B-C4'-C3'	2.75	114.25	107.17
23	C	508	CLA	CMC-C2C-C3C	2.76	133.96	125.94
23	C	504	CLA	CMB-C2B-C3B	2.76	130.49	125.09
23	C	505	CLA	CED-O2D-CGD	2.76	122.47	115.99
36	D	408	LHG	C6-O8-C23	2.77	124.59	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	401	SQD	C3-C4-C5	2.77	115.03	110.20
23	C	509	CLA	CMB-C2B-C1B	2.78	132.97	128.36
23	c	902	CLA	C4-C3-C5	2.78	119.66	115.41
23	D	402	CLA	C3B-C4B-NB	2.78	112.81	109.21
23	c	910	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	D	403	CLA	C4A-NA-C1A	2.79	109.97	106.36
30	m	101	LMT	O4'-C4B-C3B	2.79	116.62	110.34
23	D	402	CLA	C4-C3-C5	2.79	119.67	115.41
23	b	611	CLA	CMD-C2D-C3D	2.80	130.56	125.09
23	b	611	CLA	CMB-C2B-C3B	2.80	130.56	125.09
34	H	102	DGD	C6D-C5D-C4D	2.80	118.37	112.03
34	c	918	DGD	O2G-C1B-C2B	2.80	117.61	111.53
23	B	609	CLA	CMC-C2C-C1C	2.80	129.35	125.02
27	a	418	LMG	O1-C1-C2	2.80	111.58	108.04
23	C	506	CLA	CMD-C2D-C3D	2.81	130.58	125.09
26	A	418	SQD	C46-O48-C23	2.81	124.71	116.85
23	c	908	CLA	CMD-C2D-C3D	2.82	130.60	125.09
24	a	413	PHO	C3C-C4C-NC	2.83	114.81	110.24
28	a	419	PL9	C15-C14-C16	2.83	119.73	115.41
28	A	414	PL9	C53-C6-C1	2.83	121.71	114.94
23	c	910	CLA	C4A-NA-C1A	2.84	110.03	106.36
25	A	411	BCR	C27-C26-C25	2.84	126.39	122.78
23	C	503	CLA	C4-C3-C5	2.86	119.77	115.41
23	a	409	CLA	CMD-C2D-C3D	2.86	130.69	125.09
28	A	414	PL9	C45-C44-C46	2.87	119.78	115.41
36	a	417	LHG	O8-C23-C24	2.87	120.64	111.90
34	C	517	DGD	O2G-C1B-C2B	2.88	117.78	111.53
23	C	510	CLA	C4-C3-C5	2.88	119.81	115.41
30	B	623	LMT	O5B-C5B-C4B	2.88	115.09	109.68
23	a	414	CLA	CMB-C2B-C3B	2.88	130.72	125.09
30	M	101	LMT	O2'-C2'-C1'	2.89	116.35	110.02
23	D	403	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	D	402	CLA	CMB-C2B-C3B	2.91	130.78	125.09
28	a	419	PL9	C45-C44-C46	2.92	119.87	115.41
23	B	604	CLA	CMB-C2B-C3B	2.93	130.82	125.09
23	C	509	CLA	CMC-C2C-C3C	2.93	134.45	125.94
36	d	409	LHG	O4-P-O5	2.93	128.41	112.53
33	U	201	HTG	C1-S1-C1'	2.93	110.38	100.37
23	c	914	CLA	CMD-C2D-C3D	2.94	130.85	125.09
23	C	512	CLA	CMD-C2D-C3D	2.95	130.86	125.09
23	b	618	CLA	C3B-C4B-NB	2.96	113.03	109.21
24	a	412	PHO	CMC-C2C-C1C	2.96	129.87	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	907	CLA	C3B-C4B-NB	2.96	113.03	109.21
23	b	609	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	a	411	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	B	606	CLA	CAC-C3C-C4C	2.97	129.14	124.83
36	D	408	LHG	O4-P-O5	2.97	128.63	112.53
23	C	509	CLA	C4A-NA-C1A	2.97	110.20	106.36
23	c	903	CLA	C3B-C4B-NB	2.98	113.07	109.21
25	b	620	BCR	C35-C13-C12	2.99	123.06	118.10
26	f	102	SQD	C46-O48-C23	2.99	125.20	116.85
23	C	506	CLA	C4-C3-C5	2.99	119.97	115.41
23	b	611	CLA	C3B-C4B-NB	2.99	113.08	109.21
26	B	621	SQD	C4-C3-C2	3.00	116.38	110.79
23	b	613	CLA	CHB-C4A-NA	3.00	128.66	124.51
24	A	409	PHO	O2D-CGD-CBD	3.00	115.41	111.30
23	b	617	CLA	C4-C3-C5	3.00	119.99	115.41
23	b	616	CLA	C3B-C4B-NB	3.00	113.09	109.21
28	A	414	PL9	C3-C4-C5	3.00	123.02	118.62
23	b	609	CLA	CMC-C2C-C3C	3.00	134.67	125.94
23	b	615	CLA	C4A-NA-C1A	3.00	110.24	106.36
23	d	402	CLA	O2D-CGD-CBD	3.01	115.43	111.30
30	M	101	LMT	C1-O1'-C1'	3.01	119.21	113.94
37	v	201	HEM	CMD-C2D-C3D	3.02	127.69	114.35
23	b	615	CLA	C3B-C4B-NB	3.02	113.11	109.21
23	c	909	CLA	C3B-C4B-NB	3.02	113.11	109.21
34	d	406	DGD	O1G-C1G-C2G	3.02	116.83	108.69
25	b	621	BCR	C16-C17-C18	3.03	131.57	127.20
23	c	906	CLA	CMD-C2D-C3D	3.03	131.01	125.09
30	C	520	LMT	C1B-O5B-C5B	3.04	119.64	113.75
23	b	615	CLA	CMD-C2D-C3D	3.04	131.03	125.09
24	a	412	PHO	CAC-C3C-C4C	3.04	128.71	125.16
23	b	614	CLA	C4A-NA-C1A	3.05	110.30	106.36
28	D	405	PL9	C53-C6-C1	3.05	122.22	114.94
36	D	410	LHG	O4-P-O5	3.05	129.05	112.53
23	C	510	CLA	C4A-NA-C1A	3.05	110.31	106.36
25	t	101	BCR	C1-C6-C7	3.06	124.38	115.82
23	C	502	CLA	CMC-C2C-C1C	3.06	129.75	125.02
33	V	202	HTG	O2-C2-C1	3.06	116.39	110.43
23	C	505	CLA	CMC-C2C-C1C	3.06	129.76	125.02
23	b	614	CLA	CMC-C2C-C1C	3.06	129.76	125.02
25	T	101	BCR	C2-C1-C6	3.06	115.21	110.36
23	C	502	CLA	C4-C3-C5	3.06	120.09	115.41
23	b	604	CLA	C4A-NA-C1A	3.06	110.32	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	419	LMT	O1'-C1'-C2'	3.06	111.91	108.04
30	a	402	LMT	O2'-C2'-C1'	3.06	116.74	110.02
23	c	908	CLA	C4A-NA-C1A	3.08	110.34	106.36
23	C	513	CLA	C4-C3-C5	3.09	120.13	115.41
23	b	604	CLA	CMC-C2C-C1C	3.10	129.82	125.02
28	A	414	PL9	C30-C29-C31	3.10	120.15	115.41
34	c	918	DGD	C3E-C4E-C5E	3.11	115.61	110.20
23	b	617	CLA	CHB-C4A-NA	3.11	128.82	124.51
23	B	616	CLA	C4-C3-C5	3.12	120.18	115.41
30	C	520	LMT	O3'-C3'-C4'	3.13	117.28	109.87
26	f	102	SQD	O48-C23-C24	3.14	121.46	111.90
34	C	518	DGD	O1G-C1A-C2A	3.14	121.46	111.90
33	b	626	HTG	C1-O5-C5	3.14	118.73	112.74
23	b	606	CLA	CAC-C3C-C4C	3.15	129.40	124.83
33	c	924	HTG	C3-C4-C5	3.15	115.69	110.20
23	C	510	CLA	O2D-CGD-CBD	3.16	115.63	111.30
23	C	509	CLA	O2A-CGA-CBA	3.16	121.53	111.90
23	B	607	CLA	C3B-C4B-NB	3.16	113.30	109.21
34	d	406	DGD	O6D-C1D-O3G	3.16	117.67	110.05
23	C	506	CLA	CMC-C2C-C1C	3.16	129.91	125.02
23	C	506	CLA	CAC-C3C-C4C	3.16	129.42	124.83
23	A	410	CLA	CAC-C3C-C4C	3.17	129.43	124.83
23	B	608	CLA	O2D-CGD-CBD	3.17	115.64	111.30
24	A	408	PHO	C4A-NA-C1A	3.17	111.04	108.21
23	c	914	CLA	CMC-C2C-C1C	3.17	129.92	125.02
23	C	513	CLA	CMD-C2D-C3D	3.18	131.30	125.09
23	c	914	CLA	O2A-CGA-CBA	3.18	121.58	111.90
23	C	504	CLA	CAC-C3C-C4C	3.18	129.45	124.83
23	B	602	CLA	CMC-C2C-C1C	3.18	129.94	125.02
23	B	613	CLA	C4-C3-C5	3.19	120.29	115.41
23	a	414	CLA	CMC-C2C-C1C	3.20	129.98	125.02
23	c	909	CLA	O2D-CGD-CBD	3.21	115.70	111.30
23	b	617	CLA	C4A-NA-C1A	3.22	110.52	106.36
23	C	507	CLA	CMB-C2B-C3B	3.22	131.39	125.09
28	a	419	PL9	C40-C39-C41	3.22	120.33	115.41
24	a	413	PHO	C4A-NA-C1A	3.24	111.10	108.21
23	c	912	CLA	CMD-C2D-C3D	3.24	131.43	125.09
23	B	613	CLA	CMD-C2D-C3D	3.25	131.44	125.09
23	B	609	CLA	O2A-CGA-CBA	3.25	121.79	111.90
23	c	911	CLA	CMD-C2D-C3D	3.25	131.44	125.09
33	V	202	HTG	O5-C5-C6	3.25	114.57	106.36
23	B	611	CLA	C3B-C4B-NB	3.26	113.42	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	CMD-C2D-C3D	3.26	131.46	125.09
27	Z	101	LMG	C3-C4-C5	3.26	115.88	110.20
23	B	610	CLA	CMB-C2B-C3B	3.27	131.48	125.09
23	B	608	CLA	CED-O2D-CGD	3.27	123.65	115.99
34	c	919	DGD	O1G-C1A-C2A	3.27	121.86	111.90
23	D	403	CLA	CAC-C3C-C4C	3.27	129.58	124.83
37	V	201	HEM	CMD-C2D-C3D	3.27	128.83	114.35
24	a	413	PHO	C2B-C1B-NB	3.27	114.64	109.73
25	B	619	BCR	C29-C30-C25	3.28	115.56	110.36
23	B	607	CLA	C4-C3-C5	3.29	120.43	115.41
26	D	407	SQD	O48-C23-C24	3.29	121.92	111.90
23	b	617	CLA	C3B-C4B-NB	3.29	113.46	109.21
23	b	605	CLA	C4-C3-C5	3.29	120.43	115.41
34	h	102	DGD	O1G-C1A-C2A	3.29	121.93	111.90
28	a	419	PL9	C35-C34-C36	3.29	120.44	115.41
25	t	101	BCR	C35-C13-C12	3.29	123.58	118.10
23	B	605	CLA	C4-C3-C5	3.30	120.44	115.41
23	c	903	CLA	CMD-C2D-C3D	3.30	131.54	125.09
23	B	611	CLA	O2A-CGA-CBA	3.30	121.95	111.90
37	f	101	HEM	C3B-C4B-CHC	3.30	127.81	123.16
23	b	619	CLA	CMD-C2D-C3D	3.30	131.55	125.09
23	c	905	CLA	C4A-NA-C1A	3.31	110.64	106.36
25	b	621	BCR	C29-C30-C25	3.32	115.61	110.36
28	a	419	PL9	C30-C29-C31	3.32	120.48	115.41
23	c	914	CLA	CMB-C2B-C3B	3.33	131.59	125.09
23	A	405	CLA	CMB-C2B-C3B	3.33	131.59	125.09
36	L	101	LHG	O7-C7-C8	3.33	118.76	111.53
23	b	613	CLA	C4A-NA-C1A	3.34	110.67	106.36
23	B	616	CLA	CMD-C2D-C3D	3.34	131.62	125.09
23	B	616	CLA	C4A-NA-C1A	3.35	110.69	106.36
23	b	615	CLA	C4-C3-C5	3.35	120.53	115.41
26	L	103	SQD	O47-C7-C8	3.36	118.82	111.53
25	T	101	BCR	C35-C13-C12	3.36	123.69	118.10
23	B	606	CLA	CMD-C2D-C3D	3.37	131.67	125.09
23	b	618	CLA	CAC-C3C-C4C	3.37	129.72	124.83
36	E	101	LHG	O7-C7-C8	3.37	118.85	111.53
30	F	102	LMT	C2'-C3'-C4'	3.37	117.01	109.60
23	A	410	CLA	C3B-C4B-NB	3.38	113.58	109.21
23	b	606	CLA	CMD-C2D-C3D	3.38	131.70	125.09
23	b	606	CLA	C3B-C4B-NB	3.39	113.59	109.21
24	A	408	PHO	C2B-C1B-NB	3.41	114.84	109.73
23	c	905	CLA	C4-C3-C5	3.41	120.62	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	CMD-C2D-C3D	3.41	131.76	125.09
36	L	101	LHG	O4-P-O5	3.41	131.02	112.53
23	b	610	CLA	O2D-CGD-CBD	3.42	115.99	111.30
23	C	501	CLA	CAC-C3C-C4C	3.43	129.80	124.83
26	a	401	SQD	O48-C23-C24	3.44	122.37	111.90
23	b	618	CLA	C4-C3-C5	3.44	120.66	115.41
37	V	201	HEM	C2D-C3D-C4D	3.44	107.33	101.50
23	A	410	CLA	CHB-C4A-NA	3.46	129.29	124.51
23	c	905	CLA	C3B-C4B-NB	3.46	113.69	109.21
23	c	902	CLA	C3B-C4B-NB	3.48	113.72	109.21
37	F	101	HEM	CAD-C3D-C2D	3.49	123.24	113.22
23	c	905	CLA	CAC-C3C-C4C	3.49	129.90	124.83
30	B	623	LMT	O1'-C1'-C2'	3.49	112.45	108.04
23	C	507	CLA	C4-C3-C5	3.49	120.74	115.41
23	b	619	CLA	CAC-C3C-C4C	3.50	129.91	124.83
23	B	607	CLA	C4A-NA-C1A	3.51	110.90	106.36
24	A	409	PHO	C2C-C1C-NC	3.52	115.00	109.73
23	C	505	CLA	CAC-C3C-C4C	3.52	129.94	124.83
23	c	907	CLA	O2D-CGD-CBD	3.52	116.13	111.30
23	B	606	CLA	C4-C3-C5	3.52	120.79	115.41
33	V	202	HTG	O5-C1-S1	3.53	119.56	110.45
24	A	409	PHO	C4-C3-C5	3.53	120.80	115.41
34	H	102	DGD	O1G-C1A-C2A	3.53	122.65	111.90
28	a	419	PL9	C20-C19-C21	3.53	120.80	115.41
23	b	619	CLA	CMB-C2B-C3B	3.53	132.00	125.09
23	c	912	CLA	C4-C3-C5	3.54	120.82	115.41
23	b	604	CLA	O2A-CGA-CBA	3.54	122.69	111.90
23	a	414	CLA	CMD-C2D-C3D	3.54	132.02	125.09
23	b	606	CLA	CMC-C2C-C1C	3.55	130.51	125.02
23	B	617	CLA	CMD-C2D-C3D	3.55	132.03	125.09
37	v	201	HEM	C2D-C3D-C4D	3.56	107.54	101.50
23	b	604	CLA	C4-C3-C5	3.57	120.87	115.41
23	C	510	CLA	CAC-C3C-C4C	3.58	130.03	124.83
24	A	409	PHO	C4A-NA-C1A	3.59	111.41	108.21
23	b	618	CLA	CMC-C2C-C1C	3.59	130.57	125.02
23	B	609	CLA	CAC-C3C-C4C	3.59	130.04	124.83
23	b	610	CLA	C4-C3-C5	3.60	120.90	115.41
23	C	513	CLA	C4A-NA-C1A	3.60	111.01	106.36
23	A	405	CLA	C3B-C4B-NB	3.61	113.87	109.21
23	c	910	CLA	C4-C3-C5	3.61	120.92	115.41
23	c	910	CLA	C3B-C4B-NB	3.61	113.88	109.21
26	f	102	SQD	O6-C44-C45	3.63	114.83	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406	CLA	C4-C3-C5	3.64	120.96	115.41
27	c	920	LMG	O8-C28-C29	3.65	123.03	111.90
37	V	201	HEM	CAD-C3D-C4D	3.66	125.37	112.47
23	b	607	CLA	C4A-NA-C1A	3.66	111.09	106.36
36	d	407	LHG	C6-O8-C23	3.66	127.08	116.85
30	F	102	LMT	O4'-C4B-C5B	3.66	118.94	109.24
23	c	909	CLA	C4A-NA-C1A	3.67	111.10	106.36
23	A	407	CLA	C3B-C4B-NB	3.67	113.95	109.21
23	b	604	CLA	CMD-C2D-C3D	3.68	132.28	125.09
23	B	604	CLA	C6-C5-C3	3.69	120.58	112.48
24	a	413	PHO	C2C-C1C-NC	3.69	115.27	109.73
36	a	417	LHG	O7-C7-C8	3.70	119.56	111.53
23	b	614	CLA	C3B-C4B-NB	3.70	113.99	109.21
27	c	921	LMG	O1-C1-C2	3.71	112.72	108.04
23	c	906	CLA	CAC-C3C-C4C	3.71	130.22	124.83
23	C	510	CLA	C3B-C4B-NB	3.71	114.01	109.21
30	F	102	LMT	C1B-O5B-C5B	3.72	120.97	113.75
23	D	403	CLA	O2D-CGD-CBD	3.72	116.41	111.30
30	m	101	LMT	O1'-C1'-C2'	3.73	112.75	108.04
23	b	607	CLA	CMC-C2C-C1C	3.73	130.79	125.02
23	c	904	CLA	CMD-C2D-C3D	3.73	132.39	125.09
23	B	608	CLA	CMD-C2D-C3D	3.75	132.43	125.09
23	c	912	CLA	C4A-NA-C1A	3.76	111.22	106.36
23	c	907	CLA	CMC-C2C-C1C	3.76	130.83	125.02
37	v	201	HEM	CMC-C2C-C3C	3.76	125.92	116.53
23	a	414	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	B	605	CLA	CED-O2D-CGD	3.77	124.83	115.99
23	B	602	CLA	C4A-NA-C1A	3.77	111.23	106.36
23	A	407	CLA	CMC-C2C-C1C	3.77	130.85	125.02
23	C	507	CLA	C4A-NA-C1A	3.77	111.23	106.36
26	A	418	SQD	O47-C7-C8	3.77	119.72	111.53
23	c	902	CLA	C4A-NA-C1A	3.79	111.25	106.36
33	B	624	HTG	C1'-S1-C1	3.79	105.52	100.30
23	a	410	CLA	CMD-C2D-C3D	3.80	132.53	125.09
34	d	406	DGD	O2G-C1B-C2B	3.81	119.80	111.53
30	B	623	LMT	C1B-O5B-C5B	3.81	121.13	113.75
23	C	505	CLA	CMD-C2D-C3D	3.82	132.56	125.09
23	d	403	CLA	C3B-C4B-NB	3.82	114.15	109.21
37	v	201	HEM	CAD-C3D-C2D	3.82	124.21	113.22
23	D	402	CLA	CAC-C3C-C4C	3.84	130.41	124.83
27	C	519	LMG	O8-C28-C29	3.84	123.60	111.90
34	C	516	DGD	O2G-C1B-C2B	3.85	119.90	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	CMB-C2B-C3B	3.86	132.63	125.09
34	C	518	DGD	O2G-C1B-C2B	3.86	119.91	111.53
23	c	906	CLA	CMB-C2B-C3B	3.86	132.64	125.09
23	b	606	CLA	O2D-CGD-CBD	3.87	116.61	111.30
23	d	402	CLA	CMD-C2D-C3D	3.87	132.66	125.09
23	a	414	CLA	C4-C3-C5	3.88	121.34	115.41
23	B	612	CLA	CMD-C2D-C3D	3.89	132.69	125.09
27	c	921	LMG	O7-C10-C11	3.89	119.97	111.53
24	A	408	PHO	CAC-C3C-C4C	3.90	129.71	125.16
33	b	601	HTG	C1'-S1-C1	3.90	105.68	100.30
24	a	413	PHO	C4-C3-C5	3.91	121.38	115.41
23	c	911	CLA	C4-C3-C5	3.92	121.39	115.41
30	A	419	LMT	C1'-O5'-C5'	3.92	121.36	113.75
23	C	508	CLA	C4-C3-C5	3.92	121.40	115.41
23	b	619	CLA	O2A-CGA-CBA	3.92	123.85	111.90
30	c	922	LMT	O1'-C1'-C2'	3.94	113.02	108.04
23	A	407	CLA	C4-C3-C5	3.96	121.45	115.41
23	c	904	CLA	C4A-NA-C1A	3.96	111.48	106.36
27	c	920	LMG	O7-C10-C11	3.97	120.15	111.53
23	A	407	CLA	CMB-C2B-C3B	3.97	132.85	125.09
24	A	408	PHO	O2D-CGD-CBD	3.98	116.76	111.30
34	d	406	DGD	C3D-C4D-C5D	3.98	116.43	109.72
23	d	402	CLA	C3B-C4B-NB	4.00	114.38	109.21
23	b	615	CLA	O2D-CGD-CBD	4.02	116.82	111.30
23	C	511	CLA	C3B-C4B-NB	4.04	114.44	109.21
27	C	519	LMG	O7-C10-C11	4.04	120.31	111.53
23	c	907	CLA	CHB-C4A-NA	4.05	130.11	124.51
36	d	407	LHG	O8-C23-C24	4.05	124.24	111.90
23	d	403	CLA	C4-C3-C5	4.05	121.59	115.41
23	b	618	CLA	CMB-C2B-C3B	4.06	133.03	125.09
23	C	512	CLA	C4-C3-C5	4.06	121.61	115.41
23	B	603	CLA	C4-C3-C5	4.07	121.62	115.41
30	a	402	LMT	C1-O1'-C1'	4.07	121.06	113.94
26	a	401	SQD	O47-C7-C8	4.08	120.40	111.53
28	d	405	PL9	C15-C14-C16	4.08	121.64	115.41
24	a	412	PHO	C2D-C1D-ND	4.09	115.86	109.73
28	a	419	PL9	C25-C24-C26	4.09	121.66	115.41
23	b	608	CLA	CMC-C2C-C1C	4.10	131.37	125.02
23	c	908	CLA	C4-C3-C5	4.11	121.68	115.41
25	D	404	BCR	C29-C30-C25	4.11	116.87	110.36
27	b	623	LMG	O7-C10-C11	4.11	120.46	111.53
23	C	503	CLA	CMB-C2B-C3B	4.12	133.14	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	O2D-CGD-CBD	4.12	116.95	111.30
23	a	411	CLA	C4-C3-C5	4.13	121.72	115.41
23	B	608	CLA	C3B-C4B-NB	4.13	114.55	109.21
26	B	621	SQD	O48-C23-C24	4.13	124.50	111.90
23	D	403	CLA	CED-O2D-CGD	4.13	125.69	115.99
23	c	909	CLA	CMD-C2D-C3D	4.14	133.19	125.09
23	C	504	CLA	C4-C3-C5	4.15	121.74	115.41
23	b	610	CLA	CAC-C3C-C4C	4.15	130.85	124.83
26	D	407	SQD	O47-C7-C8	4.16	120.58	111.53
30	b	624	LMT	O5'-C5'-C4'	4.17	118.55	109.75
23	C	502	CLA	CAC-C3C-C4C	4.17	130.88	124.83
23	B	615	CLA	C4-C3-C5	4.19	121.80	115.41
23	A	405	CLA	CAC-C3C-C4C	4.20	130.93	124.83
30	A	419	LMT	O2'-C2'-C1'	4.22	119.26	110.02
23	b	607	CLA	CAC-C3C-C4C	4.23	130.97	124.83
23	C	513	CLA	C2C-C1C-NC	4.26	113.41	110.24
23	A	410	CLA	O2D-CGD-CBD	4.27	117.15	111.30
25	K	101	BCR	C37-C22-C23	4.28	125.22	118.10
24	a	412	PHO	C3C-C4C-NC	4.29	117.16	110.24
27	d	410	LMG	O7-C10-C11	4.29	120.85	111.53
23	B	610	CLA	CMD-C2D-C3D	4.30	133.49	125.09
23	C	507	CLA	O2D-CGD-CBD	4.30	117.20	111.30
23	C	509	CLA	O2D-CGD-CBD	4.31	117.22	111.30
23	B	604	CLA	CMC-C2C-C1C	4.32	131.70	125.02
23	B	606	CLA	O2D-CGD-CBD	4.33	117.24	111.30
23	C	505	CLA	O2D-CGD-CBD	4.34	117.26	111.30
23	B	612	CLA	CMC-C2C-C1C	4.36	131.77	125.02
24	a	413	PHO	C2D-C1D-ND	4.37	116.27	109.73
23	B	603	CLA	O2D-CGD-CBD	4.38	117.31	111.30
37	V	201	HEM	CMC-C2C-C3C	4.39	127.48	116.53
23	b	609	CLA	C4A-NA-C1A	4.41	112.06	106.36
37	f	101	HEM	CAD-C3D-C4D	4.41	128.04	112.47
24	A	409	PHO	C3C-C4C-NC	4.44	117.41	110.24
37	v	201	HEM	CAD-C3D-C4D	4.44	128.13	112.47
26	A	418	SQD	O48-C23-C24	4.44	125.43	111.90
23	c	909	CLA	C2C-C1C-NC	4.46	113.57	110.24
23	c	907	CLA	C2C-C1C-NC	4.46	113.57	110.24
23	b	609	CLA	O2D-CGD-CBD	4.47	117.43	111.30
23	c	910	CLA	O2D-CGD-CBD	4.50	117.47	111.30
37	F	101	HEM	CMB-C2B-C3B	4.50	127.77	116.53
27	b	623	LMG	O8-C28-C29	4.53	125.71	111.90
23	B	603	CLA	C2C-C1C-NC	4.54	113.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	411	CLA	O2D-CGD-CBD	4.56	117.56	111.30
23	c	914	CLA	O2D-CGD-CBD	4.59	117.60	111.30
33	c	924	HTG	O5-C5-C4	4.60	118.31	109.68
23	A	406	CLA	CMD-C2D-C3D	4.61	134.11	125.09
30	M	101	LMT	O1'-C1'-C2'	4.63	113.88	108.04
23	B	613	CLA	O2D-CGD-CBD	4.63	117.65	111.30
24	A	409	PHO	C2B-C1B-NB	4.64	116.68	109.73
23	c	914	CLA	C2C-C1C-NC	4.64	113.70	110.24
23	C	503	CLA	O2D-CGD-CBD	4.65	117.68	111.30
36	D	408	LHG	O8-C23-C24	4.66	126.08	111.90
23	A	405	CLA	C2C-C1C-NC	4.66	113.71	110.24
23	b	612	CLA	CAC-C3C-C4C	4.68	131.63	124.83
24	a	412	PHO	CMD-C2D-C1D	4.70	132.70	125.06
24	A	409	PHO	CAC-C3C-C4C	4.70	130.64	125.16
23	B	607	CLA	O2D-CGD-CBD	4.71	117.76	111.30
23	b	613	CLA	O2D-CGD-CBD	4.72	117.77	111.30
23	B	610	CLA	CAC-C3C-C4C	4.72	131.68	124.83
23	c	911	CLA	O2D-CGD-CBD	4.73	117.78	111.30
23	B	610	CLA	O2D-CGD-CBD	4.75	117.82	111.30
23	C	512	CLA	C2C-C1C-NC	4.75	113.78	110.24
30	a	402	LMT	O1'-C1'-C2'	4.76	114.05	108.04
27	Z	101	LMG	O7-C10-C11	4.76	121.88	111.53
23	B	604	CLA	C3B-C4B-NB	4.77	115.37	109.21
37	V	201	HEM	CAD-C3D-C2D	4.77	126.92	113.22
27	B	622	LMG	O8-C28-C29	4.77	126.42	111.90
30	t	102	LMT	O1'-C1'-C2'	4.77	114.06	108.04
37	v	201	HEM	CMB-C2B-C3B	4.78	128.47	116.53
23	c	913	CLA	C2C-C1C-NC	4.79	113.81	110.24
23	B	611	CLA	CHB-C4A-NA	4.79	131.13	124.51
24	A	409	PHO	C2D-C1D-ND	4.80	116.92	109.73
23	b	605	CLA	CMD-C2D-C3D	4.86	134.59	125.09
23	b	616	CLA	CAC-C3C-C4C	4.86	131.89	124.83
23	B	617	CLA	CAC-C3C-C4C	4.86	131.89	124.83
23	C	511	CLA	C4A-NA-C1A	4.88	112.67	106.36
23	D	402	CLA	CMD-C2D-C3D	4.88	134.63	125.09
23	b	614	CLA	O2D-CGD-CBD	4.89	118.01	111.30
23	B	609	CLA	C3B-C4B-NB	4.90	115.54	109.21
26	a	401	SQD	O9-S-C6	4.91	111.08	106.94
26	D	407	SQD	O7-S-C6	4.94	111.11	106.94
23	b	605	CLA	CMB-C2B-C3B	4.94	134.75	125.09
23	B	617	CLA	O2D-CGD-CBD	4.96	118.11	111.30
23	c	905	CLA	O2D-CGD-CBD	4.97	118.12	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	m	102	LMT	O1'-C1'-C2'	4.98	114.33	108.04
23	C	508	CLA	C2C-C1C-NC	4.98	113.95	110.24
23	c	911	CLA	C2C-C1C-NC	5.02	113.98	110.24
23	C	504	CLA	O2D-CGD-CBD	5.03	118.19	111.30
30	a	402	LMT	C1'-O5'-C5'	5.04	123.53	113.75
37	f	101	HEM	CMB-C2B-C3B	5.05	129.14	116.53
23	d	402	CLA	C4-C3-C5	5.06	123.13	115.41
23	B	605	CLA	O2D-CGD-CBD	5.07	118.25	111.30
24	A	408	PHO	C2C-C1C-NC	5.07	117.33	109.73
24	A	408	PHO	C3C-C4C-NC	5.09	118.46	110.24
24	a	412	PHO	C2C-C1C-NC	5.09	117.36	109.73
23	c	906	CLA	O2D-CGD-CBD	5.10	118.30	111.30
33	b	602	HTG	C1'-S1-C1	5.11	107.34	100.30
23	b	607	CLA	O2D-CGD-CBD	5.14	118.35	111.30
23	A	406	CLA	CAC-C3C-C4C	5.14	132.30	124.83
23	A	405	CLA	CMD-C2D-C3D	5.15	135.16	125.09
23	a	414	CLA	CAC-C3C-C4C	5.17	132.33	124.83
23	b	618	CLA	CMD-C2D-C3D	5.18	135.22	125.09
27	B	622	LMG	O7-C10-C11	5.18	122.79	111.53
26	a	416	SQD	O47-C7-C8	5.21	122.85	111.53
23	B	613	CLA	CAC-C3C-C4C	5.22	132.41	124.83
30	C	520	LMT	O1B-C4'-C3'	5.25	120.73	107.17
23	b	619	CLA	C2C-C1C-NC	5.27	114.17	110.24
23	b	609	CLA	C2C-C1C-NC	5.29	114.18	110.24
23	b	608	CLA	C4-C3-C5	5.29	123.49	115.41
26	A	418	SQD	O6-C1-C2	5.31	114.74	108.04
23	B	615	CLA	CAC-C3C-C4C	5.31	132.54	124.83
23	B	611	CLA	O2D-CGD-CBD	5.34	118.63	111.30
37	f	101	HEM	CAD-C3D-C2D	5.35	128.59	113.22
23	b	605	CLA	C2C-C1C-NC	5.36	114.23	110.24
23	c	903	CLA	C2C-C1C-NC	5.37	114.24	110.24
37	F	101	HEM	CMC-C2C-C3C	5.38	129.95	116.53
33	C	522	HTG	C1-O5-C5	5.38	123.00	112.74
23	b	618	CLA	O2D-CGD-CBD	5.40	118.71	111.30
33	O	303	HTG	C1'-S1-C1	5.40	107.75	100.30
26	A	412	SQD	O47-C7-C8	5.41	123.28	111.53
23	b	606	CLA	C4-C3-C5	5.42	123.69	115.41
23	A	407	CLA	CAC-C3C-C4C	5.43	132.71	124.83
23	b	604	CLA	C2C-C1C-NC	5.44	114.30	110.24
23	a	411	CLA	CAC-C3C-C4C	5.44	132.73	124.83
33	c	924	HTG	C1-O5-C5	5.47	123.17	112.74
23	a	414	CLA	O2D-CGD-CBD	5.47	118.81	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C2C-C1C-NC	5.48	114.32	110.24
23	b	617	CLA	C2C-C1C-NC	5.48	114.32	110.24
27	a	418	LMG	O7-C10-C11	5.49	123.45	111.53
23	b	610	CLA	C2C-C1C-NC	5.49	114.33	110.24
23	c	904	CLA	C2C-C1C-NC	5.50	114.33	110.24
33	D	414	HTG	C1'-S1-C1	5.53	107.92	100.30
23	D	403	CLA	C2C-C1C-NC	5.53	114.36	110.24
37	F	101	HEM	CAD-C3D-C4D	5.55	132.04	112.47
23	c	912	CLA	O2D-CGD-CBD	5.56	118.93	111.30
23	C	511	CLA	O2D-CGD-CBD	5.58	118.96	111.30
23	c	906	CLA	C2C-C1C-NC	5.59	114.41	110.24
23	A	406	CLA	O2D-CGD-CBD	5.60	118.98	111.30
26	B	621	SQD	O9-S-C6	5.60	111.66	106.94
23	C	508	CLA	O2D-CGD-CBD	5.67	119.07	111.30
23	B	602	CLA	C2C-C1C-NC	5.67	114.46	110.24
33	B	625	HTG	C1'-S1-C1	5.68	108.12	100.30
23	B	615	CLA	O2D-CGD-CBD	5.68	119.09	111.30
28	D	405	PL9	C40-C39-C41	5.75	124.19	115.41
23	b	608	CLA	O2D-CGD-CBD	5.77	119.21	111.30
37	V	201	HEM	CMB-C2B-C3B	5.81	131.04	116.53
37	f	101	HEM	CMC-C2C-C3C	5.82	131.06	116.53
23	c	905	CLA	C2C-C1C-NC	5.83	114.58	110.24
23	d	403	CLA	C2C-C1C-NC	5.84	114.59	110.24
27	A	413	LMG	O1-C1-C2	5.85	115.42	108.04
23	A	410	CLA	C4-C3-C5	5.86	124.35	115.41
23	C	512	CLA	O2D-CGD-CBD	5.86	119.34	111.30
23	b	612	CLA	O2D-CGD-CBD	5.87	119.36	111.30
23	B	614	CLA	C2C-C1C-NC	5.89	114.63	110.24
23	b	614	CLA	C2C-C1C-NC	5.90	114.63	110.24
24	A	408	PHO	C2D-C1D-ND	5.91	118.60	109.73
23	B	613	CLA	C2C-C1C-NC	5.92	114.65	110.24
28	d	405	PL9	C40-C39-C41	5.94	124.48	115.41
23	B	615	CLA	C2C-C1C-NC	5.95	114.67	110.24
24	A	408	PHO	CMD-C2D-C1D	5.98	134.79	125.06
23	C	511	CLA	C2C-C1C-NC	5.98	114.70	110.24
23	c	902	CLA	O2D-CGD-CBD	6.01	119.55	111.30
23	b	605	CLA	O2D-CGD-CBD	6.03	119.57	111.30
23	a	409	CLA	C2C-C1C-NC	6.11	114.79	110.24
23	b	615	CLA	C2C-C1C-NC	6.13	114.81	110.24
23	B	612	CLA	O2D-CGD-CBD	6.14	119.73	111.30
23	c	910	CLA	C2C-C1C-NC	6.15	114.82	110.24
26	D	407	SQD	O9-S-C6	6.16	112.13	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	409	CLA	CAC-C3C-C4C	6.18	133.80	124.83
23	A	407	CLA	O2D-CGD-CBD	6.18	119.77	111.30
34	D	406	DGD	O2G-C1B-C2B	6.18	124.96	111.53
23	b	608	CLA	CAC-C3C-C4C	6.19	133.82	124.83
23	C	502	CLA	C2C-C1C-NC	6.22	114.88	110.24
23	C	513	CLA	O2D-CGD-CBD	6.29	119.92	111.30
24	a	412	PHO	O2D-CGD-CBD	6.31	119.95	111.30
23	b	611	CLA	O2D-CGD-CBD	6.33	119.98	111.30
23	C	503	CLA	C2C-C1C-NC	6.39	115.00	110.24
24	A	409	PHO	CMD-C2D-C1D	6.40	135.47	125.06
24	a	413	PHO	CMD-C2D-C1D	6.40	135.48	125.06
26	f	102	SQD	O9-S-C6	6.42	112.38	106.91
23	C	510	CLA	C2C-C1C-NC	6.43	115.03	110.24
26	a	401	SQD	O6-C1-C2	6.46	116.20	108.04
23	b	613	CLA	C2C-C1C-NC	6.48	115.07	110.24
23	B	608	CLA	C2C-C1C-NC	6.49	115.07	110.24
23	B	604	CLA	O2D-CGD-CBD	6.51	120.23	111.30
23	c	902	CLA	C2C-C1C-NC	6.54	115.11	110.24
23	c	912	CLA	C2C-C1C-NC	6.59	115.15	110.24
23	B	611	CLA	C2C-C1C-NC	6.61	115.16	110.24
23	c	908	CLA	C2C-C1C-NC	6.64	115.18	110.24
23	b	611	CLA	C2C-C1C-NC	6.69	115.22	110.24
33	B	630	HTG	C1'-S1-C1	6.75	109.60	100.30
23	c	903	CLA	O2D-CGD-CBD	6.82	120.66	111.30
23	b	618	CLA	C2C-C1C-NC	6.86	115.35	110.24
23	B	610	CLA	C2C-C1C-NC	6.86	115.35	110.24
23	b	612	CLA	C2C-C1C-NC	6.93	115.40	110.24
26	L	103	SQD	O9-S-C6	6.96	112.81	106.94
23	B	617	CLA	C2C-C1C-NC	6.98	115.44	110.24
23	D	402	CLA	C2C-C1C-NC	6.98	115.44	110.24
26	L	103	SQD	O6-C1-C2	7.00	116.88	108.04
23	d	403	CLA	O2D-CGD-CBD	7.01	120.92	111.30
23	a	410	CLA	C2C-C1C-NC	7.01	115.46	110.24
23	c	913	CLA	O2D-CGD-CBD	7.03	120.94	111.30
23	C	501	CLA	C2C-C1C-NC	7.13	115.55	110.24
23	A	407	CLA	C2C-C1C-NC	7.16	115.57	110.24
23	B	609	CLA	O2D-CGD-CBD	7.19	121.17	111.30
23	B	607	CLA	C2C-C1C-NC	7.20	115.60	110.24
33	d	401	HTG	C1'-S1-C1	7.20	110.23	100.30
23	B	616	CLA	C2C-C1C-NC	7.24	115.63	110.24
24	a	413	PHO	O2D-CGD-CBD	7.26	121.26	111.30
33	C	521	HTG	C1'-S1-C1	7.31	110.37	100.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	O2D-CGD-CBD	7.43	121.49	111.30
23	b	615	CLA	CAC-C3C-C4C	7.50	135.72	124.83
23	b	604	CLA	O2D-CGD-CBD	7.59	121.71	111.30
23	b	616	CLA	C2C-C1C-NC	7.60	115.90	110.24
26	A	418	SQD	O9-S-C6	7.60	113.35	106.94
23	A	410	CLA	C2C-C1C-NC	7.75	116.01	110.24
26	B	621	SQD	O7-S-C6	7.81	113.52	106.94
23	C	506	CLA	C2C-C1C-NC	7.82	116.07	110.24
23	B	606	CLA	C2C-C1C-NC	7.83	116.07	110.24
23	b	607	CLA	C2C-C1C-NC	7.83	116.08	110.24
23	B	602	CLA	O2D-CGD-CBD	7.88	122.12	111.30
23	b	619	CLA	O2D-CGD-CBD	8.00	122.28	111.30
23	C	505	CLA	C2C-C1C-NC	8.07	116.25	110.24
23	b	617	CLA	O2D-CGD-CBD	8.08	122.38	111.30
23	c	908	CLA	O2D-CGD-CBD	8.08	122.39	111.30
23	B	612	CLA	C2C-C1C-NC	8.10	116.28	110.24
33	u	201	HTG	C1'-S1-C1	8.13	111.51	100.30
26	A	412	SQD	O9-S-C6	8.24	113.89	106.94
23	C	509	CLA	C2C-C1C-NC	8.37	116.48	110.24
33	c	923	HTG	C1'-S1-C1	8.46	111.96	100.30
23	C	504	CLA	C2C-C1C-NC	8.50	116.57	110.24
33	b	627	HTG	C1'-S1-C1	8.54	112.07	100.30
23	b	606	CLA	C2C-C1C-NC	8.63	116.67	110.24
23	b	608	CLA	C2C-C1C-NC	8.68	116.71	110.24
23	a	411	CLA	C2C-C1C-NC	8.72	116.73	110.24
26	A	412	SQD	O6-C1-C2	8.80	119.16	108.04
33	c	924	HTG	C1'-S1-C1	8.83	112.47	100.30
23	d	402	CLA	C2C-C1C-NC	8.90	116.87	110.24
26	L	103	SQD	O7-S-C6	8.93	114.47	106.94
26	B	621	SQD	O6-C1-C2	9.00	119.41	108.04
23	B	609	CLA	C2C-C1C-NC	9.17	117.07	110.24
23	a	414	CLA	C2C-C1C-NC	9.44	117.27	110.24
33	B	626	HTG	C1'-S1-C1	9.48	113.37	100.30
23	B	605	CLA	C2C-C1C-NC	9.55	117.35	110.24
23	A	406	CLA	C2C-C1C-NC	9.79	117.53	110.24
23	B	604	CLA	C2C-C1C-NC	9.80	117.54	110.24
33	C	522	HTG	C1'-S1-C1	9.96	114.03	100.30
26	D	407	SQD	O6-C1-C2	10.04	120.72	108.04
33	B	631	HTG	C1'-S1-C1	10.14	114.28	100.30
26	a	416	SQD	O6-C1-C2	10.43	121.21	108.04
23	C	501	CLA	O2D-CGD-CBD	10.98	126.37	111.30
26	a	416	SQD	O9-S-C6	11.53	116.66	106.94

All (168) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	c	914	CLA	NC
23	c	914	CLA	NA
23	A	406	CLA	NA
23	d	402	CLA	ND
23	d	402	CLA	NA
23	b	618	CLA	NC
23	b	618	CLA	ND
23	b	618	CLA	NA
23	d	403	CLA	NC
23	C	508	CLA	NC
23	C	508	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	ND
23	b	617	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	b	612	CLA	NC
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	B	609	CLA	NC
23	B	603	CLA	NC
23	B	603	CLA	ND
23	C	513	CLA	NC
23	a	411	CLA	NC
23	a	411	CLA	NA
23	D	402	CLA	ND
23	B	612	CLA	NC
23	B	612	CLA	NA
23	C	506	CLA	NC
23	C	506	CLA	ND
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	c	912	CLA	NC
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	c	908	CLA	NC
23	c	908	CLA	ND
23	c	908	CLA	NA

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Mol	Chain	Res	Type	Atom
23	c	911	CLA	NC
23	c	911	CLA	ND
23	c	911	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	616	CLA	NA
23	b	611	CLA	NC
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	A	410	CLA	NC
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	c	902	CLA	NC
23	c	902	CLA	ND
23	c	902	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	NA
23	a	414	CLA	NC
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	507	CLA	NA
23	c	904	CLA	NC
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	C	505	CLA	ND
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	NA
23	c	909	CLA	NC
23	c	909	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	b	609	CLA	NC
23	b	609	CLA	ND
23	c	907	CLA	ND
23	c	907	CLA	NA
23	c	910	CLA	NC
23	c	910	CLA	ND
23	c	910	CLA	NA
23	c	906	CLA	ND
23	b	614	CLA	NC
23	b	614	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	B	617	CLA	NA
23	a	410	CLA	NC
23	a	410	CLA	ND
23	a	410	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	D	403	CLA	NC

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Mol	Chain	Res	Type	Atom
23	D	403	CLA	ND
23	D	403	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	c	903	CLA	NC
23	c	903	CLA	ND
23	c	903	CLA	NA
23	C	510	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	C	501	CLA	NC
23	C	501	CLA	ND
23	C	501	CLA	NA
23	b	615	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	c	905	CLA	NC
23	c	905	CLA	ND
23	c	905	CLA	NA
23	c	913	CLA	NC
23	c	913	CLA	NA
23	c	913	CLA	ND
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C7-O47-C45-C44
26	f	102	SQD	C45-O47-C7-O49

There are no ring outliers.

83 monomers are involved in 254 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	405	CLA	4	0
23	A	406	CLA	4	0
23	A	407	CLA	1	0
24	A	408	PHO	2	0
24	A	409	PHO	3	0
23	A	410	CLA	3	0
25	A	411	BCR	2	0
26	A	412	SQD	4	0
27	A	413	LMG	3	0
28	A	414	PL9	10	0
26	A	418	SQD	1	0
31	A	422	GOL	1	0
31	A	423	GOL	3	0
23	B	602	CLA	1	0
23	B	604	CLA	3	0
23	B	605	CLA	4	0
23	B	606	CLA	7	0
23	B	607	CLA	5	0
23	B	608	CLA	3	0
23	B	609	CLA	4	0
23	B	610	CLA	1	0
23	B	611	CLA	4	0
23	B	612	CLA	5	0
23	B	613	CLA	6	0
23	B	614	CLA	4	0
23	B	615	CLA	7	0
23	B	616	CLA	4	0
23	B	617	CLA	11	0
25	B	619	BCR	3	0
25	B	620	BCR	2	0
26	B	621	SQD	5	0
27	B	622	LMG	4	0
30	B	623	LMT	4	0
33	B	626	HTG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	631	HTG	1	0
31	B	633	GOL	2	0
31	B	635	GOL	1	0
23	C	501	CLA	4	0
23	C	502	CLA	2	0
23	C	503	CLA	3	0
23	C	504	CLA	4	0
23	C	505	CLA	1	0
23	C	506	CLA	5	0
23	C	507	CLA	2	0
23	C	508	CLA	2	0
23	C	509	CLA	4	0
23	C	510	CLA	4	0
23	C	511	CLA	5	0
23	C	512	CLA	3	0
23	C	513	CLA	3	0
25	C	514	BCR	1	0
25	C	515	BCR	4	0
34	C	517	DGD	2	0
27	C	519	LMG	2	0
30	C	520	LMT	4	0
33	C	521	HTG	1	0
31	C	524	GOL	4	0
23	D	402	CLA	1	0
23	D	403	CLA	6	0
25	D	404	BCR	5	0
34	D	406	DGD	9	0
26	D	407	SQD	3	0
36	D	408	LHG	2	0
36	D	409	LHG	9	0
36	D	410	LHG	13	0
27	D	411	LMG	2	0
33	D	414	HTG	2	0
31	D	415	GOL	3	0
36	E	101	LHG	3	0
37	F	101	HEM	4	0
38	H	101	RRX	4	0
34	H	102	DGD	1	0
30	J	102	LMT	1	0
25	K	101	BCR	5	0
25	K	102	BCR	4	0
36	L	101	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	L	103	SQD	5	0
31	L	104	GOL	1	0
30	M	101	LMT	3	0
25	T	101	BCR	9	0
33	U	201	HTG	1	0
37	V	201	HEM	1	0
30	Z	102	LMT	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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%)	-0.14	5 (1%) 76 79	16, 23, 46, 69	0
1	a	334/344 (97%)	0.03	14 (4%) 40 44	19, 24, 50, 76	0
2	B	504/504 (100%)	0.11	39 (7%) 16 18	18, 27, 54, 88	0
2	b	501/504 (99%)	0.14	47 (9%) 11 12	20, 29, 58, 119	0
3	C	451/455 (99%)	-0.07	14 (3%) 52 56	21, 31, 46, 81	0
3	c	455/455 (100%)	0.18	26 (5%) 27 30	23, 34, 48, 79	0
4	D	340/342 (99%)	-0.20	7 (2%) 67 70	17, 24, 40, 70	0
4	d	340/342 (99%)	-0.16	6 (1%) 71 74	19, 26, 45, 80	0
5	E	81/83 (97%)	0.97	18 (22%) 1 1	27, 40, 62, 82	0
5	e	79/83 (95%)	1.24	23 (29%) 1 0	32, 44, 72, 82	0
6	F	34/44 (77%)	0.23	5 (14%) 3 3	26, 34, 63, 74	0
6	f	32/44 (72%)	0.38	3 (9%) 11 12	29, 37, 76, 86	0
7	H	63/63 (100%)	-0.05	1 (1%) 74 78	24, 33, 43, 70	0
7	h	63/63 (100%)	0.41	5 (7%) 15 17	27, 37, 51, 81	0
8	I	35/38 (92%)	-0.08	0 100 100	27, 34, 64, 86	0
8	i	37/38 (97%)	0.24	2 (5%) 29 33	26, 34, 71, 83	0
9	J	36/40 (90%)	0.18	4 (11%) 7 8	26, 38, 65, 79	0
9	j	39/40 (97%)	0.64	8 (20%) 1 1	30, 42, 68, 84	0
10	K	37/37 (100%)	-0.14	0 100 100	32, 38, 47, 63	0
10	k	37/37 (100%)	0.34	3 (8%) 15 16	36, 42, 55, 69	0
11	L	37/37 (100%)	-0.10	3 (8%) 15 16	17, 22, 65, 75	0
11	l	37/37 (100%)	0.16	2 (5%) 29 33	19, 23, 64, 95	0
12	M	32/36 (88%)	-0.14	1 (3%) 52 56	21, 24, 40, 56	0
12	m	33/36 (91%)	0.03	2 (6%) 25 27	20, 25, 48, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	0.34	35 (14%) 4 4	18, 33, 66, 120	0
13	o	241/244 (98%)	0.42	40 (16%) 2 2	20, 35, 71, 87	0
14	T	29/32 (90%)	0.03	1 (3%) 49 52	19, 23, 49, 85	0
14	t	29/32 (90%)	0.03	1 (3%) 49 52	20, 23, 47, 72	0
15	U	97/104 (93%)	-0.10	0 100 100	23, 30, 52, 58	0
15	u	97/104 (93%)	-0.33	1 (1%) 84 86	24, 30, 40, 66	0
16	V	137/137 (100%)	-0.35	0 100 100	22, 28, 43, 51	0
16	v	137/137 (100%)	0.48	14 (10%) 9 10	26, 37, 52, 72	0
17	Y	27/30 (90%)	1.10	5 (18%) 2 2	37, 47, 70, 77	0
17	y	28/30 (93%)	1.21	7 (25%) 1 1	45, 55, 73, 77	0
18	X	38/40 (95%)	0.74	7 (18%) 2 2	32, 39, 65, 69	0
18	x	38/40 (95%)	0.97	9 (23%) 1 1	34, 42, 83, 94	0
19	Z	62/62 (100%)	1.51	20 (32%) 1 0	37, 46, 75, 92	0
19	z	60/62 (96%)	2.02	26 (43%) 0 0	47, 57, 88, 95	0
All	All	5235/5344 (97%)	0.15	404 (7%) 16 18	16, 30, 59, 120	0

All (404) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	494	GLY	8.4
2	b	496	TYR	8.2
18	x	37	VAL	8.0
13	o	246	ALA	7.5
13	O	60	ARG	7.5
18	x	38	GLN	7.2
2	b	494	GLY	7.2
19	z	61	VAL	7.1
2	B	495	PHE	7.0
17	Y	22	LEU	6.7
19	Z	62	VAL	6.4
19	z	60	PHE	6.4
5	e	25	ILE	6.2
19	z	5	PHE	6.1
1	A	11	ALA	6.0
19	Z	3	ILE	6.0
2	b	503	THR	6.0
2	b	502	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	5.8
19	Z	33	TRP	5.7
2	b	500	GLY	5.6
19	z	4	LEU	5.6
2	b	499	VAL	5.6
2	b	495	PHE	5.6
2	b	493	TRP	5.5
2	b	484	PRO	5.5
13	o	36	GLN	5.5
13	o	25	THR	5.5
9	J	5	GLY	5.4
11	l	1	MET	5.4
1	a	13	LEU	5.4
5	E	17	VAL	5.3
2	B	496	TYR	5.3
13	O	25	THR	5.2
2	B	501	ASP	5.2
19	z	2	THR	5.2
11	L	1	MET	5.1
2	b	86	ILE	5.1
9	j	6	GLY	5.1
19	Z	7	LEU	5.1
18	x	2	THR	5.1
2	b	85	GLY	5.1
9	j	5	GLY	5.1
13	o	35	SER	5.0
19	Z	30	PRO	5.0
19	Z	32	ASP	5.0
5	E	21	VAL	5.0
19	Z	31	GLN	5.0
5	E	6	GLY	5.0
18	X	2	THR	4.9
2	b	489	GLU	4.9
2	B	486	LEU	4.9
7	h	64	ALA	4.9
2	b	487	SER	4.9
18	X	37	VAL	4.8
19	z	7	LEU	4.7
13	o	23	ASP	4.7
13	O	27	ARG	4.7
2	B	500	GLY	4.6
2	B	487	SER	4.5

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Mol	Chain	Res	Type	RSRZ
17	y	22	LEU	4.5
2	b	293	ALA	4.5
5	E	4	THR	4.5
6	F	12	SER	4.5
13	o	38	TYR	4.4
13	O	3	GLN	4.4
19	z	41	PHE	4.4
13	o	26	ALA	4.4
9	J	6	GLY	4.4
6	f	14	PRO	4.3
1	a	11	ALA	4.3
19	z	3	ILE	4.3
10	k	18	PHE	4.3
19	Z	4	LEU	4.3
2	b	504	THR	4.2
17	y	19	ILE	4.2
6	F	13	TYR	4.2
3	c	201[A]	ASN	4.2
9	j	8	ILE	4.2
2	B	504	THR	4.2
2	B	293	ALA	4.2
3	C	23	ALA	4.2
13	O	26	ALA	4.2
13	o	32	ILE	4.1
2	b	126	PRO	4.1
11	L	3	PRO	4.1
5	E	5	THR	4.1
1	A	13	LEU	4.1
19	z	6	GLN	4.1
2	B	499	VAL	4.1
17	y	20	ALA	4.0
6	F	16	PHE	4.0
3	C	143	TYR	4.0
6	f	16	PHE	4.0
15	u	8	GLU	4.0
2	b	497	GLN	3.9
2	B	503	THR	3.9
19	Z	34	ASP	3.9
13	o	34	SER	3.9
5	e	6	GLY	3.9
19	Z	60	PHE	3.9
18	x	39	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
3	c	200	THR	3.9
13	O	133	VAL	3.8
1	a	235	TYR	3.8
2	B	484	PRO	3.8
6	F	15	ILE	3.8
5	e	21	VAL	3.8
19	Z	1	MET	3.8
9	j	4	GLU	3.8
3	c	21	ILE	3.8
13	O	4	THR	3.8
2	b	488	PRO	3.7
12	M	33	GLN	3.7
13	o	27	ARG	3.7
16	v	19	ILE	3.7
5	E	84	LYS	3.7
4	D	238	THR	3.7
3	c	279	LEU	3.7
19	z	39	LEU	3.7
13	O	24	ASP	3.6
8	i	37	LEU	3.6
2	B	485	GLU	3.6
2	b	84	THR	3.6
4	d	238	THR	3.6
13	o	37	THR	3.6
2	B	295	GLY	3.6
13	O	23	ASP	3.6
16	v	14	SER	3.5
2	b	295	GLY	3.5
14	T	30	THR	3.5
1	A	12	ASN	3.5
13	o	33	ASP	3.5
3	c	433	LEU	3.5
4	d	12	ARG	3.4
13	o	204	VAL	3.4
4	D	12	ARG	3.4
18	X	39	ARG	3.4
5	e	17	VAL	3.4
19	Z	61	VAL	3.4
13	O	132	ASN	3.4
2	b	492	GLU	3.4
2	B	483	ASP	3.4
13	o	22	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
13	o	87	VAL	3.4
17	y	25	ILE	3.3
13	o	132	ASN	3.3
13	o	207	ARG	3.3
13	o	58	ASN	3.3
13	o	141[A]	ASP	3.3
16	v	8	LEU	3.3
13	o	134	THR	3.3
2	b	294	SER	3.3
2	B	497	GLN	3.3
18	X	38	GLN	3.2
5	E	83	LEU	3.2
18	x	34	ILE	3.2
13	O	89	SER	3.2
5	e	83	LEU	3.2
13	o	133	VAL	3.2
5	e	84	LYS	3.2
3	C	24	THR	3.2
5	e	20	TRP	3.2
2	b	161	LEU	3.2
3	c	432	VAL	3.1
4	D	13	GLY	3.1
13	o	30	TYR	3.1
16	v	15	GLU	3.1
18	X	3	ILE	3.1
13	o	24	ASP	3.1
17	Y	21	GLN	3.1
6	F	14	PRO	3.1
16	v	12	LEU	3.1
13	O	130	GLN	3.1
16	v	16	GLY	3.1
2	B	297	THR	3.1
16	v	18	THR	3.1
7	H	64	ALA	3.1
13	o	89	SER	3.1
2	B	502	VAL	3.1
2	b	501	ASP	3.1
13	o	4	THR	3.0
9	j	3	SER	3.0
13	O	22	LEU	3.0
1	a	12	ASN	3.0
2	b	491	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
5	e	32	ILE	3.0
9	J	8	ILE	3.0
5	e	61	ARG	3.0
2	b	298	LEU	3.0
2	B	490	GLN	3.0
18	x	36	LYS	3.0
2	b	490	GLN	2.9
2	b	296	ALA	2.9
4	d	240	ALA	2.9
1	a	224	ILE	2.9
5	E	15	THR	2.9
3	C	253	LEU	2.9
16	v	21	LEU	2.9
19	Z	42	LEU	2.9
13	O	88	ASN	2.9
13	o	243	ILE	2.9
13	o	245	PRO	2.9
2	B	296	ALA	2.9
13	o	202	ALA	2.9
11	l	3	PRO	2.8
5	e	59	GLU	2.8
19	z	57	LEU	2.8
5	E	25	ILE	2.8
14	t	29	ILE	2.8
7	h	57	GLY	2.8
19	Z	29	SER	2.8
19	z	30	PRO	2.8
13	O	87	VAL	2.8
3	C	207	ARG	2.8
19	Z	35	ARG	2.8
13	O	28	GLY	2.8
5	e	13	ILE	2.8
2	B	250	PHE	2.8
2	B	493	TRP	2.8
5	E	20	TRP	2.8
18	X	34	ILE	2.8
2	B	251	VAL	2.8
2	b	457	VAL	2.8
3	c	434	ALA	2.7
2	b	292	LEU	2.7
17	Y	41	VAL	2.7
13	O	61	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
3	c	284	PHE	2.7
19	z	43	GLY	2.7
3	c	249	ILE	2.7
2	b	290	ALA	2.7
3	c	191	PRO	2.7
3	c	20	SER	2.7
13	O	135	SER	2.7
19	z	46	LEU	2.7
7	h	6	TRP	2.7
4	D	17	ILE	2.7
5	E	18	ARG	2.7
2	B	498	LYS	2.6
3	C	155	ASN	2.6
5	E	81	GLU	2.6
5	e	10	PHE	2.6
13	O	91	GLY	2.6
19	z	9	LEU	2.6
3	c	285	ILE	2.6
18	x	3	ILE	2.6
2	b	301	ALA	2.6
19	z	34	ASP	2.6
2	b	458	PHE	2.6
3	C	257	PHE	2.6
2	B	161	LEU	2.6
4	D	116	LEU	2.6
13	O	138	THR	2.6
8	i	34	ARG	2.6
13	O	137	THR	2.6
1	a	242	GLU	2.6
2	B	294	SER	2.6
13	O	136	ILE	2.6
12	m	34	LYS	2.6
1	a	14	TRP	2.6
1	a	16	ARG	2.6
2	b	297	THR	2.6
3	c	429	SER	2.6
2	b	29	LEU	2.6
9	j	12	ILE	2.6
3	c	280	SER	2.6
2	B	253	ALA	2.5
19	z	42	LEU	2.5
5	e	12	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
18	X	31	ILE	2.5
5	E	19	TYR	2.5
16	v	26	TYR	2.5
13	o	28	GLY	2.5
3	c	253	LEU	2.5
3	c	257	PHE	2.5
18	x	35	ASP	2.5
19	z	32	ASP	2.5
2	B	489	GLU	2.5
19	z	53	VAL	2.5
5	e	7	GLU	2.5
1	a	264	SER	2.5
2	B	247	PHE	2.5
16	v	10	VAL	2.5
4	d	237	PRO	2.5
16	v	6	GLU	2.5
5	e	14	ILE	2.5
6	f	15	ILE	2.5
3	c	19	ASN	2.5
3	C	204	LEU	2.5
2	b	246	PHE	2.5
13	o	91	GLY	2.5
3	C	262	ARG	2.5
5	E	22	ILE	2.5
13	O	139	SER	2.5
9	j	10	LEU	2.5
13	O	131	PRO	2.5
1	a	243	GLU	2.4
2	b	245	VAL	2.4
13	o	130	GLN	2.4
17	y	21	GLN	2.4
19	z	35	ARG	2.4
9	j	2	MET	2.4
1	A	339	PHE	2.4
3	c	436	PHE	2.4
19	Z	36	SER	2.4
2	b	302	TRP	2.4
13	O	141	ASP	2.4
5	e	8	ARG	2.4
19	z	10	ALA	2.4
2	B	488	PRO	2.4
13	o	139	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	c	181	PHE	2.4
3	c	435	PHE	2.4
2	B	2	GLY	2.4
2	B	457	VAL	2.4
5	e	28	PRO	2.4
13	o	135	SER	2.4
2	B	459	ALA	2.4
17	y	37	PHE	2.4
13	O	207	ARG	2.4
13	o	208	THR	2.4
13	O	62	GLU	2.4
7	h	21	VAL	2.4
13	O	21	THR	2.4
5	E	82	GLN	2.3
13	o	206	GLY	2.3
10	k	11	LEU	2.3
5	e	9	PRO	2.3
13	o	31	PRO	2.3
2	b	128	THR	2.3
13	O	204	VAL	2.3
19	Z	41	PHE	2.3
1	a	225	ARG	2.3
13	O	58	ASN	2.3
2	B	505	ARG	2.3
4	D	240	ALA	2.3
2	b	483	ASP	2.3
2	b	129	GLY	2.3
3	C	182	PHE	2.3
3	c	431	PHE	2.3
5	e	26	THR	2.3
16	v	22	THR	2.3
13	O	93	LEU	2.3
4	d	154	VAL	2.3
19	z	58	ASN	2.3
2	B	479	PHE	2.3
3	C	252	ILE	2.3
2	b	459	ALA	2.3
17	y	26	ALA	2.3
19	Z	5	PHE	2.2
5	e	29	ALA	2.2
3	c	438	LEU	2.2
12	m	33	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	a	280	VAL	2.2
11	L	2	GLU	2.2
4	d	24	ARG	2.2
3	C	255	THR	2.2
3	c	155	ASN	2.2
13	O	92	SER	2.2
9	J	7	ARG	2.2
5	e	11	SER	2.2
2	B	292	LEU	2.2
5	e	36	LEU	2.2
18	x	33	GLN	2.2
3	c	278	ALA	2.2
13	O	56	PRO	2.2
13	o	131	PRO	2.2
3	c	437	PHE	2.2
4	D	158	LEU	2.2
13	O	140	THR	2.2
19	z	28	ALA	2.1
5	E	24	SER	2.1
3	C	25	ASN	2.1
2	B	248	ALA	2.1
2	B	290	ALA	2.1
10	k	12	PRO	2.1
13	o	29	ALA	2.1
16	v	62	ALA	2.1
17	Y	40	ALA	2.1
5	E	61	ARG	2.1
5	e	24	SER	2.1
2	b	460	LEU	2.1
1	a	15	GLU	2.1
2	b	250	PHE	2.1
2	b	127	ARG	2.1
16	v	17	LYS	2.1
19	Z	40	ILE	2.1
7	h	23	PRO	2.1
13	o	56	PRO	2.1
2	B	298	LEU	2.1
19	z	49	ALA	2.1
3	C	181	PHE	2.1
3	c	426	LEU	2.1
19	Z	39	LEU	2.1
13	O	142	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	b	249	ALA	2.0
5	E	16	SER	2.0
1	A	243	GLU	2.0
17	Y	24	MET	2.0
19	z	59	PHE	2.0
1	a	297	LEU	2.0
2	b	461	LEU	2.0
13	o	209	GLY	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
4	HSK	D	336[B]	11/12	0.98	0.09	-	23,26,27,29	8
14	FME	T	1	10/11	0.97	0.08	-	24,27,43,50	0
12	FME	M	1	10/11	0.96	0.11	-	27,34,51,59	0
14	FME	t	1	10/11	0.95	0.09	-	20,23,41,50	0
8	FME	I	1	10/11	0.97	0.12	-	27,34,38,39	0
4	HSK	D	336[A]	10/12	0.98	0.09	-	26,28,31,34	7
12	FME	m	1	10/11	0.92	0.12	-	31,38,54,60	0
8	FME	i	1	10/11	0.98	0.11	-	30,32,37,39	0
4	HSK	d	336[A]	10/12	0.96	0.10	-	30,33,40,44	7
4	HSK	d	336[B]	11/12	0.96	0.10	-	30,31,37,38	8

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
29	UNL	T	102	13/-	0.78	0.54	33.26	66,70,83,87	0
29	UNL	A	420	4/-	0.93	0.53	32.42	64,66,66,66	0
29	UNL	t	103	16/-	0.71	0.46	19.49	63,74,94,95	0
29	UNL	a	403	6/-	0.92	0.42	16.55	57,62,66,66	0
31	GOL	b	633	6/6	0.93	0.24	11.67	41,46,49,52	0
40	SO4	O	302	5/5	0.82	0.29	11.42	78,87,95,105	0
31	GOL	D	415	6/6	0.96	0.19	9.24	35,36,42,46	0
30	LMT	b	625	24/35	0.78	0.25	9.04	35,61,99,100	0
29	UNL	d	411	16/-	0.86	0.32	8.70	39,49,63,66	0
29	UNL	b	628	36/-	0.82	0.26	8.33	44,65,101,106	0
33	HTG	b	602	19/19	0.67	0.27	7.84	50,93,111,117	0
31	GOL	L	104	6/6	0.91	0.26	7.25	44,52,54,55	0
34	DGD	D	406	53/66	0.54	0.29	6.99	53,77,92,103	0
31	GOL	l	102	6/6	0.89	0.38	6.94	37,55,57,57	0
29	UNL	D	413	16/-	0.89	0.26	6.87	39,47,65,65	0
33	HTG	d	401	19/19	0.56	0.30	6.49	55,101,111,114	0
31	GOL	a	422	6/6	0.94	0.10	6.47	30,38,44,45	0
29	UNL	C	523	34/-	0.69	0.28	6.33	52,77,88,93	0
29	UNL	b	631	16/-	0.72	0.23	5.73	59,66,77,79	0
30	LMT	J	102	24/35	0.74	0.19	5.52	45,55,79,83	0
29	UNL	i	103	13/-	0.65	0.29	5.49	58,65,76,78	0
31	GOL	C	526	6/6	0.89	0.14	5.46	38,43,51,57	0
29	UNL	b	630	16/-	0.75	0.39	5.16	51,62,73,74	0
34	DGD	d	406	50/66	0.62	0.26	5.05	56,75,94,97	0
30	LMT	F	102	35/35	0.71	0.36	5.00	53,84,91,96	0
30	LMT	t	102	24/35	0.78	0.26	5.00	33,55,94,95	0
31	GOL	V	204	6/6	0.95	0.26	4.95	39,52,59,59	0
29	UNL	E	103	12/-	0.60	0.29	4.84	65,73,83,88	0
31	GOL	c	928	6/6	0.94	0.22	4.74	42,51,54,54	0
29	UNL	B	629	14/-	0.66	0.27	4.65	61,70,89,90	0
31	GOL	a	423	6/6	0.96	0.14	4.44	33,34,35,45	0
33	HTG	V	202	13/19	0.92	0.26	4.26	43,48,76,84	0
29	UNL	E	102	15/-	0.62	0.23	4.24	57,64,83,83	0
28	PL9	A	414	55/55	0.76	0.26	4.13	47,66,93,96	0
33	HTG	C	522	19/19	0.75	0.34	4.13	50,79,92,94	0
26	SQD	B	621	54/54	0.63	0.27	3.80	48,65,108,109	0
29	UNL	B	632	16/-	0.78	0.32	3.77	50,59,73,73	0
30	LMT	M	101	35/35	0.68	0.24	3.69	43,61,77,90	0
31	GOL	f	104	6/6	0.91	0.33	3.65	46,51,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
27	LMG	A	413	51/55	0.79	0.24	3.64	42,57,76,78	0
36	LHG	d	407	49/49	0.94	0.23	3.56	27,36,46,49	0
29	UNL	j	102	16/-	0.80	0.17	3.56	52,61,69,69	0
29	UNL	D	412	40/-	0.79	0.20	3.53	39,60,96,99	0
26	SQD	L	103	54/54	0.71	0.24	3.49	43,64,89,96	0
23	CLA	B	602	65/65	0.92	0.18	3.47	29,41,78,95	0
26	SQD	a	401	54/54	0.76	0.18	3.43	45,59,85,90	0
31	GOL	V	205	6/6	0.97	0.23	3.39	33,36,37,41	0
31	GOL	A	421	6/6	0.96	0.13	3.33	30,37,38,41	0
31	GOL	a	424	6/6	0.85	0.19	3.31	42,56,59,74	0
26	SQD	A	418	54/54	0.81	0.19	3.21	42,59,81,86	0
31	GOL	A	423	6/6	0.98	0.25	3.17	39,43,45,53	0
33	HTG	u	201	14/19	0.83	0.25	3.12	46,64,90,96	0
31	GOL	B	633	6/6	0.95	0.13	3.01	34,39,47,52	0
33	HTG	b	626	19/19	0.96	0.17	2.98	29,40,73,75	0
27	LMG	c	921	51/55	0.74	0.27	2.96	38,80,95,111	0
33	HTG	D	414	19/19	0.70	0.31	2.92	66,93,106,107	0
39	MG	j	101	1/1	0.99	0.16	2.88	35,35,35,35	0
34	DGD	C	518	62/66	0.96	0.15	2.86	20,30,68,75	0
25	BCR	T	101	40/40	0.96	0.16	2.77	24,32,47,53	0
31	GOL	b	632	6/6	0.95	0.11	2.74	35,42,46,47	0
29	UNL	x	101	16/-	0.91	0.16	2.72	36,45,70,73	0
29	UNL	z	102	16/-	0.76	0.22	2.71	51,70,89,92	0
23	CLA	b	604	65/65	0.93	0.17	2.66	34,47,73,81	0
30	LMT	A	419	35/35	0.87	0.15	2.63	37,56,73,94	0
28	PL9	a	419	55/55	0.75	0.23	2.58	52,74,98,109	0
27	LMG	D	411	51/55	0.93	0.17	2.55	23,35,91,99	0
25	BCR	B	619	40/40	0.95	0.19	2.43	19,26,42,45	0
30	LMT	C	520	35/35	0.83	0.30	2.43	52,71,83,89	0
29	UNL	A	417	13/-	0.81	0.35	2.38	56,59,66,66	0
29	UNL	X	101	16/-	0.91	0.12	2.37	34,39,58,60	0
36	LHG	D	410	46/49	0.97	0.14	2.33	24,32,82,87	0
31	GOL	A	422	6/6	0.89	0.13	2.33	42,55,58,67	0
31	GOL	C	524	6/6	0.91	0.17	2.29	36,45,47,53	0
33	HTG	U	201	9/19	0.79	0.23	2.25	54,59,82,98	0
25	BCR	D	404	40/40	0.96	0.16	2.21	24,29,55,57	0
30	LMT	m	102	35/35	0.76	0.19	2.21	41,54,72,84	0
30	LMT	c	922	35/35	0.78	0.32	2.13	61,73,85,90	0
27	LMG	d	410	51/55	0.91	0.12	2.13	29,36,80,91	0
31	GOL	c	930	6/6	0.95	0.21	2.11	49,54,57,59	0
25	BCR	B	618	40/40	0.96	0.15	2.08	20,26,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
36	LHG	D	408	49/49	0.93	0.16	2.05	26,35,45,45	0
27	LMG	Z	101	51/55	0.73	0.27	1.99	41,76,102,113	0
30	LMT	Z	102	35/35	0.78	0.28	1.97	41,87,102,107	0
26	SQD	D	407	45/54	0.82	0.28	1.96	50,78,94,101	0
34	DGD	C	516	62/66	0.94	0.20	1.96	22,32,85,87	0
30	LMT	a	402	35/35	0.84	0.17	1.93	37,54,69,80	0
29	UNL	J	104	12/-	0.85	0.17	1.87	53,65,72,74	0
33	HTG	c	924	19/19	0.78	0.41	1.86	53,85,97,100	0
23	CLA	C	505	65/65	0.96	0.14	1.86	26,31,47,51	0
27	LMG	a	418	51/55	0.75	0.22	1.84	43,60,68,73	0
29	UNL	a	421	10/-	0.89	0.29	1.80	53,57,61,64	0
25	BCR	C	515	40/40	0.96	0.14	1.80	28,34,41,44	0
28	PL9	d	405	55/55	0.95	0.16	1.78	19,25,30,34	0
33	HTG	b	601	19/19	0.87	0.14	1.78	43,51,62,68	0
31	GOL	B	638	6/6	0.93	0.10	1.78	35,47,49,53	0
30	LMT	M	102	35/35	0.64	0.24	1.71	35,52,60,63	0
30	LMT	b	624	25/35	0.71	0.21	1.70	51,71,94,98	0
36	LHG	d	409	49/49	0.96	0.16	1.69	27,32,85,91	0
27	LMG	B	622	51/55	0.87	0.18	1.67	28,37,53,63	0
23	CLA	A	407	65/65	0.97	0.16	1.66	18,21,80,92	0
25	BCR	A	411	40/40	0.97	0.12	1.64	21,26,33,36	0
36	LHG	a	417	40/49	0.69	0.25	1.64	60,109,148,151	0
29	UNL	a	420	40/-	0.57	0.33	1.64	53,72,88,94	0
34	DGD	c	919	62/66	0.91	0.14	1.64	25,35,60,71	0
25	BCR	b	621	40/40	0.96	0.20	1.63	21,28,43,46	0
33	HTG	B	630	19/19	0.84	0.15	1.60	39,52,66,79	0
31	GOL	b	636	6/6	0.87	0.12	1.55	45,56,58,60	0
23	CLA	C	509	65/65	0.96	0.13	1.54	27,31,47,51	0
23	CLA	B	611	65/65	0.96	0.14	1.52	19,25,34,39	0
26	SQD	a	416	54/54	0.91	0.17	1.50	37,55,88,90	0
36	LHG	L	101	49/49	0.94	0.14	1.49	22,31,44,49	0
29	UNL	j	103	12/-	0.71	0.25	1.47	55,65,70,71	0
25	BCR	b	620	40/40	0.97	0.16	1.47	23,27,33,33	0
24	PHO	a	413	64/64	0.97	0.13	1.46	19,25,30,35	0
31	GOL	c	927	6/6	0.86	0.13	1.46	43,53,60,68	0
36	LHG	d	408	49/49	0.95	0.14	1.45	22,27,42,47	0
34	DGD	H	102	62/66	0.91	0.20	1.43	24,31,40,45	0
23	CLA	C	508	65/65	0.96	0.13	1.43	24,29,73,81	0
31	GOL	B	636	6/6	0.95	0.14	1.42	33,43,47,56	0
23	CLA	b	611	65/65	0.98	0.18	1.42	22,27,39,43	0
27	LMG	b	623	51/55	0.88	0.19	1.41	30,39,52,63	0
31	GOL	b	635	6/6	0.81	0.14	1.40	40,43,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	BCR	d	404	40/40	0.94	0.10	1.36	25,33,56,58	0
36	LHG	l	101	49/49	0.92	0.17	1.36	22,31,47,57	0
29	UNL	A	415	36/-	0.60	0.25	1.36	58,67,75,79	0
23	CLA	c	914	65/65	0.90	0.15	1.35	38,53,90,98	0
36	LHG	D	409	49/49	0.96	0.12	1.29	22,28,40,44	0
23	CLA	A	410	65/65	0.96	0.11	1.26	20,24,99,105	0
31	GOL	C	525	6/6	0.98	0.15	1.26	26,26,27,29	0
34	DGD	C	517	62/66	0.94	0.14	1.23	22,31,78,92	0
23	CLA	b	614	65/65	0.97	0.17	1.23	20,24,36,45	0
30	LMT	z	101	32/35	0.80	0.24	1.20	46,85,90,100	0
34	DGD	h	102	62/66	0.88	0.18	1.18	27,35,45,52	0
23	CLA	c	909	65/65	0.97	0.18	1.17	25,30,82,98	0
33	HTG	B	625	19/19	0.94	0.15	1.14	31,38,71,75	0
23	CLA	B	608	65/65	0.97	0.14	1.10	17,20,34,37	0
36	LHG	E	101	49/49	0.82	0.21	1.08	50,80,94,97	0
23	CLA	C	503	65/65	0.96	0.12	1.07	26,31,38,39	0
27	LMG	c	920	51/55	0.82	0.23	1.07	30,65,100,104	0
33	HTG	b	627	19/19	0.74	0.34	1.06	53,94,104,105	0
31	GOL	v	204	6/6	0.95	0.25	1.06	46,50,61,62	0
23	CLA	a	411	65/65	0.98	0.14	1.05	18,23,106,117	0
31	GOL	V	203	6/6	0.95	0.15	1.03	26,32,36,38	0
26	SQD	A	412	54/54	0.94	0.14	1.03	35,54,71,74	0
23	CLA	c	911	65/65	0.97	0.22	1.02	24,30,41,45	0
23	CLA	a	410	65/65	0.98	0.13	1.01	17,20,28,34	0
24	PHO	A	409	64/64	0.97	0.14	1.01	19,22,29,37	0
23	CLA	c	910	65/65	0.97	0.18	1.00	25,31,49,52	0
23	CLA	b	610	65/65	0.97	0.15	0.99	18,23,32,35	0
23	CLA	B	616	65/65	0.97	0.10	0.98	23,28,48,50	0
27	LMG	C	519	51/55	0.86	0.19	0.98	29,59,97,105	0
23	CLA	C	510	65/65	0.96	0.15	0.96	22,28,38,41	0
25	BCR	t	101	40/40	0.95	0.14	0.95	23,30,42,44	0
23	CLA	b	617	65/65	0.96	0.14	0.93	20,25,71,83	0
23	CLA	B	610	65/65	0.88	0.13	0.93	23,28,33,35	0
23	CLA	B	606	65/65	0.97	0.15	0.90	17,23,35,40	0
23	CLA	C	504	65/65	0.96	0.15	0.90	23,28,62,68	0
23	CLA	B	612	65/65	0.96	0.13	0.87	18,21,34,37	0
23	CLA	B	613	65/65	0.97	0.14	0.86	19,24,31,34	0
23	CLA	b	612	65/65	0.89	0.13	0.85	26,30,36,38	0
23	CLA	B	609	65/65	0.97	0.16	0.84	18,24,31,34	0
23	CLA	B	605	65/65	0.97	0.18	0.81	19,22,53,55	0
30	LMT	m	101	35/35	0.74	0.22	0.80	32,51,61,62	0
23	CLA	C	501	65/65	0.96	0.14	0.79	25,32,46,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	CLA	b	616	65/65	0.98	0.20	0.78	20,24,46,50	0
23	CLA	B	614	65/65	0.97	0.17	0.78	18,23,48,54	0
30	LMT	B	623	35/35	0.75	0.24	0.77	43,79,117,129	0
31	GOL	B	635	6/6	0.94	0.12	0.75	38,47,49,50	0
31	GOL	B	637	6/6	0.93	0.13	0.74	36,38,45,54	0
23	CLA	b	613	65/65	0.96	0.13	0.74	24,28,35,40	0
28	PL9	D	405	55/55	0.97	0.10	0.72	18,23,31,38	0
25	BCR	b	622	40/40	0.95	0.10	0.70	25,33,43,45	0
23	CLA	d	402	65/65	0.98	0.12	0.70	18,21,39,44	0
25	BCR	K	101	40/40	0.95	0.10	0.68	30,35,40,43	0
34	DGD	c	917	62/66	0.94	0.16	0.68	24,33,77,80	0
23	CLA	c	905	65/65	0.94	0.18	0.68	24,31,64,66	0
31	GOL	b	634	6/6	0.96	0.12	0.68	32,39,44,46	0
23	CLA	b	607	65/65	0.96	0.16	0.66	20,25,54,59	0
23	CLA	c	903	65/65	0.95	0.19	0.63	22,29,42,55	0
23	CLA	a	409	65/65	0.98	0.12	0.60	18,21,31,43	0
23	CLA	b	608	65/65	0.98	0.11	0.55	20,24,33,34	0
23	CLA	B	604	65/65	0.97	0.14	0.52	17,22,34,41	0
23	CLA	c	904	65/65	0.94	0.15	0.51	24,37,42,42	0
26	SQD	f	102	33/54	0.81	0.21	0.51	63,73,113,114	0
31	GOL	v	203	6/6	0.95	0.15	0.51	31,35,41,43	0
31	GOL	c	929	6/6	0.99	0.14	0.47	25,27,30,30	0
25	BCR	k	102	40/40	0.88	0.13	0.47	29,41,48,50	0
24	PHO	A	408	64/64	0.97	0.11	0.46	16,21,25,27	0
23	CLA	a	414	65/65	0.97	0.09	0.44	19,25,99,104	0
23	CLA	C	502	65/65	0.97	0.14	0.44	21,26,39,48	0
23	CLA	b	606	65/65	0.96	0.12	0.43	20,26,37,42	0
34	DGD	c	918	62/66	0.92	0.15	0.42	27,35,79,91	0
23	CLA	c	902	65/65	0.94	0.13	0.38	27,34,46,50	0
23	CLA	A	406	65/65	0.97	0.09	0.38	13,18,29,39	0
23	CLA	b	615	65/65	0.96	0.14	0.37	19,27,33,38	0
23	CLA	B	603	65/65	0.92	0.14	0.35	23,26,34,37	0
23	CLA	c	913	65/65	0.93	0.12	0.35	33,45,67,72	0
24	PHO	a	412	64/64	0.98	0.12	0.32	17,22,26,27	0
23	CLA	C	506	65/65	0.90	0.13	0.32	25,38,94,97	0
38	RRX	H	101	41/41	0.88	0.14	0.31	25,30,44,47	0
23	CLA	c	908	65/65	0.94	0.12	0.28	26,32,52,55	0
23	CLA	b	609	65/65	0.92	0.11	0.27	23,31,57,63	0
33	HTG	O	303	19/19	0.97	0.09	0.27	27,32,50,52	0
23	CLA	C	513	65/65	0.93	0.13	0.27	35,46,78,83	0
25	BCR	K	102	40/40	0.96	0.08	0.26	28,31,39,42	0
29	UNL	J	103	14/-	0.77	0.16	0.26	61,66,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	CLA	C	512	65/65	0.94	0.10	0.26	34,41,69,74	0
23	CLA	A	405	65/65	0.97	0.10	0.25	14,19,25,42	0
35	BCT	a	408	4/4	0.96	0.09	0.25	30,32,37,46	0
23	CLA	B	617	65/65	0.96	0.10	0.24	20,28,79,83	0
37	HEM	f	101	43/43	0.98	0.19	0.23	39,47,61,77	0
23	CLA	D	402	65/65	0.96	0.11	0.20	13,18,36,39	0
39	MG	J	101	1/1	0.99	0.09	0.19	28,28,28,28	0
33	HTG	B	624	19/19	0.96	0.09	0.13	27,33,41,51	0
23	CLA	D	403	65/65	0.96	0.11	0.13	22,28,73,79	0
23	CLA	B	615	65/65	0.96	0.11	0.11	19,24,67,74	0
25	BCR	B	620	40/40	0.95	0.09	0.09	22,31,41,44	0
25	BCR	c	916	40/40	0.94	0.10	0.06	28,36,45,47	0
23	CLA	b	605	65/65	0.93	0.12	0.06	24,29,36,39	0
23	CLA	B	607	65/65	0.94	0.10	0.00	21,27,55,61	0
38	RRX	h	101	41/41	0.88	0.12	-0.04	27,35,49,54	0
22	CL	a	407	1/1	0.99	0.12	-0.09	27,27,27,27	0
35	BCT	D	401	4/4	0.98	0.08	-0.09	32,35,41,51	0
23	CLA	c	906	65/65	0.96	0.10	-0.12	26,31,46,50	0
23	CLA	b	619	65/65	0.96	0.12	-0.19	25,32,89,97	0
25	BCR	k	101	40/40	0.93	0.09	-0.22	33,39,47,49	0
23	CLA	C	507	65/65	0.95	0.10	-0.27	26,33,56,61	0
37	HEM	V	201	43/43	0.99	0.07	-0.29	22,24,28,33	0
23	CLA	d	403	65/65	0.97	0.08	-0.33	25,32,83,90	0
25	BCR	a	415	40/40	0.96	0.07	-0.34	21,25,30,31	0
25	BCR	c	915	40/40	0.92	0.10	-0.36	44,51,59,60	0
37	HEM	F	101	43/43	0.97	0.12	-0.42	36,42,49,52	0
23	CLA	c	912	65/65	0.95	0.09	-0.48	29,37,45,50	0
23	CLA	C	511	65/65	0.95	0.09	-0.48	27,34,40,42	0
23	CLA	b	618	65/65	0.95	0.08	-0.52	24,30,49,53	0
23	CLA	c	907	65/65	0.94	0.09	-0.56	28,36,76,80	0
21	FE2	a	405	1/1	0.99	0.06	-0.60	27,27,27,27	0
37	HEM	v	201	43/43	0.98	0.08	-0.66	25,31,35,38	0
25	BCR	C	514	40/40	0.95	0.07	-0.70	33,42,46,46	0
22	CL	A	404	1/1	0.99	0.13	-0.76	22,22,22,22	0
21	FE2	A	402	1/1	1.00	0.06	-0.86	26,26,26,26	0
31	GOL	B	634	6/6	0.96	0.10	-0.89	29,29,34,37	0
31	GOL	v	202	6/6	0.96	0.10	-0.94	35,36,40,41	0
20	OEX	a	404	10/10	1.00	0.07	-1.51	22,26,28,29	0
20	OEX	A	401	10/10	1.00	0.07	-1.52	21,23,27,28	0
22	CL	A	403	1/1	0.99	0.06	-1.71	25,25,25,25	0
32	CA	O	301	1/1	0.95	0.14	-1.92	49,49,49,49	0
32	CA	o	301	1/1	0.95	0.11	-2.03	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	CA	c	901	1/1	0.96	0.07	-4.10	46,46,46,46	0
22	CL	a	406	1/1	0.99	0.04	-4.85	29,29,29,29	0
29	UNL	b	629	16/-	0.89	0.11	-	43,48,56,60	0
29	UNL	e	800	11/-	0.76	0.29	-	53,60,68,68	0
33	HTG	C	521	19/19	0.92	0.18	-	56,63,76,80	0
29	UNL	c	926	10/-	0.75	0.17	-	65,67,71,72	0
29	UNL	A	416	16/-	0.90	0.14	-	41,46,73,73	0
31	GOL	h	103	6/6	0.56	0.28	-	78,83,83,84	0
29	UNL	i	104	10/-	0.74	0.28	-	67,72,77,78	0
29	UNL	I	102	11/-	0.83	0.22	-	62,65,66,68	0
29	UNL	H	103	10/-	0.75	0.23	-	60,69,74,76	0
32	CA	F	103	1/1	0.96	0.15	-	55,55,55,55	0
32	CA	b	603	1/1	0.90	0.09	-	82,82,82,82	0
32	CA	B	601	1/1	0.82	0.09	-	81,81,81,81	0
29	UNL	B	627	16/-	0.83	0.14	-	43,47,69,69	0
29	UNL	i	102	16/-	0.79	0.23	-	54,65,83,84	0
29	UNL	L	102	14/-	0.89	0.22	-	52,58,66,69	0
33	HTG	B	626	19/19	0.74	0.41	-	48,87,92,93	0
32	CA	f	103	1/1	0.97	0.19	-	56,56,56,56	0
33	HTG	c	923	19/19	0.85	0.24	-	64,75,82,83	0
33	HTG	B	631	19/19	0.69	0.26	-	49,111,120,125	0
31	GOL	O	304	6/6	0.79	0.17	-	52,60,61,63	0
29	UNL	c	925	30/-	0.74	0.18	-	59,72,89,95	0
29	UNL	I	101	13/-	0.78	0.22	-	44,53,61,63	0
29	UNL	B	628	10/-	0.86	0.27	-	52,56,70,74	0
29	UNL	Z	103	16/-	0.74	0.21	-	48,63,81,81	0
29	UNL	M	103	16/-	0.85	0.23	-	49,58,77,79	0
29	UNL	i	101	16/-	0.92	0.13	-	40,46,56,62	0

6.5 Other polymers (i)

There are no such residues in this entry.