Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:04 PM GMT

PDB ID	:	4UB6
Title	:	Native structure of photosystem II (dataset-1) by a femtosecond X-ray laser
Authors	:	Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on	:	2014-08-12
Resolution	:	1.95 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:

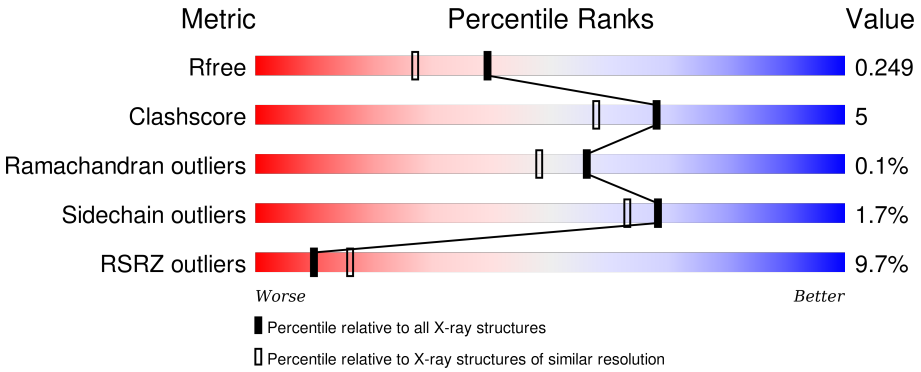
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	6% 89% 8%
1	a	344	11% 96%
2	B	505	5% 87% 12%
2	b	505	7% 98%
3	C	455	4% 89% 9%

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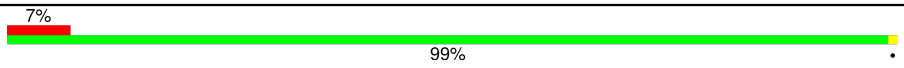
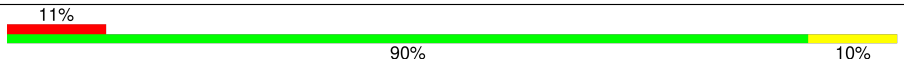
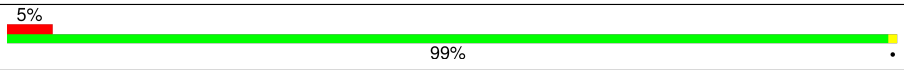
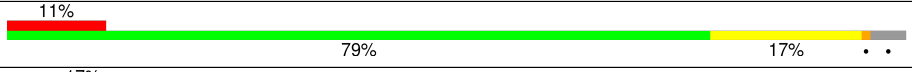
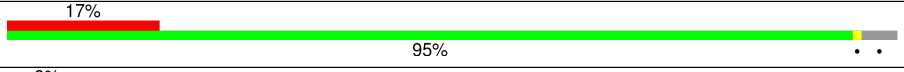
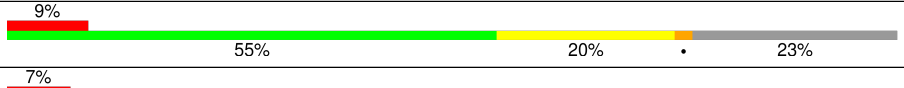
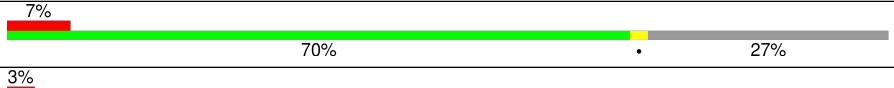
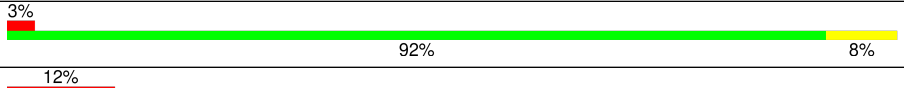
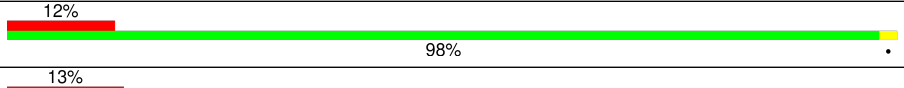
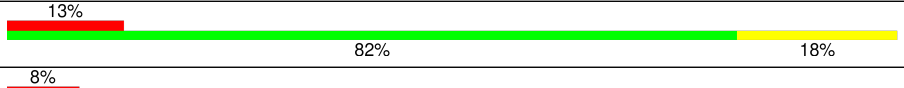
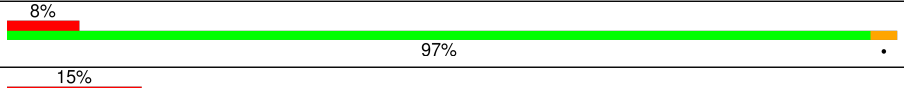
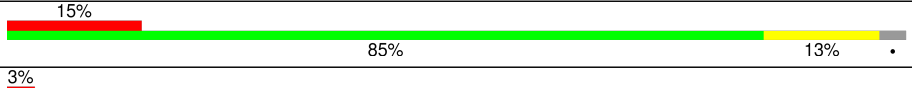
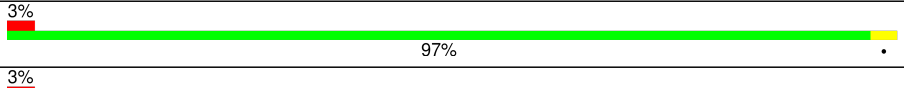
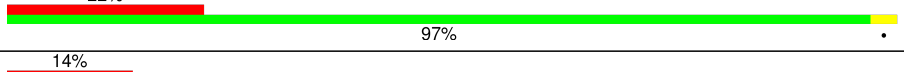
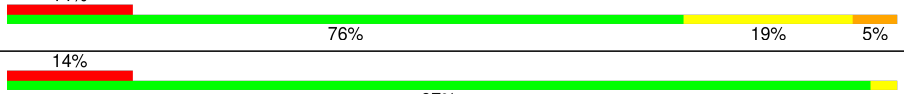
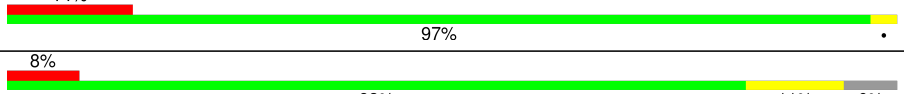
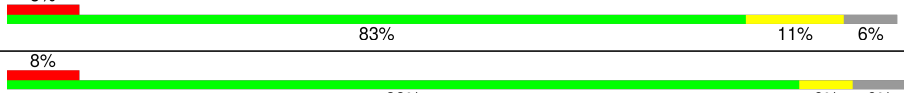
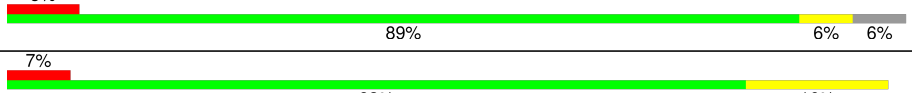
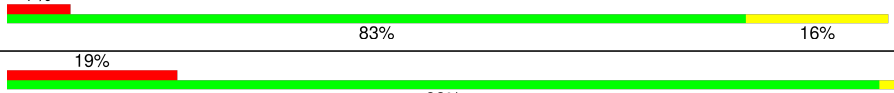
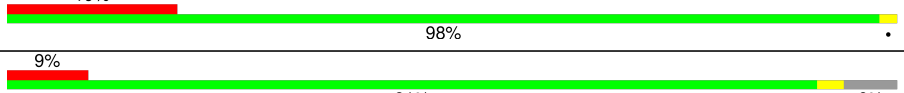
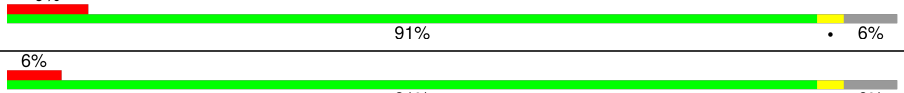
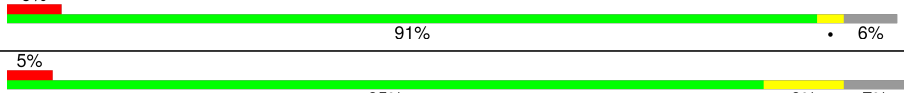
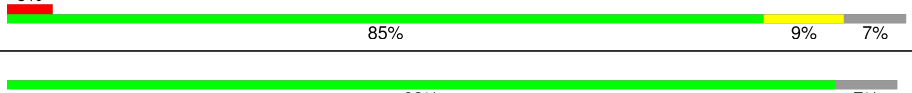
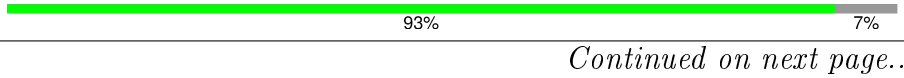
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	93% 6%
16	v	137	8% 100%
17	Y	30	23% 70% 27%
17	y	30	27% 87% 10%
18	X	40	15% 95%
18	x	40	28% 98%
19	Z	62	29% 81% 19%
19	z	62	56% 97%
20	R	34	100% 88% 9%

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
22	CL	U	201	-	-	X	-
23	BCT	A	404	-	-	-	X
23	BCT	a	419	-	-	-	X
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	407	X	-	-	-
24	CLA	A	410	X	-	-	-
24	CLA	B	602	X	-	-	X
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	605	X	-	-	X
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	912	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
25	PHO	a	420	-	-	-	X
26	BCR	b	622	-	-	-	X
26	BCR	d	404	-	-	-	X
27	SQD	A	416	-	-	-	X
27	SQD	B	621	-	-	-	X
27	SQD	L	102	-	-	-	X
27	SQD	a	402	-	-	-	X
27	SQD	a	411	-	-	-	X
28	GOL	A	413	-	-	-	X
28	GOL	A	414	-	-	-	X
28	GOL	A	415	-	-	-	X
28	GOL	B	627	-	-	-	X
28	GOL	B	628	-	-	-	X
28	GOL	B	629	-	-	-	X
28	GOL	B	631	-	-	-	X
28	GOL	C	525	-	-	-	X
28	GOL	C	526	-	-	-	X
28	GOL	F	103	-	-	-	X
28	GOL	T	101	-	-	-	X
28	GOL	V	203	-	-	-	X
28	GOL	V	206	-	-	-	X
28	GOL	a	415	-	-	-	X
28	GOL	b	628	-	-	-	X
28	GOL	b	631	-	-	-	X
28	GOL	b	632	-	-	-	X
28	GOL	b	633	-	-	-	X
28	GOL	c	925	-	-	-	X
28	GOL	f	101	-	-	-	X
28	GOL	t	102	-	-	-	X
28	GOL	v	203	-	-	-	X
29	LMT	A	417	-	-	-	X
29	LMT	B	636	-	-	-	X
29	LMT	C	522	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	LMT	E	102	-	-	-	X
29	LMT	a	401	-	-	-	X
29	LMT	b	601	-	-	-	X
29	LMT	c	921	-	-	-	X
29	LMT	f	103	-	-	-	X
29	LMT	m	102	-	-	-	X
29	LMT	m	104	-	-	-	X
31	PL9	A	419	-	-	-	X
31	PL9	a	417	-	-	-	X
32	UNL	D	410	-	-	-	X
32	UNL	I	101	-	-	-	X
32	UNL	J	102	-	-	-	X
32	UNL	K	101	-	-	-	X
32	UNL	d	410	-	-	-	X
32	UNL	d	411	-	-	-	X
32	UNL	d	413	-	-	-	X
32	UNL	i	101	-	-	-	X
32	UNL	j	102	-	-	-	X
34	LMG	C	501	-	-	-	X
34	LMG	J	101	-	-	-	X
34	LMG	Z	101	-	-	-	X
34	LMG	a	412	-	-	-	X
34	LMG	b	624	-	-	-	X
34	LMG	j	101	-	-	-	X
34	LMG	z	101	-	-	-	X
35	HTG	B	625	-	-	-	X
35	HTG	C	524	-	-	-	X
35	HTG	D	411	-	-	-	X
35	HTG	V	202	-	-	-	X
35	HTG	b	626	-	-	-	X
35	HTG	c	923	-	-	-	X
35	HTG	d	412	-	-	-	X
36	DGD	D	405	-	-	-	X
36	DGD	d	406	-	-	-	X
37	LHG	l	101	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 54195 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	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

- 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	11	0
			4027	2643	668	703	13			
2	b	504	Total	C	N	O	S	0	12	0
			4033	2650	668	702	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	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 668	C 436	N 107	O 125	0	2	0
5	e	81	Total 670	C 439	N 107	O 124	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0	0
6	f	32	Total 257	C 175	N 43	O 38	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 519	C 346	N 85	O 86	S 2	0	1	0
7	h	65	Total 511	C 341	N 82	O 86	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total 314	C 211	N 48	O 54	S 1	0	0	0
8	i	38	Total 314	C 211	N 48	O 54	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total 272	C 182	N 42	O 47	S 1	0	0	0
9	j	39	Total 280	C 187	N 43	O 48	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 293	C 204	N 43	O 46	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

- 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	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

- 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	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	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
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- 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	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

- 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
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

- 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		

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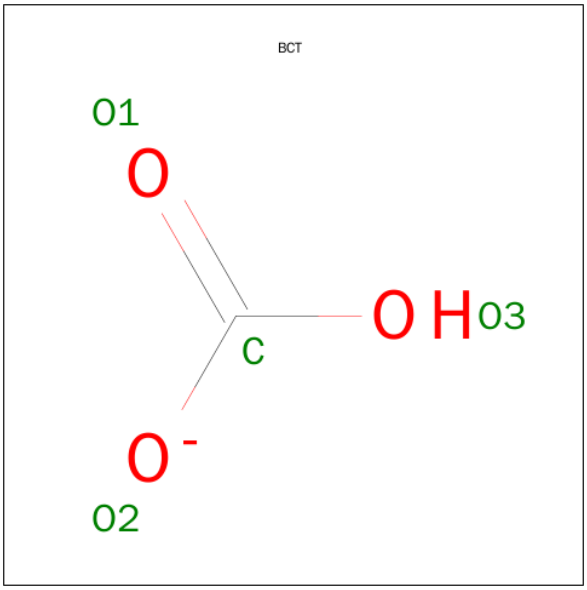
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

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

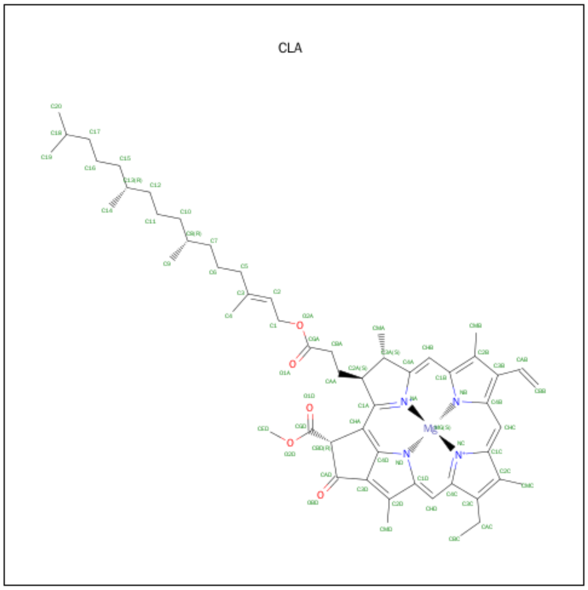
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	v	1	Total Cl 1 1	0	0
22	a	2	Total Cl 2 2	0	0
22	U	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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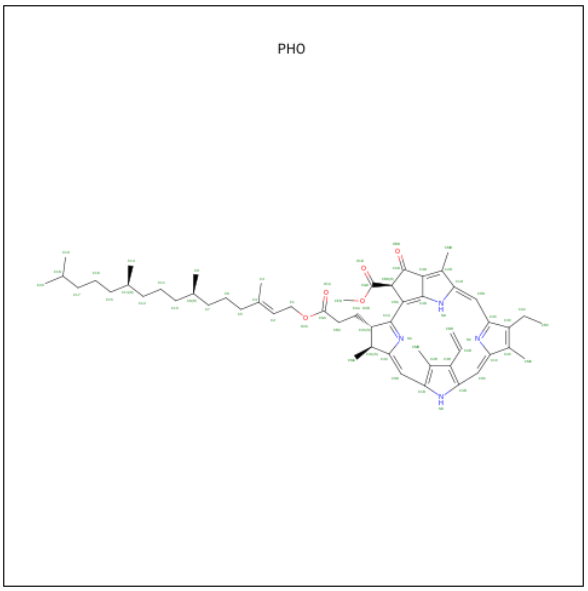
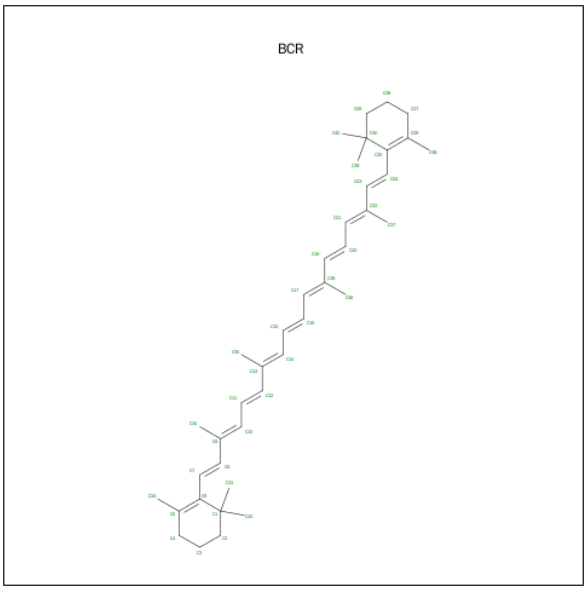
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



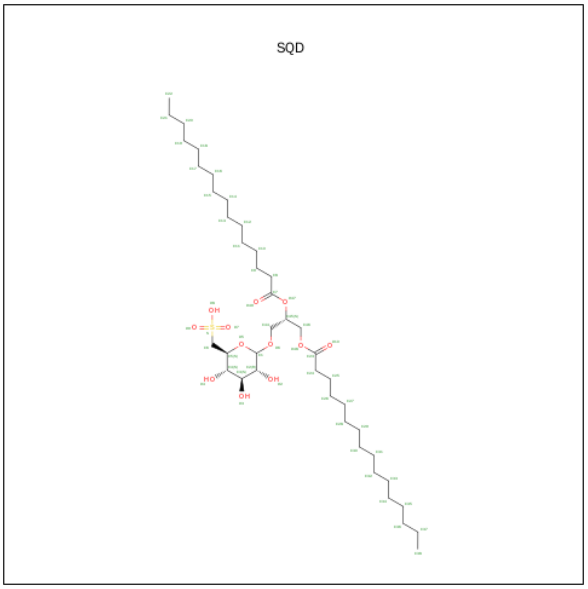
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



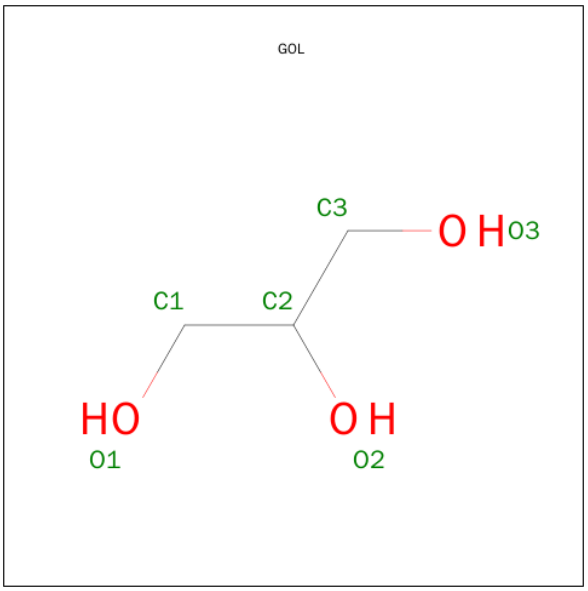
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0

- Molecule 27 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
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	f	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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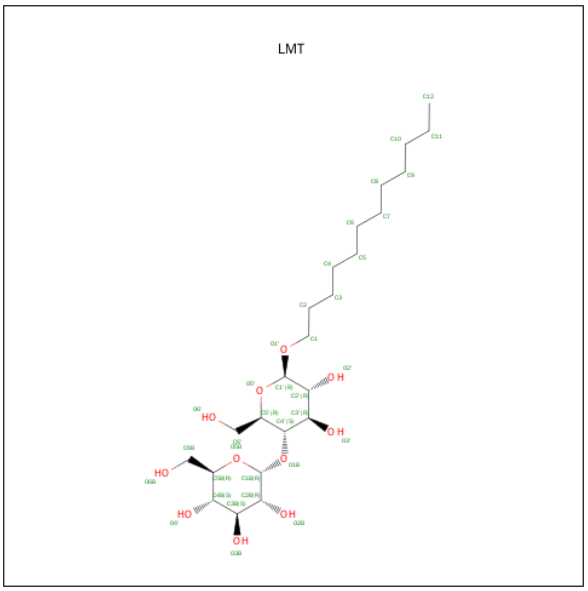
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	v	1	Total C O 6 3 3	0	0
28	v	1	Total C O 6 3 3	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 35 24 11	0	0
29	B	1	Total C O 35 24 11	0	0
29	B	1	Total C O 25 19 6	0	0
29	C	1	Total C O 35 24 11	0	0
29	E	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24 11	0	0
29	b	1	Total C O 25 19 6	0	0
29	b	1	Total C O 25 19 6	0	0

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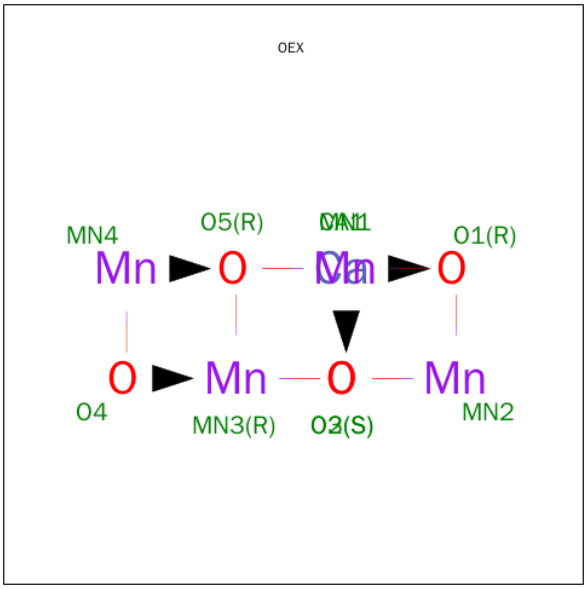
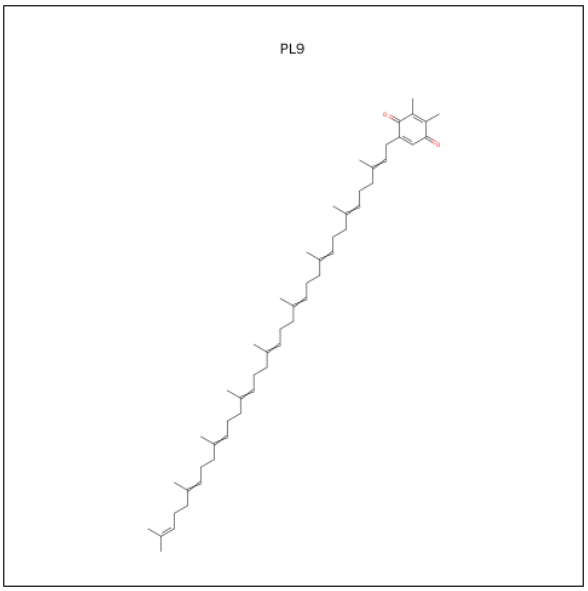
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C O 35 24 11	0	0
29	f	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0
29	m	1	Total C O 35 24 11	0	0

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



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

- Molecule 31 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
31	A	1	Total C O 55 53 2	0	0
31	D	1	Total C O 55 53 2	0	0
31	a	1	Total C O 55 53 2	0	0
31	d	1	Total C O 55 53 2	0	0

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	J	1	Total C 10 10	0	0
32	i	1	Total C O 40 35 5	0	0
32	D	2	Total C O 57 51 6	0	0
32	K	1	Total C O 34 29 5	0	0
32	B	1	Total C O 33 28 5	0	0
32	I	1	Total C O 40 35 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	a	1	Total C O 30 25 5	0	0

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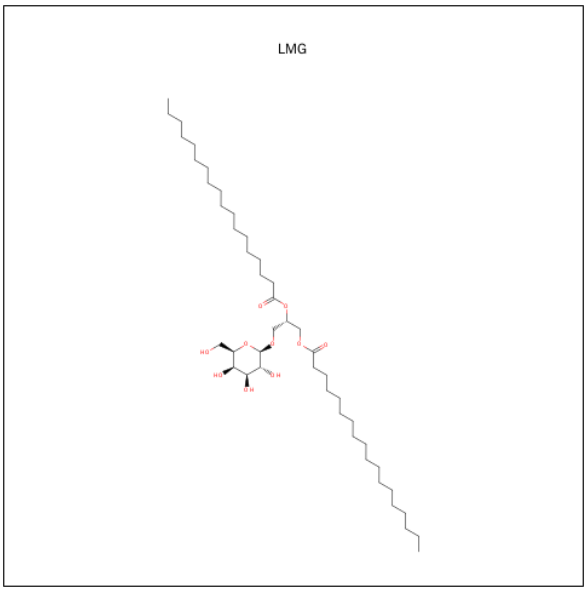
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	j	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	d	3	Total C O 71 63 8	0	0
32	m	1	Total C 10 10	0	0
32	b	1	Total C O 33 28 5	0	0
32	M	1	Total C 10 10	0	0

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

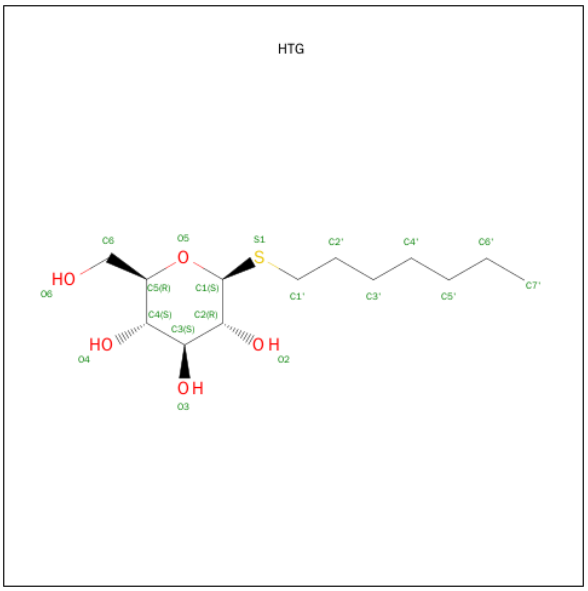
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	J	1	Total C O 51 41 10	0	0
34	Z	1	Total C O 37 27 10	0	0
34	a	1	Total C O 51 41 10	0	0
34	b	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	j	1	Total C O 51 41 10	0	0
34	z	1	Total C O 39 29 10	0	0

- Molecule 35 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

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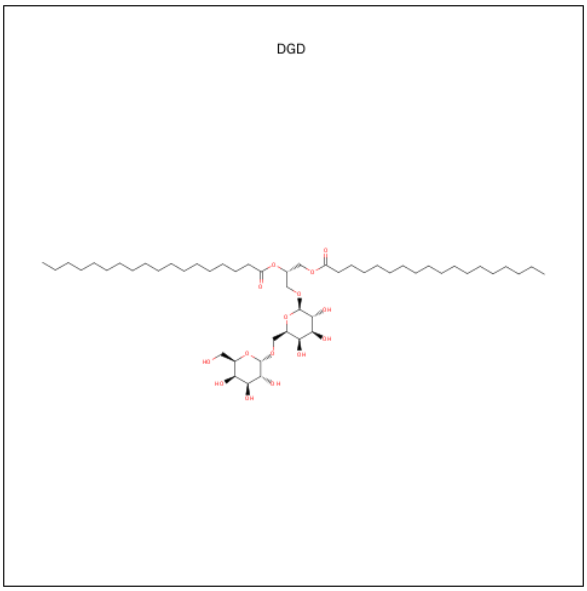
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

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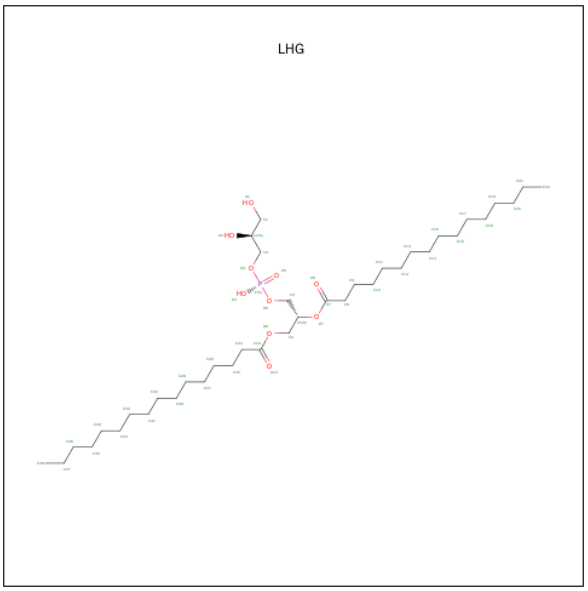
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	e	1	Total C O P 42 31 10 1	0	0

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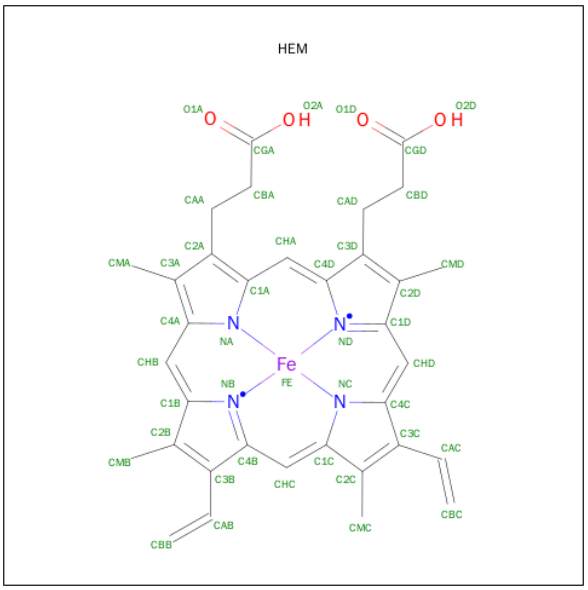
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	165	Total O 167 167	0	2
40	B	289	Total O 293 293	0	4
40	C	233	Total O 235 235	0	2
40	D	138	Total O 143 143	0	5
40	E	31	Total O 31 31	0	0
40	F	9	Total O 9 9	0	0
40	H	48	Total O 49 49	0	1
40	I	4	Total O 4 4	0	0
40	J	13	Total O 13 13	0	0
40	K	8	Total O 8 8	0	0
40	L	16	Total O 17 17	0	1
40	M	8	Total O 8 8	0	0
40	O	188	Total O 191 191	0	3
40	T	16	Total O 17 17	0	1
40	U	81	Total O 81 81	0	0
40	V	116	Total O 118 118	0	2
40	Y	4	Total O 4 4	0	0
40	X	9	Total O 9 9	0	0
40	Z	1	Total O 1 1	0	0
40	a	153	Total O 154 154	0	1
40	b	261	Total O 264 264	0	3
40	c	197	Total O 199 199	0	2

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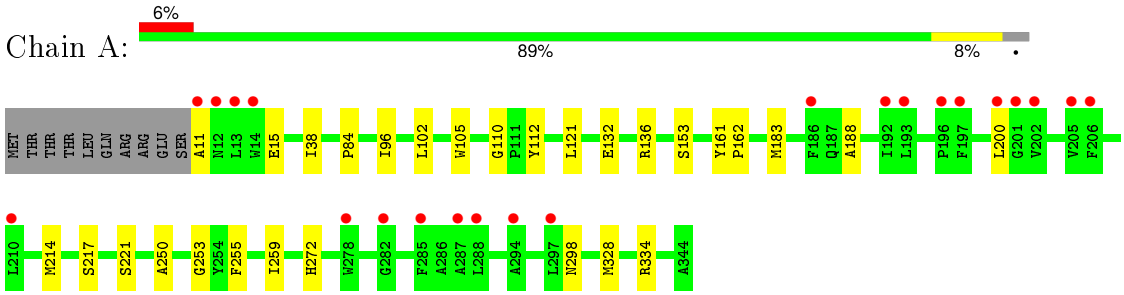
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	d	132	Total O 137 137	0	5
40	e	17	Total O 17 17	0	0
40	f	5	Total O 5 5	0	0
40	h	41	Total O 41 41	0	0
40	i	6	Total O 6 6	0	0
40	j	7	Total O 7 7	0	0
40	k	6	Total O 6 6	0	0
40	l	10	Total O 10 10	0	0
40	m	18	Total O 18 18	0	0
40	o	154	Total O 155 155	0	1
40	t	12	Total O 12 12	0	0
40	u	97	Total O 97 97	0	0
40	v	89	Total O 90 90	0	1
40	y	4	Total O 4 4	0	0
40	x	4	Total O 4 4	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.

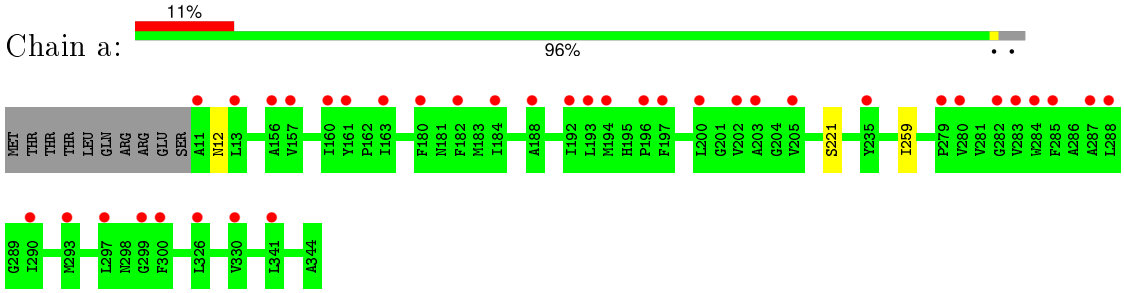
- Molecule 1: Photosystem Q(B) protein

Chain A:



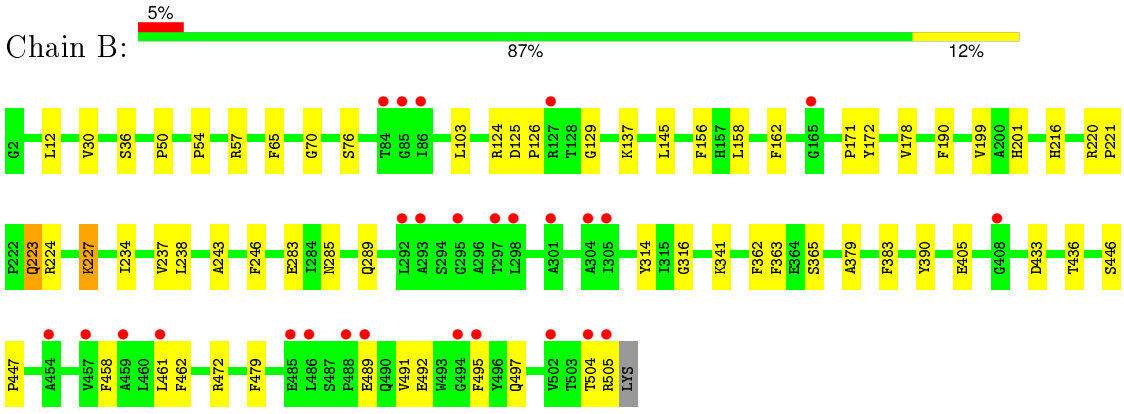
- Molecule 1: Photosystem Q(B) protein

Chain a:



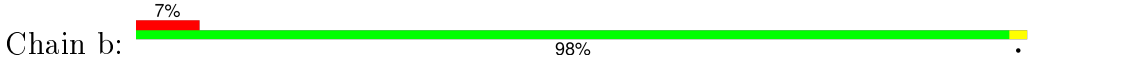
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

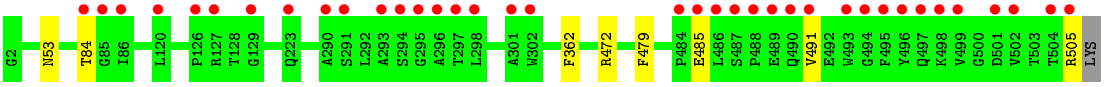
Chain B:



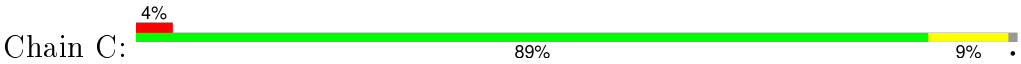
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

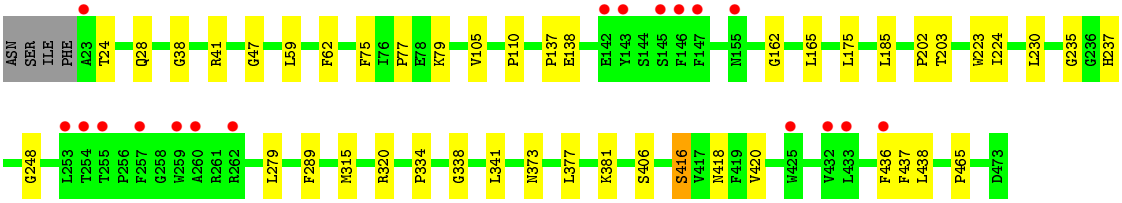
Chain b:



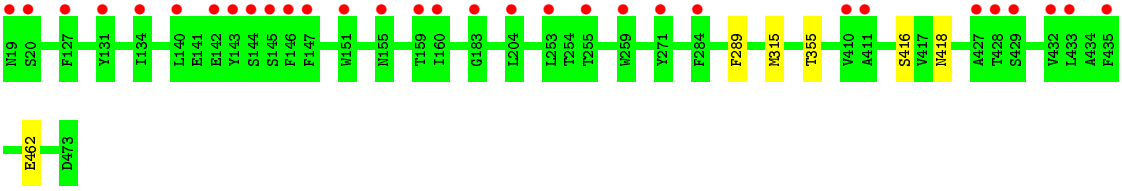


• Molecule 3: Photosystem II 44 kDa reaction center protein

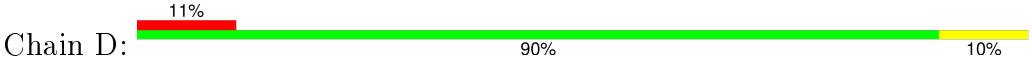


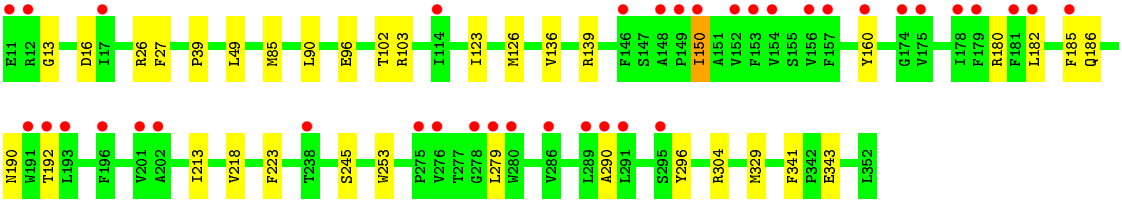


• Molecule 3: Photosystem II 44 kDa reaction center protein

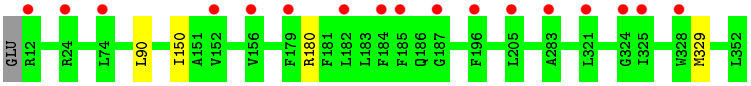


• Molecule 4: Photosystem II D2 protein

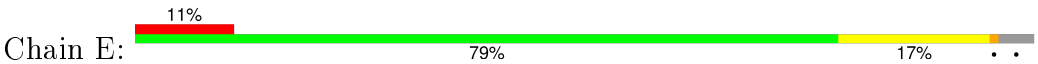




• Molecule 4: Photosystem II D2 protein

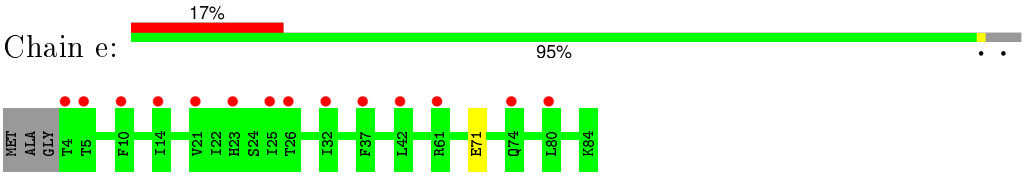


• Molecule 5: Cytochrome b559 subunit alpha



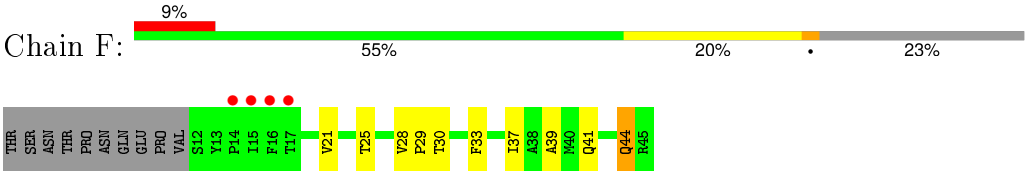
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



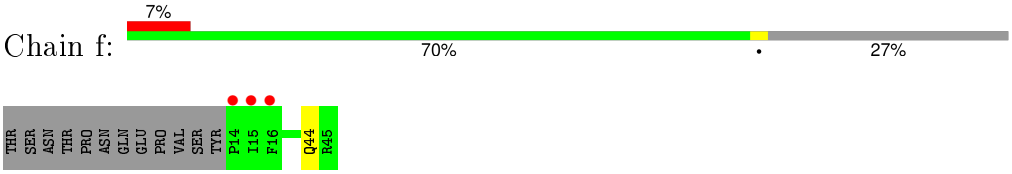
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



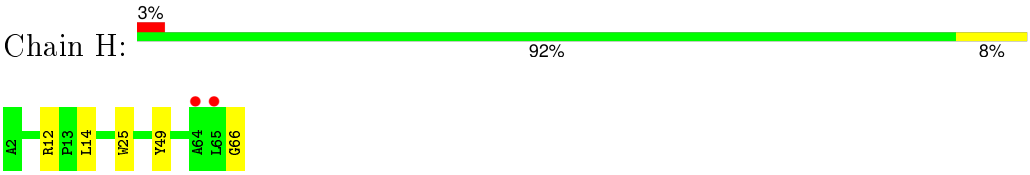
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



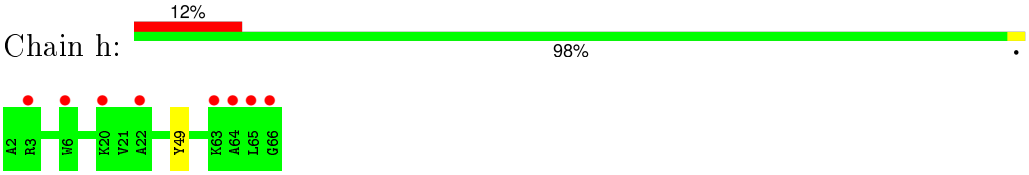
• Molecule 7: Photosystem II reaction center protein H

Chain H:



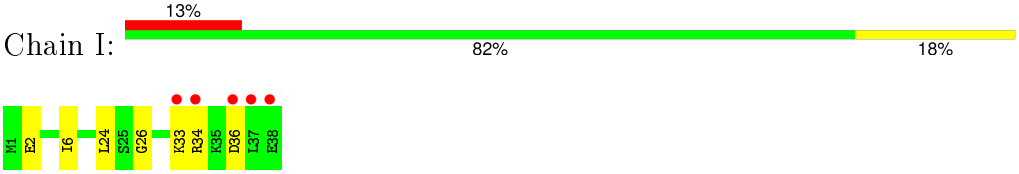
• Molecule 7: Photosystem II reaction center protein H

Chain h:



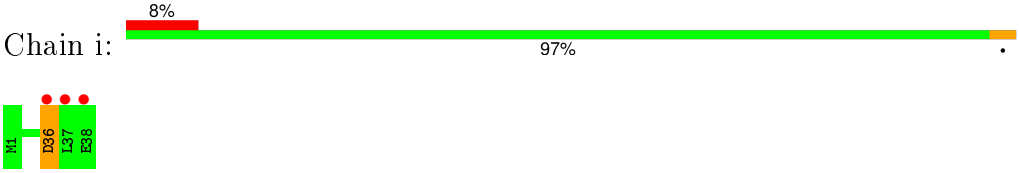
• Molecule 8: Photosystem II reaction center protein I

Chain I:



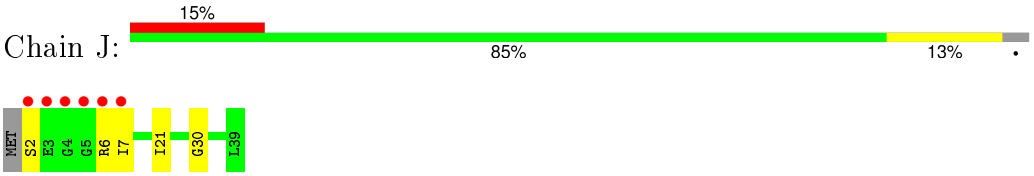
• Molecule 8: Photosystem II reaction center protein I

Chain i:



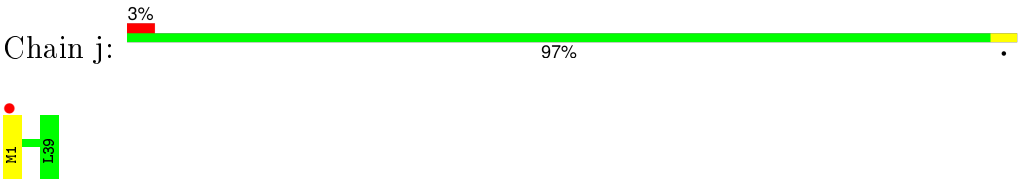
• Molecule 9: Photosystem II reaction center protein J

Chain J:



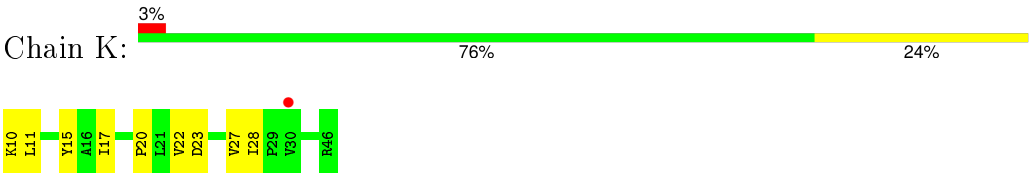
• Molecule 9: Photosystem II reaction center protein J

Chain j:



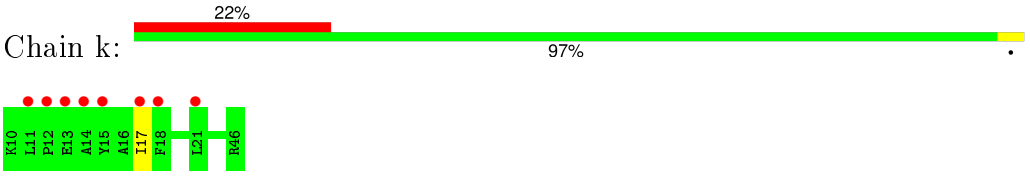
• Molecule 10: Photosystem II reaction center protein K

Chain K:



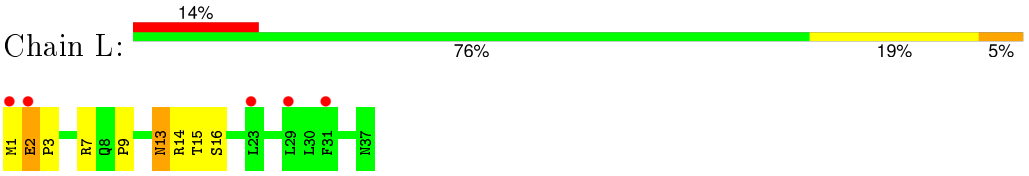
• Molecule 10: Photosystem II reaction center protein K

Chain k:



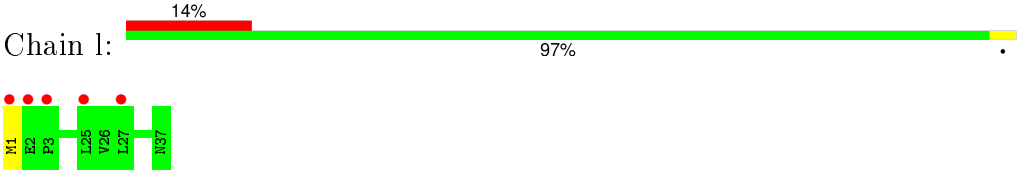
• Molecule 11: Photosystem II reaction center protein L

Chain L:



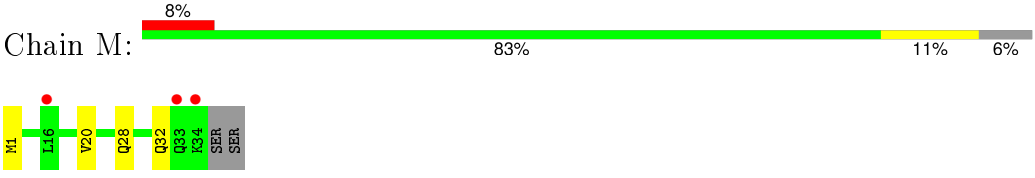
• Molecule 11: Photosystem II reaction center protein L

Chain l:



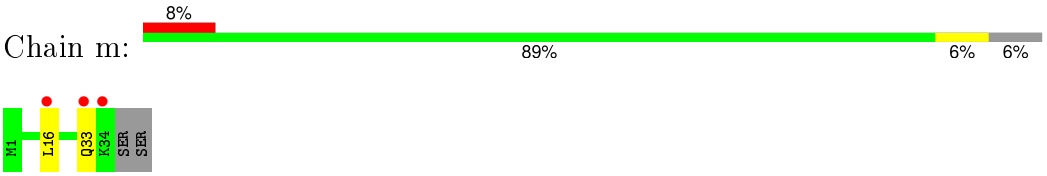
• Molecule 12: Photosystem II reaction center protein M

Chain M:



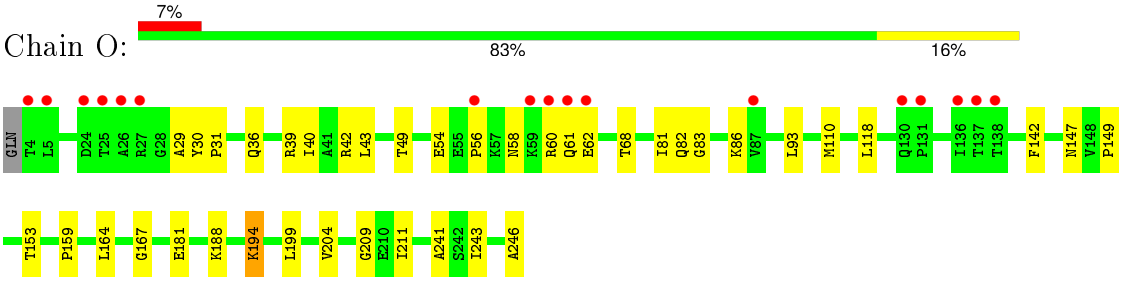
• Molecule 12: Photosystem II reaction center protein M

Chain m:



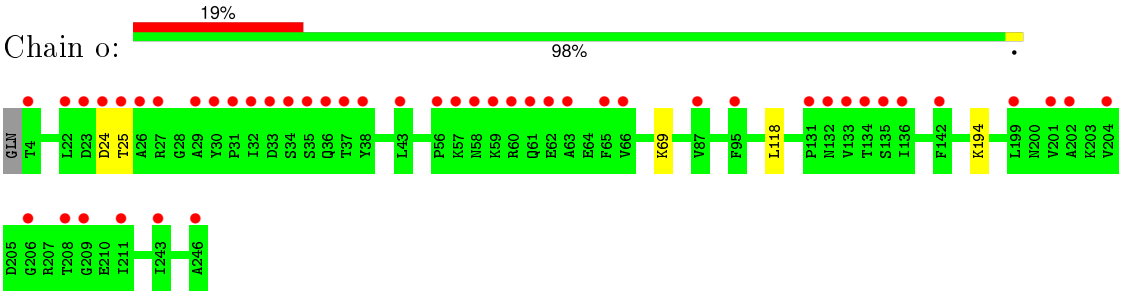
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



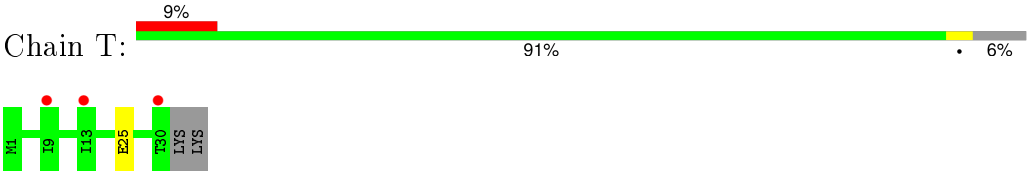
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



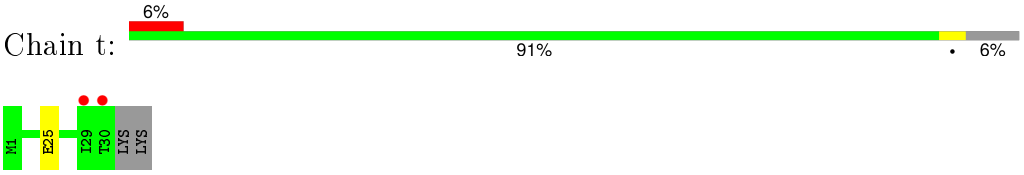
• Molecule 14: Photosystem II reaction center protein T

Chain T:



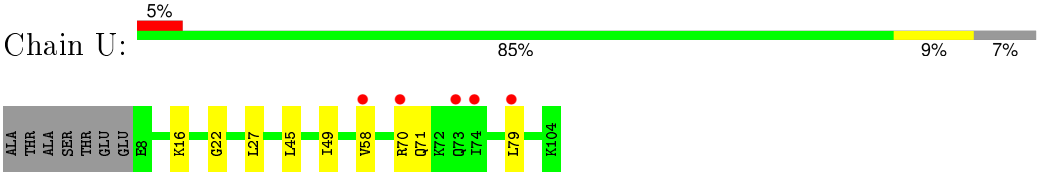
• Molecule 14: Photosystem II reaction center protein T

Chain t:



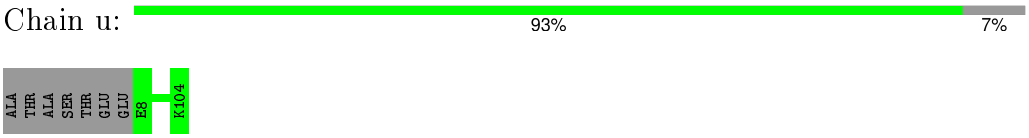
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



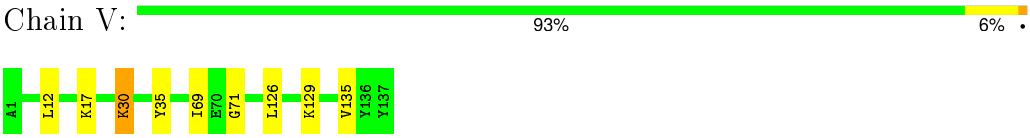
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



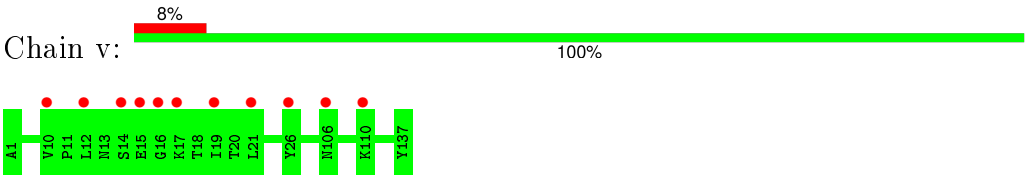
• Molecule 16: Cytochrome c-550

Chain V:



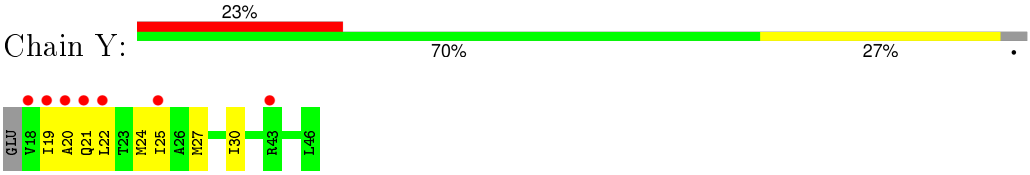
• Molecule 16: Cytochrome c-550

Chain v:



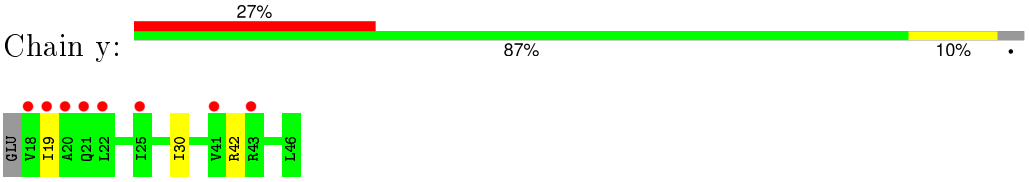
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



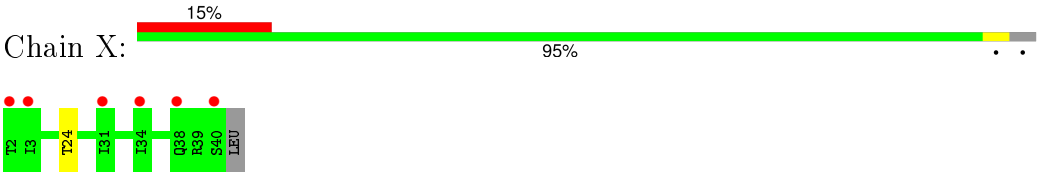
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



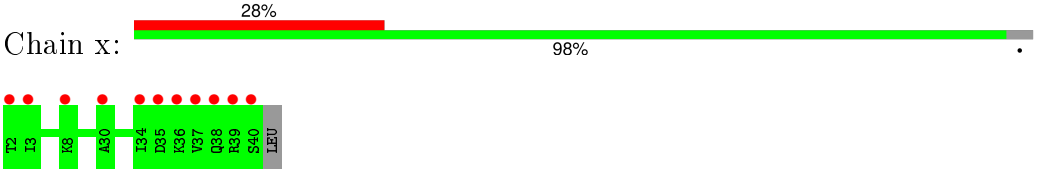
• Molecule 18: Photosystem II reaction center protein X

Chain X:



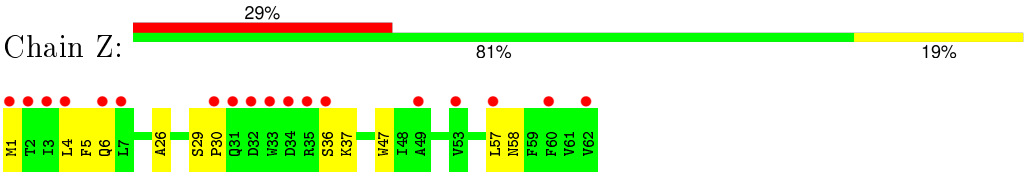
• Molecule 18: Photosystem II reaction center protein X

Chain x:



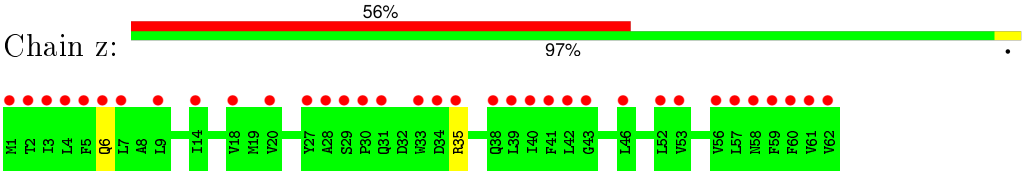
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



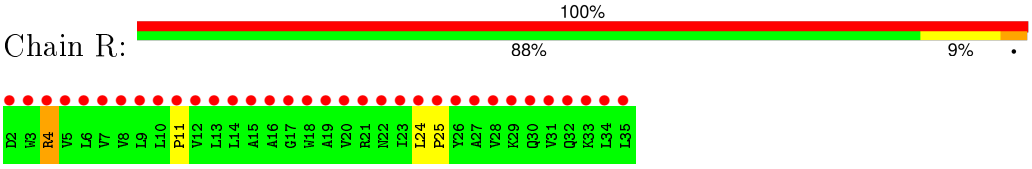
- Molecule 19: Photosystem II reaction center protein Z

Chain z:



- Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.74Å 229.99Å 288.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.29 – 1.95 62.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.29-1.95) 92.0 (62.29-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.198 , 0.238 0.210 , 0.249	Depositor DCC
R_{free} test set	29303 reflections (5.64%)	DCC
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 69.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 585327 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	54195	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, HTG, BCR, 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	0.52	0/2728	0.59	0/3719
1	a	0.52	0/2748	0.57	0/3746
2	B	0.49	0/4200	0.56	0/5721
2	b	0.47	0/4209	0.56	0/5734
3	C	0.45	0/3626	0.54	0/4936
3	c	0.45	0/3676	0.53	0/5004
4	D	0.53	0/2827	0.57	0/3852
4	d	0.51	0/2818	0.56	0/3840
5	E	0.37	0/693	0.54	0/944
5	e	0.35	0/695	0.50	0/948
6	F	0.40	0/284	0.52	0/387
6	f	0.39	0/265	0.52	0/360
7	H	0.37	0/535	0.53	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.38	0/311	0.55	0/419
8	i	0.38	0/311	0.51	0/419
9	J	0.42	0/278	0.47	0/376
9	j	0.41	0/286	0.47	0/386
10	K	0.33	0/303	0.52	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.47	0/319	0.51	0/433
11	l	0.45	0/319	0.50	0/433
12	M	0.45	0/270	0.58	0/368
12	m	0.55	0/262	0.63	0/357
13	O	0.40	0/1958	0.58	0/2654
13	o	0.39	0/1937	0.58	0/2625
14	T	0.55	0/266	0.54	0/362
14	t	0.56	0/266	0.57	0/362
15	U	0.45	0/785	0.58	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.42	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.39	0/1085	0.52	0/1473
17	Y	0.32	0/216	0.46	0/289
17	y	0.33	0/216	0.51	0/289
18	X	0.37	0/290	0.42	0/392
18	x	0.35	0/290	0.46	0/392
19	Z	0.33	0/490	0.43	0/669
19	z	0.33	0/490	0.45	0/669
20	R	0.26	0/279	0.38	0/383
All	All	0.46	0/43239	0.55	0/58829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2634	0	2546	24	0
1	a	2645	0	2567	0	0
2	B	4027	0	3906	53	0
2	b	4033	0	3921	0	0
3	C	3501	0	3428	29	0
3	c	3544	0	3480	0	0
4	D	2729	0	2632	36	0
4	d	2720	0	2626	0	0
5	E	668	0	658	14	0
5	e	670	0	664	0	0
6	F	275	0	282	7	0
6	f	257	0	269	0	0
7	H	519	0	545	5	0
7	h	511	0	532	0	0
8	I	314	0	328	6	0
8	i	314	0	328	0	0
9	J	272	0	279	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	280	0	291	0	0
10	K	293	0	305	9	0
10	k	293	0	305	0	0
11	L	309	0	327	10	0
11	l	309	0	327	0	0
12	M	274	0	299	4	0
12	m	269	0	288	0	0
13	O	1903	0	1886	23	0
13	o	1891	0	1870	0	0
14	T	264	0	267	2	0
14	t	264	0	267	0	0
15	U	774	0	773	6	0
15	u	774	0	773	0	0
16	V	1072	0	1086	7	0
16	v	1064	0	1073	0	0
17	Y	215	0	246	5	0
17	y	215	0	246	0	0
18	X	287	0	317	1	0
18	x	287	0	317	0	0
19	Z	479	0	516	9	0
19	z	479	0	516	0	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	U	1	0	0	3	0
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	14	0
24	B	1040	0	1152	56	0
24	C	845	0	936	35	0
24	D	130	0	144	10	0
24	a	195	0	216	0	0
24	b	1040	0	1152	0	0
24	c	845	0	936	0	0
24	d	195	0	216	0	0
25	A	128	0	148	3	0
25	a	128	0	148	0	0
26	A	40	0	56	1	0
26	B	120	0	168	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C	80	0	112	1	0
26	D	40	0	56	2	0
26	H	40	0	56	4	0
26	K	80	0	112	5	0
26	T	40	0	56	3	0
26	a	40	0	56	0	0
26	b	120	0	168	0	0
26	c	40	0	56	0	0
26	d	40	0	56	0	0
26	h	40	0	56	0	0
26	k	80	0	112	0	0
26	t	40	0	56	0	0
26	y	40	0	56	0	0
27	A	108	0	156	7	0
27	B	54	0	78	3	0
27	F	43	0	52	3	0
27	L	54	0	78	2	0
27	a	108	0	156	0	0
27	f	43	0	53	0	0
28	A	18	0	24	2	0
28	B	42	0	56	5	0
28	C	12	0	16	2	0
28	F	6	0	7	0	0
28	O	6	0	8	0	0
28	T	12	0	16	1	0
28	V	24	0	32	1	0
28	a	18	0	24	0	0
28	b	36	0	48	0	0
28	c	12	0	16	0	0
28	f	6	0	6	0	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	18	0	24	0	0
29	A	35	0	46	0	0
29	B	60	0	81	2	0
29	C	35	0	46	2	0
29	E	35	0	46	1	0
29	M	35	0	46	3	0
29	a	35	0	46	0	0
29	b	50	0	70	0	0
29	c	35	0	46	0	0
29	f	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	m	105	0	138	0	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	55	0	80	5	0
31	D	55	0	80	1	0
31	a	55	0	80	0	0
31	d	55	0	80	0	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	1	0
34	C	153	0	216	7	0
34	J	51	0	72	7	0
34	Z	37	0	44	5	0
34	a	51	0	72	0	0
34	b	51	0	72	0	0
34	c	102	0	144	0	0
34	j	51	0	72	0	0
34	z	39	0	48	0	0
35	B	95	0	130	3	0
35	C	38	0	52	1	0
35	D	16	0	17	2	0
35	O	19	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	V	19	0	26	0	0
35	b	76	0	104	0	0
35	c	38	0	52	0	0
35	d	16	0	17	0	0
36	C	186	0	246	8	0
36	D	62	0	82	5	0
36	H	62	0	82	1	0
36	c	186	0	246	0	0
36	d	62	0	82	0	0
36	h	62	0	82	0	0
37	D	147	0	222	10	0
37	E	42	0	57	2	0
37	L	49	0	74	2	0
37	d	147	0	222	0	0
37	e	42	0	57	0	0
37	l	49	0	74	0	0
38	E	43	0	30	0	0
38	V	43	0	30	0	0
38	e	43	0	30	0	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	167	0	0	2	0
40	B	293	0	0	3	0
40	C	235	0	0	1	0
40	D	143	0	0	4	0
40	E	31	0	0	0	0
40	F	9	0	0	0	0
40	H	49	0	0	0	0
40	I	4	0	0	0	0
40	J	13	0	0	1	0
40	K	8	0	0	1	0
40	L	17	0	0	0	0
40	M	8	0	0	0	0
40	O	191	0	0	4	0
40	T	17	0	0	0	0
40	U	81	0	0	3	0
40	V	118	0	0	1	0
40	X	9	0	0	0	0
40	Y	4	0	0	0	0
40	Z	1	0	0	1	0
40	a	154	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	b	264	0	0	0	0
40	c	199	0	0	0	0
40	d	137	0	0	0	0
40	e	17	0	0	0	0
40	f	5	0	0	0	0
40	h	41	0	0	0	0
40	i	6	0	0	0	0
40	j	7	0	0	0	0
40	k	6	0	0	0	0
40	l	10	0	0	0	0
40	m	18	0	0	0	0
40	o	155	0	0	0	0
40	t	12	0	0	0	0
40	u	97	0	0	0	0
40	v	90	0	0	0	0
40	x	4	0	0	0	0
40	y	4	0	0	0	0
All	All	54195	0	52838	356	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 5.

All (356) 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)
1:A:214:MET:HG2	31:A:419:PL9:H102	1.48	0.95
5:E:67:THR:H	5:E:75:GLN:HE22	2.76	0.94
1:A:253:GLY:HA3	2:B:491:VAL:HG12	3.66	0.87
22:U:201:CL:CL	40:U:305:HOH:O	2.35	0.82
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.45	0.81
24:C:514:CLA:H202	34:C:521:LMG:H402	1.66	0.76
28:A:414:GOL:H11	12:M:1:FME:HG2	1.71	0.73
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.70	0.72
37:D:408:LHG:H132	37:D:408:LHG:H372	1.72	0.72
34:J:101:LMG:H342	34:J:101:LMG:H241	5.12	0.72
22:U:201:CL:CL	40:V:407:HOH:O	2.46	0.70
24:C:507:CLA:HMC2	24:C:508:CLA:H102	1.74	0.70
2:B:223[B]:GLN:NE2	40:B:943:HOH:O	2.23	0.70
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.23	0.69
27:A:412:SQD:H251	37:D:408:LHG:H131	1.74	0.68
36:D:405:DGD:O1B	36:D:405:DGD:O2D	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.27	0.68
34:J:101:LMG:H321	34:J:101:LMG:H221	7.28	0.68
24:C:507:CLA:HMB1	24:C:507:CLA:HBB1	1.76	0.67
22:U:201:CL:CL	40:U:331:HOH:O	2.49	0.67
36:C:519:DGD:HA32	34:J:101:LMG:H121	1.77	0.67
24:C:510:CLA:HBB1	24:C:510:CLA:HMB1	1.77	0.66
24:C:509:CLA:H92	37:D:408:LHG:H371	1.77	0.65
4:D:139:ARG:NH2	40:D:629:HOH:O	2.30	0.65
24:B:615:CLA:H142	37:L:101:LHG:H361	9.71	0.65
26:K:102:BCR:H321	26:K:102:BCR:HC8	1.80	0.64
26:H:101:BCR:HC8	26:H:101:BCR:H331	1.79	0.63
13:O:40:ILE:HG12	13:O:243:ILE:HD13	2.07	0.63
2:B:103:LEU:HD21	24:B:609:CLA:HMC3	29.99	0.63
24:B:605:CLA:HMB1	24:B:605:CLA:HBB1	1.81	0.62
34:J:101:LMG:H142	34:J:101:LMG:H292	3.78	0.61
11:L:2:GLU:HG2	11:L:3:PRO:HD2	1.82	0.61
24:A:406:CLA:HBB1	24:A:406:CLA:HMB1	1.84	0.61
4:D:192:THR:HG23	24:D:402:CLA:HBC2	40.91	0.61
16:V:71:GLY:HA2	28:V:203:GOL:H32	2.42	0.60
6:F:30:THR:HG21	34:J:101:LMG:H412	1.82	0.60
36:D:405:DGD:HD4	5:E:45:ASP:HB3	1.83	0.60
28:A:414:GOL:O1	40:A:523:HOH:O	27.09	0.59
1:A:121[B]:LEU:HD11	24:C:506:CLA:H122	1.85	0.59
24:B:613:CLA:HBB1	24:B:613:CLA:HHC	4.54	0.58
1:A:298:ASN:ND2	40:A:578:HOH:O	51.61	0.58
1:A:183:MET:HA	24:A:405:CLA:HMD2	1.85	0.58
24:C:503:CLA:H61	24:C:513:CLA:H42	1.85	0.58
29:B:636:LMT:H2'	28:B:637:GOL:H2	1.85	0.57
36:D:405:DGD:HB22	36:D:405:DGD:HA42	1.86	0.57
16:V:12:LEU:HD23	16:V:17:LYS:HD3	1.85	0.57
24:B:616:CLA:H71	24:B:617:CLA:H192	1.85	0.57
24:B:602:CLA:H12	24:B:602:CLA:H71	1.85	0.57
24:B:617:CLA:HMB1	24:B:617:CLA:HBB1	1.86	0.56
2:B:234:ILE:HB	28:B:632:GOL:H31	48.49	0.56
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	1.88	0.56
13:O:204:VAL:HG22	13:O:211:ILE:HG22	2.00	0.56
3:C:320:ARG:HB2	28:C:525:GOL:H32	1.88	0.55
11:L:13:ASN:ND2	11:L:16:SER:H	2.03	0.55
3:C:406:SER:HA	3:C:420:VAL:HG23	1.89	0.55
24:B:617:CLA:H121	26:B:620:BCR:H12C	1.89	0.55
34:C:501:LMG:H161	36:C:517:DGD:HA62	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:36:ASP:OD1	8:I:36:ASP:N	3.86	0.54
27:L:102:SQD:H462	27:L:102:SQD:H1	1.88	0.54
25:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.90	0.54
13:O:82:GLN:NE2	40:O:566:HOH:O	2.40	0.53
3:C:377:LEU:HG	3:C:381:LYS:HE3	2.39	0.53
24:A:410:CLA:H193	24:C:507:CLA:H93	1.91	0.53
1:A:84:PRO:HA	1:A:112:TYR:CG	2.44	0.53
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.96	0.53
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.90	0.53
11:L:9:PRO:HB3	29:M:101:LMT:H6'1	14.16	0.53
3:C:334:PRO:HA	13:O:153:THR:OG1	2.18	0.52
3:C:465:PRO:HG3	8:I:33:LYS:HE2	1.91	0.52
1:A:102:LEU:HD12	35:B:633:HTG:H61	72.35	0.52
26:H:101:BCR:H331	26:H:101:BCR:C8	2.37	0.52
24:A:410:CLA:H171	24:C:507:CLA:H142	1.90	0.52
34:J:101:LMG:H292	34:J:101:LMG:H152	1.92	0.52
24:C:502:CLA:HMD2	24:C:503:CLA:H101	1.92	0.52
24:C:511:CLA:H43	37:D:408:LHG:H383	1.92	0.52
28:B:631:GOL:H11	15:U:22:GLY:HA2	49.63	0.52
24:A:407:CLA:HMD3	4:D:182:LEU:HD11	1.91	0.52
2:B:76[A]:SER:HG	35:O:303:HTG:HO6	56.28	0.51
31:A:419:PL9:H502	4:D:39:PRO:HG3	1.93	0.51
11:L:13:ASN:C	11:L:13:ASN:HD22	2.14	0.51
34:C:501:LMG:H382	36:C:517:DGD:HB51	1.91	0.51
3:C:438:LEU:HD11	24:C:506:CLA:HBB1	1.92	0.51
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.02	0.51
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.21	0.51
24:B:609:CLA:HBB2	4:D:150:ILE:HD12	1.91	0.51
4:D:123:ILE:HD11	36:H:102:DGD:HAE1	1.91	0.51
2:B:462:PHE:CE1	24:B:614:CLA:HMB3	2.46	0.51
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.93	0.51
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.92	0.51
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.93	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51
2:B:145:LEU:HD22	24:B:608:CLA:H192	41.00	0.50
1:A:183:MET:HA	24:A:406:CLA:HMD2	8.30	0.50
25:A:409:PHO:HBB1	25:A:409:PHO:HMB1	1.92	0.50
12:M:32:GLN:HG2	29:M:101:LMT:H6'2	7.99	0.50
8:I:2:GLU:O	8:I:6:ILE:HG12	2.25	0.50
26:B:620:BCR:C8	26:B:620:BCR:H331	2.42	0.50
27:A:412:SQD:H381	9:J:21:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.50
2:B:162:PHE:O	24:B:607:CLA:HHD	2.11	0.50
4:D:139:ARG:NH2	40:D:627:HOH:O	48.77	0.50
3:C:279:LEU:HD22	24:C:510:CLA:HED2	1.93	0.50
24:C:511:CLA:HBB1	24:C:511:CLA:HMB1	1.93	0.50
29:B:623:LMT:O6'	4:D:16:ASP:OD2	2.30	0.50
2:B:201:HIS:HB2	24:B:606:CLA:CHB	19.39	0.49
6:F:21:VAL:O	6:F:25:THR:HG23	2.12	0.49
2:B:491:VAL:HG13	4:D:136:VAL:HG13	3.31	0.49
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.50	0.49
24:C:507:CLA:CBB	24:C:508:CLA:HMA3	2.43	0.49
24:C:514:CLA:HMB1	24:C:514:CLA:HBB1	1.94	0.49
2:B:216:HIS:HE1	24:B:613:CLA:C1A	19.52	0.49
17:Y:20:ALA:O	17:Y:24:MET:HG2	2.47	0.49
2:B:497:GLN:HB2	2:B:504:THR:HB	1.95	0.49
1:A:38:ILE:HG12	27:A:416:SQD:H142	1.94	0.49
4:D:103:ARG:HG3	5:E:73:LYS:HE2	1.96	0.48
13:O:58:ASN:HD21	13:O:61:GLN:HB2	1.86	0.48
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.48	0.48
37:D:408:LHG:H382	37:D:408:LHG:H112	1.96	0.48
12:M:20:VAL:HG11	12:M:20:VAL:HG22	2.99	0.48
24:C:502:CLA:H42	24:C:503:CLA:HMD1	1.95	0.48
19:Z:47:TRP:CE2	34:Z:101:LMG:H241	4.80	0.48
27:B:621:SQD:H462	27:B:621:SQD:H1	1.94	0.48
29:C:522:LMT:H6'1	8:I:26:GLY:HA3	1.95	0.48
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.95	0.48
13:O:42:ARG:O	13:O:241:ALA:HA	2.14	0.48
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.96	0.47
26:K:102:BCR:H371	26:K:102:BCR:H24C	2.04	0.47
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.27	0.47
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.66	0.47
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.96	0.47
4:D:49:LEU:HD13	26:D:403:BCR:C15	2.44	0.47
9:J:6:ARG:NH2	9:J:6:ARG:HA	6.05	0.47
2:B:462:PHE:CE1	24:B:617:CLA:HMB3	23.17	0.47
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.47
16:V:12:LEU:HD12	16:V:69:ILE:HB	2.14	0.47
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.96	0.47
26:T:102:BCR:H311	26:T:102:BCR:HC8	1.96	0.47
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.97	0.47
3:C:24:THR:HB	3:C:138:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:PHE:HD1	37:E:101:LHG:HC12	1.80	0.46
3:C:203:THR:O	3:C:235:GLY:HA3	2.15	0.46
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.50	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.46
29:C:522:LMT:H31	8:I:24:LEU:HD13	1.98	0.46
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.96	0.46
19:Z:26:ALA:HB1	19:Z:36:SER:HB3	2.24	0.46
1:A:153:SER:HB2	24:A:406:CLA:H43	13.60	0.46
34:C:521:LMG:HC8	34:C:521:LMG:HC1	1.74	0.46
36:C:518:DGD:HA81	36:C:518:DGD:HAE2	1.61	0.46
13:O:30:TYR:CD1	13:O:209:GLY:HA2	2.69	0.46
34:C:520:LMG:H192	10:K:27:VAL:HG11	1.97	0.46
24:D:402:CLA:HAC1	27:F:101:SQD:H383	1.98	0.46
27:A:412:SQD:O7	3:C:28:GLN:NE2	2.30	0.46
2:B:285:ASN:O	2:B:289:GLN:HG2	2.30	0.46
26:K:103:BCR:H371	26:K:103:BCR:H24C	1.73	0.46
3:C:59:LEU:HD21	26:K:103:BCR:H372	1.97	0.46
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.98	0.46
19:Z:47:TRP:CE3	34:Z:101:LMG:H221	4.82	0.46
2:B:12:LEU:HB2	24:B:616:CLA:HMC2	18.50	0.46
37:D:406:LHG:H101	37:D:406:LHG:H351	1.98	0.46
11:L:13:ASN:HD22	11:L:16:SER:H	1.64	0.46
11:L:7:ARG:NH1	27:L:102:SQD:H62	29.89	0.45
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.76	0.45
4:D:223:PHE:CZ	4:D:245:SER:HB2	2.57	0.45
4:D:341:PHE:O	40:D:614:HOH:O	33.28	0.45
31:A:419:PL9:H271	31:A:419:PL9:H251	1.62	0.45
24:B:614:CLA:H143	24:B:614:CLA:H111	1.84	0.45
24:B:605:CLA:H202	26:H:101:BCR:H353	22.37	0.45
2:B:156:PHE:HB3	2:B:162:PHE:HB3	2.37	0.45
3:C:62:PHE:HZ	10:K:28:ILE:HD12	2.13	0.45
4:D:304:ARG:NH1	40:D:504:HOH:O	2.29	0.45
37:D:408:LHG:HC62	11:L:15:THR:HG23	27.47	0.45
3:C:436:PHE:CE1	24:C:505:CLA:H161	2.51	0.45
29:E:102:LMT:O2B	29:E:102:LMT:O3'	2.30	0.45
36:C:518:DGD:HA31	36:C:518:DGD:HA62	1.80	0.45
15:U:45:LEU:HD21	15:U:71:GLN:HB3	2.20	0.45
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.51	0.45
24:B:616:CLA:H112	24:B:616:CLA:H152	1.63	0.45
19:Z:30:PRO:HD2	40:Z:201:HOH:O	2.16	0.45
2:B:220:ARG:NH1	40:B:703:HOH:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:29:ALA:O	13:O:31:PRO:HD3	2.32	0.45
1:A:200:LEU:HG	36:C:519:DGD:HAT2	1.98	0.45
24:A:410:CLA:H61	24:A:410:CLA:H41	1.76	0.45
26:T:102:BCR:H321	26:T:102:BCR:HC8	1.99	0.45
15:U:45:LEU:O	15:U:49:ILE:HG13	2.17	0.45
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.99	0.45
4:D:185:PHE:CG	24:D:401:CLA:HMD3	2.51	0.45
24:C:508:CLA:H61	24:C:508:CLA:H92	1.84	0.45
28:C:525:GOL:H2	40:C:708:HOH:O	2.16	0.45
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.66	0.45
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.08	0.45
3:C:47:GLY:HA3	3:C:137:PRO:O	2.17	0.45
4:D:13:GLY:HA3	35:D:411:HTG:H62	1.99	0.45
10:K:10:LYS:N	40:K:204:HOH:O	2.50	0.45
27:F:101:SQD:H331	18:X:24:THR:HA	1.99	0.45
24:B:612:CLA:HMB1	4:D:126:MET:HB3	22.36	0.45
35:D:411:HTG:H1	7:H:25:TRP:CD1	2.52	0.45
2:B:363:PHE:HB3	2:B:365:SER:O	2.25	0.45
10:K:11:LEU:HD11	10:K:22:VAL:HG21	2.15	0.45
4:D:192:THR:HG23	24:D:401:CLA:HBC2	1.99	0.44
3:C:437:PHE:CE1	24:C:511:CLA:HMB3	2.51	0.44
27:B:621:SQD:H383	27:B:621:SQD:H352	1.78	0.44
2:B:65:PHE:HE1	24:B:605:CLA:HED2	1.83	0.44
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	2.34	0.44
12:M:28:GLN:O	12:M:32:GLN:HG3	2.18	0.44
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.52	0.44
3:C:79:LYS:HD2	16:V:35:TYR:HE1	2.00	0.44
26:B:619:BCR:C8	26:B:619:BCR:H331	2.47	0.44
24:B:610:CLA:H122	24:B:610:CLA:H162	4.26	0.44
34:C:520:LMG:H172	17:Y:25:ILE:HG12	2.00	0.44
13:O:39:ARG:HG3	13:O:83:GLY:O	2.18	0.44
2:B:158:LEU:HB3	2:B:199:VAL:HG22	2.23	0.44
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.53	0.44
13:O:181[A]:GLU:CD	13:O:181[A]:GLU:H	3.95	0.44
2:B:461:LEU:HD22	37:D:406:LHG:H301	1.99	0.44
3:C:41:ARG:NH1	24:C:512:CLA:HMD1	2.33	0.44
13:O:36:GLN:O	40:O:557:HOH:O	2.20	0.44
2:B:124:ARG:HD2	2:B:129:GLY:O	2.18	0.44
4:D:185:PHE:CG	24:D:402:CLA:HMD3	30.19	0.44
24:C:502:CLA:H192	24:C:507:CLA:C1B	2.47	0.44
35:B:633:HTG:O2	35:B:634:HTG:S1	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.54	0.44
1:A:334:ARG:NH2	13:O:159:PRO:HA	2.46	0.44
4:D:85:MET:CE	4:D:96:GLU:HG2	2.51	0.44
2:B:50:PRO:HB2	28:B:631:GOL:H12	2.00	0.44
4:D:102:THR:OG1	36:D:405:DGD:HG31	2.18	0.44
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.08	0.44
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.07	0.44
2:B:433:ASP:OD1	2:B:436:THR:OG1	2.36	0.44
24:B:612:CLA:HAB	4:D:123:ILE:HG12	19.69	0.43
36:C:517:DGD:HAT2	36:C:517:DGD:HAH1	1.78	0.43
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.07	0.43
6:F:44:GLN:HE21	6:F:44:GLN:HB2	1.60	0.43
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.13	0.43
2:B:201:HIS:HB2	24:B:606:CLA:C1B	19.80	0.43
5:E:40:THR:HB	20:R:4:ARG:HG2	1.99	0.43
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.00	0.43
24:B:603:CLA:H162	24:B:603:CLA:H203	1.83	0.43
13:O:164:LEU:HB2	13:O:188:LYS:HB2	2.01	0.43
2:B:30:VAL:HG12	24:B:609:CLA:HHD	23.95	0.43
26:B:618:BCR:H341	26:B:618:BCR:H11C	1.89	0.43
24:C:510:CLA:H191	24:C:513:CLA:HAC1	2.01	0.43
26:T:102:BCR:H331	26:T:102:BCR:HC7	1.51	0.43
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.15	0.43
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.53	0.43
27:A:412:SQD:H171	37:D:408:LHG:H181	2.01	0.43
1:A:153:SER:CB	24:A:406:CLA:H43	14.31	0.43
3:C:202:PRO:HD2	35:C:524:HTG:H62	1.99	0.43
13:O:54:GLU:O	13:O:56:PRO:HD3	2.19	0.43
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.43
20:R:24:LEU:N	20:R:25:PRO:HD2	2.34	0.43
2:B:137:LYS:HD2	7:H:14:LEU:O	2.61	0.43
5:E:33:ALA:HB2	20:R:11:PRO:HB2	2.00	0.43
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.00	0.43
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.54	0.42
15:U:27:LEU:HD22	15:U:49:ILE:HG21	2.24	0.42
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.01	0.42
10:K:15:TYR:CZ	19:Z:5:PHE:HZ	2.58	0.42
3:C:38:GLY:HA3	24:C:512:CLA:HMD3	2.00	0.42
5:E:68:ASP:OD1	5:E:71:GLU:HB2	2.31	0.42
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.42
24:D:402:CLA:H201	34:J:101:LMG:H222	44.05	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:609:CLA:H162	24:D:402:CLA:H3A	2.01	0.42
3:C:110:PRO:HG3	34:C:521:LMG:H121	2.01	0.42
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	2.01	0.42
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.49	0.42
24:B:610:CLA:HHC	24:B:610:CLA:HBB1	2.02	0.42
24:B:605:CLA:H93	24:B:605:CLA:H111	3.63	0.42
3:C:373:ASN:HB3	40:O:558:HOH:O	2.19	0.42
24:B:609:CLA:HBB1	24:B:609:CLA:HHC	4.62	0.42
24:B:609:CLA:HMB1	24:B:609:CLA:HBB1	2.01	0.42
24:D:401:CLA:HMB1	24:D:401:CLA:HBB1	2.81	0.42
24:C:514:CLA:HBA1	24:C:514:CLA:H3A	1.67	0.42
24:C:514:CLA:HBC1	34:Z:101:LMG:H171	2.02	0.42
2:B:221:PRO:HA	24:B:613:CLA:HED3	20.59	0.42
2:B:190:PHE:CZ	24:B:603:CLA:HBB1	2.54	0.42
6:F:33:PHE:O	6:F:37:ILE:HG13	2.32	0.42
4:D:186:GLN:HB2	24:D:402:CLA:HBC1	40.38	0.42
4:D:27:PHE:CD1	37:E:101:LHG:HC12	2.54	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.51	0.42
26:C:515:BCR:H24C	26:C:515:BCR:H371	1.88	0.42
31:A:419:PL9:H321	31:A:419:PL9:H28	1.87	0.42
24:D:401:CLA:H203	24:D:401:CLA:H162	4.58	0.42
24:B:608:CLA:C4A	24:B:608:CLA:HBA2	2.49	0.42
24:A:406:CLA:H162	24:A:406:CLA:H203	1.80	0.42
24:B:607:CLA:H3A	24:B:607:CLA:CGA	2.86	0.42
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.07	0.42
5:E:17:VAL:O	5:E:21:VAL:HG23	2.34	0.42
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.64	0.42
24:A:406:CLA:C4A	24:A:406:CLA:HBA1	2.49	0.42
26:K:103:BCR:H15C	26:K:103:BCR:H351	1.90	0.42
13:O:147:ASN:ND2	13:O:194:LYS:HE2	2.49	0.42
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.42
13:O:86:LYS:O	13:O:93:LEU:HA	2.32	0.42
24:B:614:CLA:H162	24:B:614:CLA:H121	1.67	0.42
2:B:238:LEU:N	24:B:616:CLA:HMD3	11.93	0.42
24:B:605:CLA:C1B	24:B:605:CLA:H143	20.39	0.42
5:E:18:ARG:H	9:J:2:SER:N	2.18	0.42
24:C:506:CLA:HBD	24:C:506:CLA:HAA1	2.02	0.41
24:B:617:CLA:H91	24:B:617:CLA:H112	1.60	0.41
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.19	0.41
40:J:206:HOH:O	16:V:30:LYS:HE3	2.20	0.41
13:O:142:PHE:HB2	13:O:199:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:407:CLA:HMB3	25:A:409:PHO:H152	2.01	0.41
26:A:411:BCR:H24C	26:A:411:BCR:H371	1.80	0.41
35:B:625:HTG:H1	35:B:625:HTG:H2'2	1.88	0.41
24:B:602:CLA:HBA2	24:B:602:CLA:C4A	2.50	0.41
15:U:16:LYS:NZ	40:U:347:HOH:O	2.30	0.41
24:C:508:CLA:H61	24:C:508:CLA:H41	1.87	0.41
10:K:10:LYS:N	10:K:10:LYS:HD2	2.36	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.55	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	2.00	0.41
4:D:26:ARG:HA	5:E:5:THR:HB	2.09	0.41
31:A:419:PL9:H512	27:F:101:SQD:H302	2.02	0.41
36:C:517:DGD:HA81	36:C:517:DGD:HAE1	1.79	0.41
27:A:412:SQD:H122	27:A:412:SQD:H152	1.61	0.41
3:C:165:LEU:HD21	24:C:507:CLA:CAB	2.51	0.41
24:B:602:CLA:H142	24:B:602:CLA:H112	1.80	0.41
3:C:338:GLY:HA3	3:C:341:LEU:O	2.20	0.41
1:A:11:ALA:HA	1:A:15:GLU:OE2	3.96	0.41
13:O:149:PRO:HB2	40:O:409:HOH:O	2.21	0.41
26:D:403:BCR:H11C	26:D:403:BCR:H341	1.93	0.41
34:Z:101:LMG:HC8	34:Z:101:LMG:H111	1.64	0.41
28:B:632:GOL:H32	40:B:961:HOH:O	47.45	0.41
24:B:607:CLA:H122	24:B:607:CLA:H161	1.81	0.41
24:C:503:CLA:H111	24:C:504:CLA:HMB2	2.02	0.41
24:C:506:CLA:H111	24:C:506:CLA:H93	1.87	0.41
24:C:508:CLA:HBD	24:C:508:CLA:HAA2	2.02	0.41
24:B:614:CLA:H122	34:B:622:LMG:H232	2.02	0.41
13:O:39:ARG:HB2	13:O:246:ALA:HB2	2.02	0.41
2:B:458:PHE:HB3	24:B:608:CLA:HBC2	15.61	0.41
24:B:617:CLA:H152	24:B:617:CLA:H111	1.75	0.41
37:D:408:LHG:C38	37:D:408:LHG:H112	2.51	0.41
2:B:223[A]:GLN:OE1	2:B:227:LYS:HD2	2.21	0.41
36:D:405:DGD:HBT1	36:D:405:DGD:HBH1	1.85	0.41
1:A:217:SER:O	1:A:221[A]:SER:HB3	2.30	0.41
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.26	0.41
24:B:612:CLA:H142	37:L:101:LHG:H362	2.02	0.41
2:B:237:VAL:HG12	24:B:613:CLA:HMD1	2.03	0.41
24:B:602:CLA:HAA1	24:B:602:CLA:HBD	2.02	0.41
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.88	0.41
3:C:75:PHE:CZ	3:C:77:PRO:HA	2.79	0.41
24:B:604:CLA:CGA	24:B:604:CLA:H3A	2.51	0.41
5:E:20:TRP:HD1	9:J:7:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:608:CLA:HMD2	24:B:616:CLA:H203	36.96	0.40
24:B:605:CLA:H112	24:B:605:CLA:H142	4.13	0.40
19:Z:37:LYS:NZ	34:Z:101:LMG:HC61	2.36	0.40
26:B:619:BCR:H371	26:B:619:BCR:H24C	1.77	0.40
24:C:513:CLA:H101	24:C:514:CLA:H141	2.03	0.40
27:B:621:SQD:O8	11:L:7:ARG:HD3	2.21	0.40
24:A:406:CLA:H192	27:A:416:SQD:H223	2.02	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.04	0.40
31:D:404:PL9:H401	31:D:404:PL9:H422	1.74	0.40
11:L:9:PRO:HA	29:M:101:LMT:H6D	16.75	0.40
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	46	35
1	a	338/344 (98%)	333 (98%)	4 (1%)	1 (0%)	46	35
2	B	513/505 (102%)	506 (99%)	7 (1%)	0	100	100
2	b	514/505 (102%)	506 (98%)	8 (2%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	39	27
3	c	459/455 (101%)	445 (97%)	12 (3%)	2 (0%)	39	27
4	D	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	1
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	240 (96%)	8 (3%)	1 (0%)	39	27
13	o	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5290/5384 (98%)	5170 (98%)	112 (2%)	8 (0%)	56	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
13	O	62	GLU
8	i	36	ASP
1	a	259	ILE
1	A	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	272 (99%)	3 (1%)	80	77
2	B	413/403 (102%)	405 (98%)	8 (2%)	65	58
2	b	414/403 (103%)	406 (98%)	8 (2%)	65	58
3	C	356/356 (100%)	351 (99%)	5 (1%)	74	70
3	c	362/356 (102%)	356 (98%)	6 (2%)	68	63
4	D	278/277 (100%)	274 (99%)	4 (1%)	74	70
4	d	277/277 (100%)	273 (99%)	4 (1%)	74	70
5	E	74/73 (101%)	73 (99%)	1 (1%)	74	70
5	e	74/73 (101%)	73 (99%)	1 (1%)	74	70
6	F	28/38 (74%)	27 (96%)	1 (4%)	42	28
6	f	26/38 (68%)	25 (96%)	1 (4%)	40	25
7	H	55/54 (102%)	52 (94%)	3 (6%)	27	12
7	h	54/54 (100%)	53 (98%)	1 (2%)	65	58
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	50	38
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	41	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	K	30/30 (100%)	29 (97%)	1 (3%)	45 32
10	k	30/30 (100%)	29 (97%)	1 (3%)	45 32
11	L	36/35 (103%)	33 (92%)	3 (8%)	14 4
11	l	36/35 (103%)	35 (97%)	1 (3%)	51 39
12	M	31/32 (97%)	31 (100%)	0	100 100
12	m	30/32 (94%)	28 (93%)	2 (7%)	20 7
13	O	214/207 (103%)	210 (98%)	4 (2%)	65 58
13	o	211/207 (102%)	206 (98%)	5 (2%)	57 47
14	T	27/28 (96%)	27 (100%)	0	100 100
14	t	27/28 (96%)	25 (93%)	2 (7%)	17 5
15	U	84/89 (94%)	83 (99%)	1 (1%)	78 75
15	u	84/89 (94%)	84 (100%)	0	100 100
16	V	118/117 (101%)	117 (99%)	1 (1%)	86 85
16	v	117/117 (100%)	117 (100%)	0	100 100
17	Y	22/23 (96%)	19 (86%)	3 (14%)	5 1
17	y	22/23 (96%)	19 (86%)	3 (14%)	5 1
18	X	32/33 (97%)	32 (100%)	0	100 100
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	40 25
19	z	52/52 (100%)	50 (96%)	2 (4%)	40 25
20	R	29/29 (100%)	28 (97%)	1 (3%)	44 30
All	All	4395/4403 (100%)	4315 (98%)	80 (2%)	68 60

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	223[A]	GLN
2	B	223[B]	GLN
2	B	227	LYS
2	B	362	PHE
2	B	472	ARG
2	B	479	PHE
2	B	492	GLU
2	B	505	ARG
3	C	289	PHE

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Mol	Chain	Res	Type
3	C	315	MET
3	C	416[A]	SER
3	C	416[B]	SER
3	C	418	ASN
4	D	90	LEU
4	D	150	ILE
4	D	180	ARG
4	D	329	MET
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	17	ILE
11	L	1	MET
11	L	2	GLU
11	L	13	ASN
13	O	49[A]	THR
13	O	49[B]	THR
13	O	118	LEU
13	O	194	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	19	ILE
17	Y	27	MET
17	Y	30	ILE
19	Z	1	MET
19	Z	6	GLN
20	R	4	ARG
1	a	12	ASN
1	a	221[A]	SER
1	a	221[B]	SER
2	b	53	ASN
2	b	84	THR
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
2	b	485	GLU
2	b	491	VAL
2	b	505	ARG
3	c	289	PHE
3	c	315	MET

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Mol	Chain	Res	Type
3	c	355	THR
3	c	418	ASN
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	150	ILE
4	d	180	ARG
4	d	329	MET
5	e	71	GLU
6	f	44	GLN
7	h	49	TYR
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
11	l	1	MET
12	m	16	LEU
12	m	33	GLN
13	o	24	ASP
13	o	25	THR
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
17	y	19	ILE
17	y	30	ILE
17	y	42	ARG
19	z	6	GLN
19	z	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	331	ASN
2	B	490	GLN
4	D	83	ASN
4	D	332	GLN
6	F	44	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN

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Mol	Chain	Res	Type
16	V	86	GLN
19	Z	31	GLN
19	Z	58	ASN
1	a	315	ASN
2	b	53	ASN
2	b	289	GLN
2	b	331	ASN
2	b	490	GLN
3	c	201	ASN
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
5	e	75	GLN
6	f	44	GLN
13	o	124	ASN
13	o	147	ASN
16	v	118	HIS
19	z	6	GLN
19	z	31	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.51	0	6,9,11	1.57	2 (33%)
12	FME	M	1	12	8,9,10	0.58	0	6,9,11	1.47	2 (33%)
14	FME	T	1	14	8,9,10	0.56	0	6,9,11	1.55	2 (33%)
8	FME	i	1	8	8,9,10	0.62	0	6,9,11	1.82	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	FME	m	1	12	8,9,10	0.65	0	6,9,11	1.41	2 (33%)
14	FME	t	1	14	8,9,10	0.58	0	6,9,11	2.19	4 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
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
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 (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O1-CN-N	-3.08	120.32	124.76
8	i	1	FME	O1-CN-N	-3.06	120.36	124.76
14	t	1	FME	O-C-CA	-2.86	117.88	125.44
8	I	1	FME	O-C-CA	-2.59	118.59	125.44
14	t	1	FME	CA-N-CN	-2.56	118.89	122.82
14	T	1	FME	O1-CN-N	-2.47	121.20	124.76
12	M	1	FME	O1-CN-N	-2.43	121.26	124.76
12	m	1	FME	O-C-CA	-2.39	119.12	125.44
8	i	1	FME	CA-N-CN	-2.29	119.30	122.82
14	T	1	FME	O-C-CA	-2.22	119.59	125.44
8	I	1	FME	CA-N-CN	-2.19	119.45	122.82
8	i	1	FME	O-C-CA	-2.18	119.67	125.44
12	M	1	FME	O-C-CA	-2.16	119.73	125.44
12	m	1	FME	O1-CN-N	-2.11	121.72	124.76
14	t	1	FME	CE-SD-CG	-2.01	93.52	100.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 251 ligands modelled in this entry, 18 are unknown and 17 are monoatomic - leaving 216 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	$\#\|Z\| > 2$
23	BCT	A	404	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	405	-	55,73,73	1.91	12 (21%)	61,113,113	2.04	17 (27%)
24	CLA	A	406	40	55,73,73	1.89	10 (18%)	61,113,113	2.37	23 (37%)
24	CLA	A	407	40	55,73,73	1.94	12 (21%)	61,113,113	2.12	20 (32%)
25	PHO	A	408	-	67,69,69	2.13	15 (22%)	84,99,99	2.04	22 (26%)
25	PHO	A	409	-	67,69,69	2.10	15 (22%)	84,99,99	1.83	21 (25%)
24	CLA	A	410	-	55,73,73	1.96	11 (20%)	61,113,113	2.02	19 (31%)
26	BCR	A	411	-	41,41,41	0.98	1 (2%)	56,56,56	1.21	4 (7%)
27	SQD	A	412	-	53,54,54	1.31	3 (5%)	61,65,65	1.87	12 (19%)
28	GOL	A	413	-	5,5,5	0.21	0	5,5,5	0.48	0
28	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.30	0
28	GOL	A	415	-	5,5,5	0.39	0	5,5,5	0.26	0
27	SQD	A	416	-	53,54,54	1.39	3 (5%)	61,65,65	1.23	7 (11%)
29	LMT	A	417	-	36,36,36	0.48	1 (2%)	47,47,47	1.07	2 (4%)
30	OEX	A	418	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
31	PL9	A	419	-	55,55,55	0.62	2 (3%)	68,69,69	1.97	25 (36%)
24	CLA	B	602	40	55,73,73	1.91	12 (21%)	61,113,113	2.14	19 (31%)
24	CLA	B	603	-	55,73,73	1.94	12 (21%)	61,113,113	2.24	24 (39%)
24	CLA	B	604	-	55,73,73	1.97	11 (20%)	61,113,113	2.30	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	605	-	55,73,73	1.87	11 (20%)	61,113,113	2.07	18 (29%)
24	CLA	B	606	-	55,73,73	1.90	12 (21%)	61,113,113	2.25	19 (31%)
24	CLA	B	607	-	55,73,73	1.94	12 (21%)	61,113,113	2.33	23 (37%)
24	CLA	B	608	40	55,73,73	1.97	12 (21%)	61,113,113	2.13	20 (32%)
24	CLA	B	609	-	55,73,73	2.00	12 (21%)	61,113,113	2.12	19 (31%)
24	CLA	B	610	-	55,73,73	1.85	11 (20%)	61,113,113	2.10	19 (31%)
24	CLA	B	611	40	55,73,73	1.93	11 (20%)	61,113,113	2.16	18 (29%)
24	CLA	B	612	-	55,73,73	1.94	12 (21%)	61,113,113	2.10	20 (32%)
24	CLA	B	613	-	55,73,73	1.94	11 (20%)	61,113,113	2.16	17 (27%)
24	CLA	B	614	-	55,73,73	2.00	12 (21%)	61,113,113	1.99	18 (29%)
24	CLA	B	615	-	55,73,73	1.89	11 (20%)	61,113,113	2.29	20 (32%)
24	CLA	B	616	-	55,73,73	1.83	12 (21%)	61,113,113	2.07	22 (36%)
24	CLA	B	617	-	55,73,73	1.94	10 (18%)	61,113,113	2.26	20 (32%)
26	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.24	7 (12%)
26	BCR	B	619	-	41,41,41	1.02	1 (2%)	56,56,56	1.24	7 (12%)
26	BCR	B	620	-	41,41,41	1.06	1 (2%)	56,56,56	1.26	4 (7%)
27	SQD	B	621	-	53,54,54	1.34	4 (7%)	61,65,65	1.63	6 (9%)
34	LMG	B	622	-	51,51,55	0.89	2 (3%)	59,59,63	1.16	4 (6%)
29	LMT	B	623	-	36,36,36	0.42	0	47,47,47	1.42	5 (10%)
35	HTG	B	624	-	19,19,19	1.05	1 (5%)	22,24,24	1.56	2 (9%)
35	HTG	B	625	-	19,19,19	0.77	1 (5%)	22,24,24	1.33	1 (4%)
35	HTG	B	626	-	19,19,19	0.93	1 (5%)	22,24,24	2.11	2 (9%)
28	GOL	B	627	-	5,5,5	0.39	0	5,5,5	0.54	0
28	GOL	B	628	-	5,5,5	0.22	0	5,5,5	0.41	0
28	GOL	B	629	-	5,5,5	0.38	0	5,5,5	0.50	0
28	GOL	B	630	-	5,5,5	0.28	0	5,5,5	0.37	0
28	GOL	B	631	-	5,5,5	0.39	0	5,5,5	0.52	0
28	GOL	B	632	-	5,5,5	0.32	0	5,5,5	0.31	0
35	HTG	B	633	-	19,19,19	1.04	2 (10%)	22,24,24	1.55	1 (4%)
35	HTG	B	634	-	19,19,19	0.97	1 (5%)	22,24,24	1.96	3 (13%)
29	LMT	B	636	-	25,25,36	0.41	0	30,30,47	0.67	0
28	GOL	B	637	-	5,5,5	0.36	0	5,5,5	0.34	0
34	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.13	5 (8%)
24	CLA	C	502	-	55,73,73	1.94	12 (21%)	61,113,113	2.23	22 (36%)
24	CLA	C	503	-	55,73,73	1.92	12 (21%)	61,113,113	2.09	21 (34%)
24	CLA	C	504	-	55,73,73	1.92	12 (21%)	61,113,113	2.03	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	505	40	55,73,73	1.96	12 (21%)	61,113,113	2.21	20 (32%)
24	CLA	C	506	-	55,73,73	1.93	12 (21%)	61,113,113	2.19	17 (27%)
24	CLA	C	507	-	55,73,73	1.93	12 (21%)	61,113,113	2.15	18 (29%)
24	CLA	C	508	40	55,73,73	1.88	12 (21%)	61,113,113	2.13	19 (31%)
24	CLA	C	509	-	55,73,73	1.96	12 (21%)	61,113,113	2.33	22 (36%)
24	CLA	C	510	-	55,73,73	1.99	12 (21%)	61,113,113	2.18	21 (34%)
24	CLA	C	511	-	55,73,73	1.96	12 (21%)	61,113,113	2.14	18 (29%)
24	CLA	C	512	3	55,73,73	1.91	13 (23%)	61,113,113	2.04	17 (27%)
24	CLA	C	513	-	55,73,73	1.92	11 (20%)	61,113,113	2.16	20 (32%)
24	CLA	C	514	-	55,73,73	1.94	12 (21%)	61,113,113	2.09	19 (31%)
26	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.36	4 (7%)
26	BCR	C	516	-	41,41,41	0.98	1 (2%)	56,56,56	1.41	5 (8%)
36	DGD	C	517	-	63,63,67	0.83	3 (4%)	77,77,81	1.06	7 (9%)
36	DGD	C	518	-	63,63,67	0.82	2 (3%)	77,77,81	1.02	6 (7%)
36	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	0.96	4 (5%)
34	LMG	C	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	5 (8%)
34	LMG	C	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.09	4 (6%)
29	LMT	C	522	-	36,36,36	0.47	0	47,47,47	1.31	5 (10%)
35	HTG	C	523	-	19,19,19	0.91	2 (10%)	22,24,24	1.64	1 (4%)
35	HTG	C	524	-	19,19,19	0.95	2 (10%)	22,24,24	1.87	4 (18%)
28	GOL	C	525	-	5,5,5	0.34	0	5,5,5	0.61	0
28	GOL	C	526	-	5,5,5	0.18	0	5,5,5	0.40	0
24	CLA	D	401	-	55,73,73	1.88	12 (21%)	61,113,113	2.18	20 (32%)
24	CLA	D	402	-	55,73,73	1.90	12 (21%)	61,113,113	2.01	18 (29%)
26	BCR	D	403	-	41,41,41	1.02	1 (2%)	56,56,56	1.76	13 (23%)
31	PL9	D	404	-	55,55,55	0.75	2 (3%)	68,69,69	1.71	21 (30%)
36	DGD	D	405	-	63,63,67	0.94	3 (4%)	77,77,81	1.26	8 (10%)
37	LHG	D	406	-	48,48,48	0.84	2 (4%)	49,54,54	1.11	4 (8%)
37	LHG	D	407	-	48,48,48	0.84	2 (4%)	49,54,54	0.86	2 (4%)
37	LHG	D	408	-	48,48,48	0.85	2 (4%)	49,54,54	1.08	3 (6%)
35	HTG	D	411	-	16,16,19	1.08	2 (12%)	19,21,24	1.16	1 (5%)
37	LHG	E	101	-	41,41,48	1.02	2 (4%)	42,47,54	1.12	3 (7%)
29	LMT	E	102	-	36,36,36	0.47	0	47,47,47	0.90	1 (2%)
38	HEM	E	103	5,6	30,50,50	2.29	7 (23%)	24,82,82	2.56	11 (45%)
27	SQD	F	101	-	42,43,54	1.45	3 (7%)	50,54,65	2.21	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	F	103	33	5,5,5	0.30	0	5,5,5	0.29	0
26	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.39	7 (12%)
36	DGD	H	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.93	4 (5%)
34	LMG	J	101	39	51,51,55	0.85	2 (3%)	59,59,63	0.89	3 (5%)
26	BCR	K	102	-	41,41,41	0.98	1 (2%)	56,56,56	1.47	7 (12%)
26	BCR	K	103	-	41,41,41	0.99	1 (2%)	56,56,56	1.41	6 (10%)
37	LHG	L	101	-	48,48,48	0.88	2 (4%)	49,54,54	1.05	4 (8%)
27	SQD	L	102	-	53,54,54	1.31	3 (5%)	61,65,65	1.78	9 (14%)
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	0.93	1 (2%)
28	GOL	O	302	-	5,5,5	0.29	0	5,5,5	0.43	0
35	HTG	O	303	-	19,19,19	0.88	1 (5%)	22,24,24	0.76	1 (4%)
28	GOL	T	101	-	5,5,5	0.40	0	5,5,5	0.30	0
26	BCR	T	102	-	41,41,41	0.93	1 (2%)	56,56,56	1.41	10 (17%)
28	GOL	T	103	-	5,5,5	0.37	0	5,5,5	0.21	0
38	HEM	V	201	16	30,50,50	2.14	7 (23%)	24,82,82	2.47	9 (37%)
35	HTG	V	202	-	19,19,19	0.94	2 (10%)	22,24,24	1.67	3 (13%)
28	GOL	V	203	-	5,5,5	0.35	0	5,5,5	0.17	0
28	GOL	V	204	-	5,5,5	0.39	0	5,5,5	0.40	0
28	GOL	V	205	-	5,5,5	0.34	0	5,5,5	0.37	0
28	GOL	V	206	-	5,5,5	0.30	0	5,5,5	0.25	0
34	LMG	Z	101	-	37,37,55	0.95	2 (5%)	45,45,63	1.32	8 (17%)
29	LMT	a	401	-	36,36,36	0.51	1 (2%)	47,47,47	0.97	3 (6%)
27	SQD	a	402	-	53,54,54	1.44	3 (5%)	61,65,65	1.20	7 (11%)
24	CLA	a	406	-	55,73,73	1.99	12 (21%)	61,113,113	2.21	21 (34%)
24	CLA	a	407	40	55,73,73	1.90	12 (21%)	61,113,113	2.15	21 (34%)
25	PHO	a	408	-	67,69,69	1.99	14 (20%)	84,99,99	1.94	22 (26%)
24	CLA	a	409	-	55,73,73	1.89	11 (20%)	61,113,113	2.20	23 (37%)
26	BCR	a	410	-	41,41,41	1.04	2 (4%)	56,56,56	1.28	4 (7%)
27	SQD	a	411	-	53,54,54	1.29	3 (5%)	61,65,65	1.70	10 (16%)
34	LMG	a	412	-	51,51,55	0.87	2 (3%)	59,59,63	1.17	5 (8%)
28	GOL	a	413	-	5,5,5	0.28	0	5,5,5	0.58	0
28	GOL	a	414	-	5,5,5	0.38	0	5,5,5	0.39	0
28	GOL	a	415	-	5,5,5	0.37	0	5,5,5	0.42	0
30	OEX	a	416	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
31	PL9	a	417	-	55,55,55	0.62	2 (3%)	68,69,69	2.05	22 (32%)
23	BCT	a	419	21	0,3,3	0.00	-	0,3,3	0.00	-
25	PHO	a	420	-	67,69,69	2.17	17 (25%)	84,99,99	2.02	20 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMT	b	601	-	25,25,36	0.45	0	30,30,47	1.36	3 (10%)
35	HTG	b	602	-	19,19,19	1.06	2 (10%)	22,24,24	1.37	1 (4%)
35	HTG	b	603	-	19,19,19	0.96	2 (10%)	22,24,24	1.82	3 (13%)
24	CLA	b	605	40	55,73,73	1.95	11 (20%)	61,113,113	2.09	17 (27%)
24	CLA	b	606	-	55,73,73	1.92	12 (21%)	61,113,113	2.22	20 (32%)
24	CLA	b	607	-	55,73,73	1.94	12 (21%)	61,113,113	2.35	21 (34%)
24	CLA	b	608	-	55,73,73	1.94	12 (21%)	61,113,113	2.22	18 (29%)
24	CLA	b	609	-	55,73,73	1.92	11 (20%)	61,113,113	2.23	18 (29%)
24	CLA	b	610	-	55,73,73	1.87	11 (20%)	61,113,113	2.28	20 (32%)
24	CLA	b	611	40	55,73,73	1.95	13 (23%)	61,113,113	2.27	20 (32%)
24	CLA	b	612	-	55,73,73	1.94	12 (21%)	61,113,113	2.07	20 (32%)
24	CLA	b	613	-	55,73,73	1.87	12 (21%)	61,113,113	2.06	20 (32%)
24	CLA	b	614	40	55,73,73	1.97	12 (21%)	61,113,113	2.14	21 (34%)
24	CLA	b	615	-	55,73,73	1.90	12 (21%)	61,113,113	2.21	18 (29%)
24	CLA	b	616	-	55,73,73	1.89	12 (21%)	61,113,113	2.11	17 (27%)
24	CLA	b	617	-	55,73,73	1.94	12 (21%)	61,113,113	2.15	21 (34%)
24	CLA	b	618	-	55,73,73	1.90	12 (21%)	61,113,113	2.28	22 (36%)
24	CLA	b	619	-	55,73,73	1.93	11 (20%)	61,113,113	2.17	19 (31%)
24	CLA	b	620	-	55,73,73	1.96	12 (21%)	61,113,113	2.16	18 (29%)
26	BCR	b	621	-	41,41,41	1.08	1 (2%)	56,56,56	1.21	2 (3%)
26	BCR	b	622	-	41,41,41	1.02	1 (2%)	56,56,56	1.27	4 (7%)
26	BCR	b	623	-	41,41,41	0.95	1 (2%)	56,56,56	1.45	9 (16%)
34	LMG	b	624	-	51,51,55	0.88	3 (5%)	59,59,63	1.05	4 (6%)
29	LMT	b	625	-	25,25,36	0.51	0	30,30,47	0.65	0
35	HTG	b	626	-	19,19,19	0.83	1 (5%)	22,24,24	1.77	2 (9%)
35	HTG	b	627	-	19,19,19	1.02	1 (5%)	22,24,24	2.14	4 (18%)
28	GOL	b	628	-	5,5,5	0.35	0	5,5,5	0.27	0
28	GOL	b	629	-	5,5,5	0.30	0	5,5,5	0.18	0
28	GOL	b	630	-	5,5,5	0.28	0	5,5,5	0.47	0
28	GOL	b	631	-	5,5,5	0.30	0	5,5,5	0.46	0
28	GOL	b	632	-	5,5,5	0.33	0	5,5,5	0.61	0
28	GOL	b	633	-	5,5,5	0.34	0	5,5,5	0.29	0
24	CLA	c	902	-	55,73,73	1.90	12 (21%)	61,113,113	2.18	18 (29%)
24	CLA	c	903	-	55,73,73	1.88	11 (20%)	61,113,113	2.08	16 (26%)
24	CLA	c	904	-	55,73,73	1.87	12 (21%)	61,113,113	2.09	18 (29%)
24	CLA	c	905	40	55,73,73	1.94	12 (21%)	61,113,113	2.17	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	906	-	55,73,73	1.86	12 (21%)	61,113,113	2.23	17 (27%)
24	CLA	c	907	-	55,73,73	1.90	12 (21%)	61,113,113	2.21	21 (34%)
24	CLA	c	908	40	55,73,73	1.91	12 (21%)	61,113,113	2.33	18 (29%)
24	CLA	c	909	-	55,73,73	1.97	12 (21%)	61,113,113	2.14	17 (27%)
24	CLA	c	910	-	55,73,73	1.98	12 (21%)	61,113,113	2.15	16 (26%)
24	CLA	c	911	-	55,73,73	1.94	12 (21%)	61,113,113	2.06	16 (26%)
24	CLA	c	912	3	55,73,73	1.92	12 (21%)	61,113,113	1.97	16 (26%)
24	CLA	c	913	-	55,73,73	1.89	12 (21%)	61,113,113	2.15	18 (29%)
24	CLA	c	914	-	55,73,73	1.92	12 (21%)	61,113,113	2.01	18 (29%)
26	BCR	c	915	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	8 (14%)
36	DGD	c	916	-	63,63,67	0.80	2 (3%)	77,77,81	1.11	5 (6%)
36	DGD	c	917	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	3 (3%)
36	DGD	c	918	-	63,63,67	0.83	2 (3%)	77,77,81	0.95	3 (3%)
34	LMG	c	919	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	2 (3%)
34	LMG	c	920	-	51,51,55	0.92	2 (3%)	59,59,63	1.23	6 (10%)
29	LMT	c	921	-	36,36,36	0.44	0	47,47,47	0.84	0
35	HTG	c	922	-	19,19,19	0.84	1 (5%)	22,24,24	1.66	1 (4%)
35	HTG	c	923	-	19,19,19	1.06	2 (10%)	22,24,24	2.11	4 (18%)
28	GOL	c	924	-	5,5,5	0.35	0	5,5,5	0.24	0
28	GOL	c	925	-	5,5,5	0.33	0	5,5,5	0.55	0
24	CLA	d	401	40	55,73,73	1.90	10 (18%)	61,113,113	2.24	22 (36%)
24	CLA	d	402	-	55,73,73	1.83	12 (21%)	61,113,113	2.21	18 (29%)
24	CLA	d	403	-	55,73,73	1.93	12 (21%)	61,113,113	2.12	20 (32%)
26	BCR	d	404	-	41,41,41	1.00	1 (2%)	56,56,56	1.84	17 (30%)
31	PL9	d	405	-	55,55,55	0.75	2 (3%)	68,69,69	1.66	18 (26%)
36	DGD	d	406	-	63,63,67	0.90	2 (3%)	77,77,81	1.25	6 (7%)
37	LHG	d	407	-	48,48,48	0.90	2 (4%)	49,54,54	1.01	3 (6%)
37	LHG	d	408	-	48,48,48	0.85	2 (4%)	49,54,54	0.93	3 (6%)
37	LHG	d	409	-	48,48,48	0.92	2 (4%)	49,54,54	1.07	3 (6%)
35	HTG	d	412	-	16,16,19	1.03	2 (12%)	19,21,24	1.68	1 (5%)
37	LHG	e	101	-	41,41,48	0.98	2 (4%)	42,47,54	0.99	2 (4%)
38	HEM	e	102	5,6	30,50,50	2.29	7 (23%)	24,82,82	2.56	12 (50%)
28	GOL	f	101	33	5,5,5	0.33	0	5,5,5	0.42	0
27	SQD	f	102	-	42,43,54	1.58	3 (7%)	50,54,65	1.51	7 (14%)
29	LMT	f	103	-	36,36,36	0.52	0	47,47,47	0.93	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.31	5 (8%)
36	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	1.00	5 (6%)
34	LMG	j	101	39	51,51,55	0.86	2 (3%)	59,59,63	0.98	3 (5%)
26	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	9 (16%)
26	BCR	k	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.37	7 (12%)
37	LHG	l	101	-	48,48,48	0.89	2 (4%)	49,54,54	1.13	4 (8%)
29	LMT	m	102	-	36,36,36	0.47	0	47,47,47	0.91	1 (2%)
29	LMT	m	103	-	36,36,36	0.47	0	47,47,47	1.02	2 (4%)
29	LMT	m	104	-	36,36,36	0.49	0	47,47,47	1.03	2 (4%)
28	GOL	o	302	-	5,5,5	0.37	0	5,5,5	0.48	0
26	BCR	t	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.39	7 (12%)
28	GOL	t	102	-	5,5,5	0.37	0	5,5,5	0.28	0
38	HEM	v	202	16	30,50,50	2.18	7 (23%)	24,82,82	2.31	9 (37%)
28	GOL	v	203	-	5,5,5	0.22	0	5,5,5	0.59	0
28	GOL	v	204	-	5,5,5	0.35	0	5,5,5	0.33	0
28	GOL	v	205	-	5,5,5	0.37	0	5,5,5	0.30	0
26	BCR	y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.64	11 (19%)
34	LMG	z	101	-	39,39,55	1.06	2 (5%)	47,47,63	1.50	9 (19%)

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
23	BCT	A	404	21	-	0/0/0/0	0/0/0/0
24	CLA	A	405	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	A	406	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	407	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	A	408	-	-	0/53/103/103	0/1/6/6
25	PHO	A	409	-	-	0/53/103/103	0/1/6/6
24	CLA	A	410	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
27	SQD	A	412	-	-	0/49/69/69	0/1/1/1
28	GOL	A	413	-	-	0/4/4/4	0/0/0/0
28	GOL	A	414	-	-	0/4/4/4	0/0/0/0
28	GOL	A	415	-	-	0/4/4/4	0/0/0/0
27	SQD	A	416	-	-	0/49/69/69	0/1/1/1
29	LMT	A	417	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OEX	A	418	1,3,40	-	0/0/68/68	0/0/6/6
31	PL9	A	419	-	-	0/53/73/73	0/1/1/1
24	CLA	B	602	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
27	SQD	B	621	-	-	0/49/69/69	0/1/1/1
34	LMG	B	622	-	-	0/46/66/70	0/1/1/1
29	LMT	B	623	-	-	0/21/61/61	0/2/2/2
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
35	HTG	B	625	-	-	0/10/30/30	0/1/1/1
35	HTG	B	626	-	-	0/10/30/30	0/1/1/1
28	GOL	B	627	-	-	0/4/4/4	0/0/0/0
28	GOL	B	628	-	-	0/4/4/4	0/0/0/0
28	GOL	B	629	-	-	0/4/4/4	0/0/0/0
28	GOL	B	630	-	-	0/4/4/4	0/0/0/0
28	GOL	B	631	-	-	0/4/4/4	0/0/0/0
28	GOL	B	632	-	-	0/4/4/4	0/0/0/0
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
35	HTG	B	634	-	-	0/10/30/30	0/1/1/1
29	LMT	B	636	-	-	0/17/37/61	0/1/1/2
28	GOL	B	637	-	-	0/4/4/4	0/0/0/0
34	LMG	C	501	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	514	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2
36	DGD	C	518	-	-	0/51/91/95	0/2/2/2
36	DGD	C	519	-	-	0/51/91/95	0/2/2/2
34	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	LMG	C	521	-	-	0/46/66/70	0/1/1/1
29	LMT	C	522	-	-	0/21/61/61	0/2/2/2
35	HTG	C	523	-	-	0/10/30/30	0/1/1/1
35	HTG	C	524	-	-	0/10/30/30	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	0/0/0/0
28	GOL	C	526	-	-	0/4/4/4	0/0/0/0
24	CLA	D	401	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	403	-	-	0/29/63/63	0/2/2/2
31	PL9	D	404	-	-	0/53/73/73	0/1/1/1
36	DGD	D	405	-	-	0/51/91/95	0/2/2/2
37	LHG	D	406	-	-	0/53/53/53	0/0/0/0
37	LHG	D	407	-	-	0/53/53/53	0/0/0/0
37	LHG	D	408	-	-	0/53/53/53	0/0/0/0
35	HTG	D	411	-	-	0/7/27/30	0/1/1/1
37	LHG	E	101	-	-	0/46/46/53	0/0/0/0
29	LMT	E	102	-	-	0/21/61/61	0/2/2/2
38	HEM	E	103	5,6	-	0/10/54/54	0/0/8/8
27	SQD	F	101	-	-	2/38/58/69	0/1/1/1
28	GOL	F	103	33	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
34	LMG	J	101	39	-	0/46/66/70	0/1/1/1
26	BCR	K	102	-	-	0/29/63/63	0/2/2/2
26	BCR	K	103	-	-	0/29/63/63	0/2/2/2
37	LHG	L	101	-	-	0/53/53/53	0/0/0/0
27	SQD	L	102	-	-	1/49/69/69	0/1/1/1
29	LMT	M	101	-	-	0/21/61/61	0/2/2/2
28	GOL	O	302	-	-	0/4/4/4	0/0/0/0
35	HTG	O	303	-	-	0/10/30/30	0/1/1/1
28	GOL	T	101	-	-	0/4/4/4	0/0/0/0
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
28	GOL	T	103	-	-	0/4/4/4	0/0/0/0
38	HEM	V	201	16	-	0/10/54/54	0/0/8/8
35	HTG	V	202	-	-	0/10/30/30	0/1/1/1
28	GOL	V	203	-	-	0/4/4/4	0/0/0/0
28	GOL	V	204	-	-	0/4/4/4	0/0/0/0
28	GOL	V	205	-	-	0/4/4/4	0/0/0/0
28	GOL	V	206	-	-	0/4/4/4	0/0/0/0
34	LMG	Z	101	-	-	2/31/51/70	0/1/1/1
29	LMT	a	401	-	-	0/21/61/61	0/2/2/2
27	SQD	a	402	-	-	0/49/69/69	0/1/1/1
24	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	407	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	a	408	-	-	0/53/103/103	0/1/6/6
24	CLA	a	409	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
27	SQD	a	411	-	-	0/49/69/69	0/1/1/1
34	LMG	a	412	-	-	0/46/66/70	0/1/1/1
28	GOL	a	413	-	-	0/4/4/4	0/0/0/0
28	GOL	a	414	-	-	0/4/4/4	0/0/0/0
28	GOL	a	415	-	-	0/4/4/4	0/0/0/0
30	OEX	a	416	1,3,40	-	0/0/68/68	0/0/6/6
31	PL9	a	417	-	-	0/53/73/73	0/1/1/1
23	BCT	a	419	21	-	0/0/0/0	0/0/0/0
25	PHO	a	420	-	-	0/53/103/103	0/1/6/6
29	LMT	b	601	-	-	0/17/37/61	0/1/1/2
35	HTG	b	602	-	-	0/10/30/30	0/1/1/1
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
24	CLA	b	605	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	607	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	40	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	618	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	621	-	-	0/29/63/63	0/2/2/2
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
34	LMG	b	624	-	-	0/46/66/70	0/1/1/1
29	LMT	b	625	-	-	0/17/37/61	0/1/1/2
35	HTG	b	626	-	-	0/10/30/30	0/1/1/1
35	HTG	b	627	-	-	0/10/30/30	0/1/1/1
28	GOL	b	628	-	-	0/4/4/4	0/0/0/0
28	GOL	b	629	-	-	0/4/4/4	0/0/0/0
28	GOL	b	630	-	-	0/4/4/4	0/0/0/0
28	GOL	b	631	-	-	0/4/4/4	0/0/0/0
28	GOL	b	632	-	-	0/4/4/4	0/0/0/0
28	GOL	b	633	-	-	0/4/4/4	0/0/0/0
24	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	903	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	904	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	905	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	906	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	907	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	908	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	909	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	912	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	913	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	914	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	c	915	-	-	0/29/63/63	0/2/2/2
36	DGD	c	916	-	-	0/51/91/95	0/2/2/2
36	DGD	c	917	-	-	0/51/91/95	0/2/2/2
36	DGD	c	918	-	-	0/51/91/95	0/2/2/2
34	LMG	c	919	-	-	0/46/66/70	0/1/1/1
34	LMG	c	920	-	-	0/46/66/70	0/1/1/1
29	LMT	c	921	-	-	0/21/61/61	0/2/2/2
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
35	HTG	c	923	-	-	0/10/30/30	0/1/1/1
28	GOL	c	924	-	-	0/4/4/4	0/0/0/0
28	GOL	c	925	-	-	0/4/4/4	0/0/0/0
24	CLA	d	401	40	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	d	402	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	d	404	-	-	0/29/63/63	0/2/2/2
31	PL9	d	405	-	-	0/53/73/73	0/1/1/1
36	DGD	d	406	-	-	1/51/91/95	0/2/2/2
37	LHG	d	407	-	-	0/53/53/53	0/0/0/0
37	LHG	d	408	-	-	0/53/53/53	0/0/0/0
37	LHG	d	409	-	-	0/53/53/53	0/0/0/0
35	HTG	d	412	-	-	0/7/27/30	0/1/1/1
37	LHG	e	101	-	-	0/46/46/53	0/0/0/0
38	HEM	e	102	5,6	-	0/10/54/54	0/0/8/8
28	GOL	f	101	33	-	0/4/4/4	0/0/0/0
27	SQD	f	102	-	-	2/38/58/69	0/1/1/1
29	LMT	f	103	-	-	0/21/61/61	0/2/2/2
26	BCR	h	101	-	-	0/29/63/63	0/2/2/2
36	DGD	h	102	-	-	0/51/91/95	0/2/2/2
34	LMG	j	101	39	-	0/46/66/70	0/1/1/1
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	BCR	k	102	-	-	0/29/63/63	0/2/2/2
37	LHG	l	101	-	-	0/53/53/53	0/0/0/0
29	LMT	m	102	-	-	0/21/61/61	0/2/2/2
29	LMT	m	103	-	-	0/21/61/61	0/2/2/2
29	LMT	m	104	-	-	0/21/61/61	0/2/2/2
28	GOL	o	302	-	-	0/4/4/4	0/0/0/0
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
28	GOL	t	102	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HEM	v	202	16	-	0/10/54/54	0/0/8/8
28	GOL	v	203	-	-	0/4/4/4	0/0/0/0
28	GOL	v	204	-	-	0/4/4/4	0/0/0/0
28	GOL	v	205	-	-	0/4/4/4	0/0/0/0
26	BCR	y	101	-	-	0/29/63/63	0/2/2/2
34	LMG	z	101	-	-	0/34/54/70	0/1/1/1

All (1064) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	402	SQD	C6-S	-8.02	1.66	1.77
27	f	102	SQD	C6-S	-7.66	1.66	1.77
27	A	416	SQD	C6-S	-7.62	1.66	1.77
27	a	411	SQD	C6-S	-7.12	1.67	1.77
27	A	412	SQD	C6-S	-7.07	1.67	1.77
27	B	621	SQD	C6-S	-6.82	1.67	1.77
38	V	201	HEM	C2D-C3D	-6.80	1.34	1.54
38	e	102	HEM	C2D-C3D	-6.77	1.34	1.54
27	L	102	SQD	C6-S	-6.74	1.67	1.77
38	E	103	HEM	C2D-C3D	-6.64	1.34	1.54
27	F	101	SQD	C6-S	-6.52	1.68	1.77
38	v	202	HEM	C2D-C3D	-6.50	1.35	1.54
38	e	102	HEM	C2C-C1C	-6.36	1.40	1.52
38	E	103	HEM	C2C-C1C	-6.21	1.40	1.52
38	v	202	HEM	C2C-C1C	-6.13	1.40	1.52
38	V	201	HEM	C2C-C1C	-5.65	1.41	1.52
26	k	101	BCR	C23-C22	-4.93	1.35	1.45
26	t	101	BCR	C23-C22	-4.89	1.35	1.45
26	B	620	BCR	C23-C22	-4.84	1.35	1.45
26	b	622	BCR	C23-C22	-4.83	1.35	1.45
26	k	102	BCR	C23-C22	-4.77	1.35	1.45
26	d	404	BCR	C23-C22	-4.67	1.35	1.45
26	D	403	BCR	C23-C22	-4.67	1.35	1.45
26	C	515	BCR	C23-C22	-4.63	1.35	1.45
26	C	516	BCR	C23-C22	-4.62	1.35	1.45
26	h	101	BCR	C23-C22	-4.58	1.35	1.45
26	b	623	BCR	C23-C22	-4.55	1.35	1.45
26	K	103	BCR	C23-C22	-4.54	1.35	1.45
26	y	101	BCR	C23-C22	-4.47	1.36	1.45
26	b	621	BCR	C23-C22	-4.47	1.36	1.45
26	H	101	BCR	C23-C22	-4.42	1.36	1.45
26	c	915	BCR	C23-C22	-4.38	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	102	BCR	C23-C22	-4.35	1.36	1.45
26	A	411	BCR	C23-C22	-4.33	1.36	1.45
26	B	619	BCR	C23-C22	-4.30	1.36	1.45
26	a	410	BCR	C23-C22	-4.29	1.36	1.45
26	K	102	BCR	C23-C22	-4.20	1.36	1.45
38	E	103	HEM	C3B-C4B	-4.10	1.48	1.51
38	e	102	HEM	C3D-C4D	-3.97	1.46	1.51
35	b	602	HTG	C1'-S1	-3.95	1.76	1.81
35	B	624	HTG	C1'-S1	-3.95	1.76	1.81
26	B	618	BCR	C23-C22	-3.87	1.37	1.45
38	E	103	HEM	C3D-C4D	-3.85	1.46	1.51
35	c	923	HTG	C1'-S1	-3.69	1.76	1.81
25	A	408	PHO	C4A-NA	-3.62	1.26	1.34
35	B	633	HTG	C1'-S1	-3.62	1.76	1.81
35	D	411	HTG	C1'-S1	-3.55	1.76	1.81
35	B	634	HTG	C1'-S1	-3.49	1.76	1.81
35	b	627	HTG	C1'-S1	-3.49	1.76	1.81
38	v	202	HEM	C3D-C4D	-3.32	1.47	1.51
25	A	409	PHO	C4A-NA	-3.32	1.27	1.34
35	b	603	HTG	C1'-S1	-3.25	1.76	1.81
35	C	524	HTG	C1'-S1	-3.24	1.77	1.81
35	d	412	HTG	C1'-S1	-3.23	1.77	1.81
35	B	626	HTG	C1'-S1	-3.22	1.77	1.81
35	V	202	HTG	C1'-S1	-3.17	1.77	1.81
38	e	102	HEM	C3B-C4B	-3.17	1.49	1.51
38	v	202	HEM	C3B-C4B	-3.14	1.49	1.51
35	C	523	HTG	C1'-S1	-3.10	1.77	1.81
35	O	303	HTG	C1'-S1	-3.02	1.77	1.81
35	b	626	HTG	C1'-S1	-3.01	1.77	1.81
25	a	420	PHO	C4A-NA	-2.98	1.27	1.34
25	a	408	PHO	C4A-NA	-2.95	1.27	1.34
35	B	625	HTG	C1'-S1	-2.90	1.77	1.81
38	V	201	HEM	C2B-C1B	-2.90	1.42	1.51
35	c	922	HTG	C1'-S1	-2.75	1.77	1.81
38	v	202	HEM	C2B-C1B	-2.68	1.43	1.51
38	e	102	HEM	C2B-C1B	-2.67	1.43	1.51
38	E	103	HEM	C2B-C1B	-2.67	1.43	1.51
38	V	201	HEM	C3B-C4B	-2.56	1.49	1.51
35	c	923	HTG	C1-S1	-2.49	1.76	1.80
35	B	633	HTG	C1-S1	-2.45	1.76	1.80
38	V	201	HEM	C3D-C4D	-2.39	1.48	1.51
35	d	412	HTG	C1-S1	-2.33	1.76	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	420	PHO	C1C-NC	-2.30	1.33	1.38
25	a	420	PHO	C1A-NA	-2.25	1.32	1.37
25	A	409	PHO	C1A-NA	-2.23	1.32	1.37
35	V	202	HTG	C1-S1	-2.15	1.77	1.80
35	b	602	HTG	C1-S1	-2.11	1.77	1.80
35	D	411	HTG	C1-S1	-2.10	1.77	1.80
35	b	603	HTG	C1-S1	-2.07	1.77	1.80
24	C	512	CLA	C1C-NC	-2.07	1.34	1.37
25	A	408	PHO	C1A-NA	-2.07	1.32	1.37
35	C	523	HTG	C1-S1	-2.05	1.77	1.80
34	b	624	LMG	O7-C8	-2.03	1.41	1.46
35	C	524	HTG	C1-S1	-2.01	1.77	1.80
31	d	405	PL9	C2-C3	2.03	1.40	1.34
36	C	517	DGD	O5D-C1E	2.03	1.43	1.40
24	c	912	CLA	C4C-C3C	2.03	1.48	1.45
24	B	612	CLA	C1C-C2C	2.04	1.48	1.44
24	b	611	CLA	C1A-CHA	2.04	1.51	1.43
24	B	608	CLA	C1C-C2C	2.05	1.48	1.44
24	c	912	CLA	C1C-C2C	2.05	1.48	1.44
31	A	419	PL9	C2-C3	2.06	1.40	1.34
24	B	616	CLA	C4C-C3C	2.07	1.48	1.45
24	d	403	CLA	C1C-C2C	2.07	1.48	1.44
24	A	407	CLA	C4C-C3C	2.08	1.48	1.45
24	b	613	CLA	C4C-C3C	2.08	1.48	1.45
26	a	410	BCR	C12-C13	2.09	1.50	1.45
24	b	616	CLA	C4C-C3C	2.10	1.48	1.45
24	c	907	CLA	C1C-C2C	2.11	1.48	1.44
31	D	404	PL9	C2-C3	2.11	1.40	1.34
24	b	611	CLA	C4C-C3C	2.12	1.48	1.45
24	B	602	CLA	C4C-C3C	2.12	1.48	1.45
24	B	602	CLA	C1C-C2C	2.13	1.48	1.44
24	C	514	CLA	C1C-C2C	2.14	1.48	1.44
31	a	417	PL9	C2-C3	2.14	1.40	1.34
24	C	508	CLA	C4C-C3C	2.14	1.48	1.45
24	b	620	CLA	C1C-C2C	2.15	1.48	1.44
29	A	417	LMT	O1'-C1'	2.15	1.44	1.40
24	c	907	CLA	C4C-C3C	2.18	1.49	1.45
24	C	507	CLA	C1C-C2C	2.18	1.49	1.44
24	a	406	CLA	C1C-C2C	2.19	1.49	1.44
24	C	514	CLA	C4C-C3C	2.20	1.49	1.45
24	c	910	CLA	C4C-C3C	2.20	1.49	1.45
24	a	407	CLA	C4C-C3C	2.21	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C1C-C2C	2.22	1.49	1.44
27	B	621	SQD	O6-C1	2.22	1.44	1.40
24	A	407	CLA	C1C-C2C	2.23	1.49	1.44
24	b	605	CLA	C1C-C2C	2.23	1.49	1.44
24	A	405	CLA	C1C-C2C	2.24	1.49	1.44
24	b	620	CLA	C4C-C3C	2.25	1.49	1.45
24	a	409	CLA	C1C-C2C	2.26	1.49	1.44
24	b	616	CLA	CHD-C4C	2.26	1.46	1.41
24	b	615	CLA	C1C-C2C	2.27	1.49	1.44
24	C	512	CLA	C1C-C2C	2.27	1.49	1.44
24	B	606	CLA	CHD-C4C	2.27	1.46	1.41
24	b	618	CLA	C4C-C3C	2.27	1.49	1.45
24	c	909	CLA	C1C-C2C	2.28	1.49	1.44
24	A	405	CLA	C4C-C3C	2.29	1.49	1.45
36	D	405	DGD	O3G-C1D	2.29	1.44	1.40
24	D	401	CLA	C1C-C2C	2.30	1.49	1.44
24	a	407	CLA	C1C-C2C	2.31	1.49	1.44
24	c	911	CLA	C4C-C3C	2.31	1.49	1.45
24	b	606	CLA	C4C-C3C	2.32	1.49	1.45
24	c	914	CLA	C4C-C3C	2.32	1.49	1.45
29	a	401	LMT	O1'-C1'	2.32	1.44	1.40
31	D	404	PL9	C6-C5	2.33	1.48	1.35
31	d	405	PL9	C6-C5	2.33	1.48	1.35
24	c	905	CLA	C4C-C3C	2.33	1.49	1.45
24	B	617	CLA	CHD-C4C	2.33	1.46	1.41
24	b	612	CLA	C1C-C2C	2.33	1.49	1.44
24	A	406	CLA	C1B-CHB	2.34	1.46	1.39
24	b	617	CLA	C4C-C3C	2.35	1.49	1.45
24	d	403	CLA	C4C-C3C	2.36	1.49	1.45
31	a	417	PL9	C6-C5	2.36	1.49	1.35
24	C	508	CLA	C1C-C2C	2.36	1.49	1.44
31	A	419	PL9	C6-C5	2.36	1.49	1.35
24	b	614	CLA	C1C-C2C	2.36	1.49	1.44
24	C	505	CLA	C4C-C3C	2.37	1.49	1.45
24	c	908	CLA	C1C-C2C	2.37	1.49	1.44
25	a	408	PHO	C3B-C4B	2.37	1.48	1.43
24	B	609	CLA	C1B-CHB	2.37	1.46	1.39
24	c	913	CLA	C4C-C3C	2.37	1.49	1.45
24	C	512	CLA	C4C-C3C	2.38	1.49	1.45
25	a	420	PHO	C4D-CHA	2.38	1.51	1.44
24	c	906	CLA	C4B-CHC	2.38	1.46	1.39
24	c	908	CLA	C4C-C3C	2.38	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	C1C-C2C	2.38	1.49	1.44
24	B	616	CLA	C1B-CHB	2.38	1.46	1.39
24	c	902	CLA	C4C-C3C	2.39	1.49	1.45
24	b	614	CLA	C4C-C3C	2.39	1.49	1.45
24	b	615	CLA	C4C-C3C	2.39	1.49	1.45
24	B	610	CLA	C1C-C2C	2.40	1.49	1.44
24	c	903	CLA	C1C-C2C	2.40	1.49	1.44
24	B	606	CLA	C1C-C2C	2.40	1.49	1.44
24	C	502	CLA	C4C-C3C	2.42	1.49	1.45
24	C	511	CLA	C4C-C3C	2.42	1.49	1.45
24	b	612	CLA	C4C-C3C	2.42	1.49	1.45
36	h	102	DGD	O5D-C1E	2.43	1.44	1.40
24	c	902	CLA	C4B-CHC	2.43	1.46	1.39
24	b	607	CLA	C1C-C2C	2.44	1.49	1.44
24	A	410	CLA	C1C-C2C	2.44	1.49	1.44
24	B	603	CLA	C4C-C3C	2.44	1.49	1.45
24	C	506	CLA	C1C-C2C	2.44	1.49	1.44
24	B	615	CLA	C4B-CHC	2.45	1.46	1.39
24	C	512	CLA	C4B-CHC	2.45	1.46	1.39
24	C	504	CLA	C1B-CHB	2.45	1.46	1.39
24	b	607	CLA	C4C-C3C	2.45	1.49	1.45
24	c	908	CLA	C4B-CHC	2.46	1.46	1.39
24	b	619	CLA	C4C-C3C	2.46	1.49	1.45
38	E	103	HEM	FE-NB	2.47	2.10	1.97
24	b	618	CLA	C1C-C2C	2.48	1.49	1.44
24	C	509	CLA	C1C-C2C	2.48	1.49	1.44
24	c	902	CLA	C1C-C2C	2.48	1.49	1.44
24	c	904	CLA	C1C-C2C	2.49	1.49	1.44
24	b	610	CLA	C1B-CHB	2.49	1.46	1.39
24	B	609	CLA	C4C-C3C	2.50	1.49	1.45
24	D	402	CLA	C1C-C2C	2.50	1.49	1.44
24	c	906	CLA	C1C-C2C	2.50	1.49	1.44
24	B	611	CLA	C4C-C3C	2.51	1.49	1.45
34	Z	101	LMG	O8-C28	2.51	1.46	1.33
24	B	604	CLA	C1C-C2C	2.51	1.49	1.44
24	c	911	CLA	C1C-C2C	2.51	1.49	1.44
24	C	507	CLA	C4B-CHC	2.52	1.46	1.39
24	b	611	CLA	CHD-C4C	2.52	1.47	1.41
24	B	605	CLA	C1C-C2C	2.53	1.49	1.44
24	B	617	CLA	C4B-CHC	2.53	1.46	1.39
24	b	619	CLA	C4B-CHC	2.54	1.46	1.39
24	b	606	CLA	C1C-C2C	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C1C-C2C	2.54	1.49	1.44
24	B	614	CLA	C4C-C3C	2.54	1.49	1.45
24	c	914	CLA	C1C-C2C	2.54	1.49	1.44
24	D	401	CLA	C4B-CHC	2.54	1.46	1.39
24	b	617	CLA	C1C-C2C	2.55	1.49	1.44
24	b	617	CLA	CHD-C4C	2.55	1.47	1.41
24	C	507	CLA	C4C-C3C	2.55	1.49	1.45
24	B	607	CLA	C4B-CHC	2.55	1.46	1.39
24	b	616	CLA	C1C-C2C	2.55	1.49	1.44
24	C	510	CLA	C1C-C2C	2.57	1.49	1.44
38	v	202	HEM	FE-NB	2.57	2.11	1.97
24	B	609	CLA	C4B-CHC	2.58	1.46	1.39
24	C	504	CLA	C4C-C3C	2.58	1.49	1.45
24	A	405	CLA	CHD-C4C	2.59	1.47	1.41
24	c	905	CLA	CHD-C4C	2.59	1.47	1.41
24	B	615	CLA	C1C-C2C	2.60	1.49	1.44
24	B	602	CLA	C1B-CHB	2.61	1.47	1.39
24	B	613	CLA	CHD-C4C	2.61	1.47	1.41
36	H	102	DGD	O5D-C1E	2.61	1.44	1.40
24	c	907	CLA	C4B-CHC	2.62	1.47	1.39
24	a	409	CLA	C4B-CHC	2.62	1.47	1.39
24	C	503	CLA	C4C-C3C	2.62	1.49	1.45
24	B	614	CLA	C1C-C2C	2.62	1.49	1.44
24	b	615	CLA	CHD-C4C	2.62	1.47	1.41
24	b	611	CLA	C1C-C2C	2.62	1.49	1.44
24	c	910	CLA	C1C-C2C	2.62	1.49	1.44
24	b	619	CLA	C1B-CHB	2.62	1.47	1.39
24	d	402	CLA	C4C-C3C	2.62	1.49	1.45
24	c	905	CLA	C4B-CHC	2.63	1.47	1.39
24	C	502	CLA	C1C-C2C	2.63	1.49	1.44
24	b	607	CLA	C1B-CHB	2.64	1.47	1.39
24	D	401	CLA	CHD-C4C	2.64	1.47	1.41
24	c	914	CLA	C1B-CHB	2.64	1.47	1.39
24	d	401	CLA	C4B-CHC	2.64	1.47	1.39
24	C	514	CLA	C4B-CHC	2.64	1.47	1.39
24	D	402	CLA	C4C-C3C	2.64	1.49	1.45
24	b	620	CLA	C4B-CHC	2.64	1.47	1.39
24	b	610	CLA	C4B-CHC	2.64	1.47	1.39
38	V	201	HEM	FE-NB	2.64	2.11	1.97
24	B	607	CLA	C1C-C2C	2.64	1.49	1.44
24	B	612	CLA	C4C-C3C	2.64	1.49	1.45
24	c	913	CLA	C1C-C2C	2.65	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	C4B-CHC	2.65	1.47	1.39
24	d	402	CLA	CHD-C4C	2.65	1.47	1.41
24	B	606	CLA	C4C-C3C	2.67	1.49	1.45
24	a	406	CLA	C4C-C3C	2.67	1.49	1.45
24	a	409	CLA	C1B-CHB	2.67	1.47	1.39
24	c	904	CLA	C4C-C3C	2.67	1.49	1.45
24	D	402	CLA	CHD-C4C	2.67	1.47	1.41
24	c	913	CLA	C1B-CHB	2.68	1.47	1.39
24	B	603	CLA	C1C-C2C	2.68	1.50	1.44
24	c	902	CLA	CHD-C4C	2.69	1.47	1.41
24	d	403	CLA	C4B-CHC	2.69	1.47	1.39
24	C	504	CLA	C1C-C2C	2.69	1.50	1.44
24	B	604	CLA	CHD-C4C	2.69	1.47	1.41
24	C	503	CLA	C1C-C2C	2.69	1.50	1.44
24	C	505	CLA	C1C-C2C	2.70	1.50	1.44
24	B	613	CLA	C1C-C2C	2.70	1.50	1.44
24	c	909	CLA	C1B-CHB	2.70	1.47	1.39
24	C	513	CLA	CHD-C4C	2.70	1.47	1.41
24	c	909	CLA	C4C-C3C	2.70	1.49	1.45
24	B	606	CLA	C4B-CHC	2.70	1.47	1.39
38	e	102	HEM	FE-NB	2.70	2.11	1.97
24	C	511	CLA	C1C-C2C	2.71	1.50	1.44
24	c	909	CLA	C4B-CHC	2.71	1.47	1.39
24	B	614	CLA	CHD-C4C	2.72	1.47	1.41
24	b	615	CLA	C4B-CHC	2.72	1.47	1.39
24	C	513	CLA	C1B-CHB	2.72	1.47	1.39
24	b	617	CLA	C4B-CHC	2.72	1.47	1.39
24	a	409	CLA	CHD-C4C	2.72	1.47	1.41
24	c	909	CLA	CHD-C4C	2.72	1.47	1.41
24	B	607	CLA	C4C-C3C	2.73	1.49	1.45
24	B	610	CLA	CHD-C4C	2.73	1.47	1.41
24	b	618	CLA	C4B-CHC	2.73	1.47	1.39
24	B	616	CLA	CHD-C4C	2.74	1.47	1.41
24	c	914	CLA	C4B-CHC	2.74	1.47	1.39
24	a	406	CLA	C4B-CHC	2.74	1.47	1.39
24	b	606	CLA	CHD-C4C	2.74	1.47	1.41
24	C	506	CLA	C4C-C3C	2.74	1.50	1.45
24	c	905	CLA	C1C-C2C	2.75	1.50	1.44
24	d	402	CLA	C1B-CHB	2.75	1.47	1.39
24	B	604	CLA	C1B-CHB	2.75	1.47	1.39
24	C	506	CLA	C1B-CHB	2.75	1.47	1.39
24	B	607	CLA	C1B-CHB	2.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C4B-CHC	2.76	1.47	1.39
24	C	505	CLA	C4B-CHC	2.76	1.47	1.39
24	D	401	CLA	C4C-C3C	2.76	1.50	1.45
24	A	406	CLA	C4B-CHC	2.77	1.47	1.39
24	d	402	CLA	C4B-CHC	2.77	1.47	1.39
24	B	613	CLA	C4B-CHC	2.78	1.47	1.39
24	C	513	CLA	C1C-C2C	2.78	1.50	1.44
24	c	912	CLA	C4B-CHC	2.78	1.47	1.39
24	B	616	CLA	C4B-CHC	2.78	1.47	1.39
24	b	605	CLA	C1B-CHB	2.78	1.47	1.39
24	D	402	CLA	C4B-CHC	2.79	1.47	1.39
24	C	503	CLA	C4B-CHC	2.79	1.47	1.39
24	A	410	CLA	C1B-CHB	2.79	1.47	1.39
24	a	407	CLA	C1B-CHB	2.79	1.47	1.39
24	b	611	CLA	C4B-CHC	2.79	1.47	1.39
24	c	904	CLA	C1B-CHB	2.79	1.47	1.39
24	C	509	CLA	C4C-C3C	2.79	1.50	1.45
24	b	609	CLA	C1C-C2C	2.79	1.50	1.44
24	B	614	CLA	C4B-CHC	2.80	1.47	1.39
24	B	607	CLA	CHD-C4C	2.80	1.47	1.41
24	B	603	CLA	C4B-CHC	2.80	1.47	1.39
24	b	620	CLA	CHD-C4C	2.80	1.47	1.41
24	C	508	CLA	C1B-CHB	2.80	1.47	1.39
24	c	913	CLA	CHD-C4C	2.80	1.47	1.41
24	b	619	CLA	CHD-C4C	2.80	1.47	1.41
24	d	401	CLA	CHD-C4C	2.80	1.47	1.41
24	c	906	CLA	CHD-C4C	2.81	1.47	1.41
24	d	403	CLA	CHD-C4C	2.81	1.47	1.41
24	B	603	CLA	CHD-C4C	2.81	1.47	1.41
24	C	509	CLA	C4B-CHC	2.81	1.47	1.39
24	B	610	CLA	C4B-CHC	2.82	1.47	1.39
24	b	607	CLA	C4B-CHC	2.82	1.47	1.39
24	b	613	CLA	C1C-C2C	2.82	1.50	1.44
24	B	608	CLA	C1B-CHB	2.82	1.47	1.39
24	C	514	CLA	CHD-C4C	2.82	1.47	1.41
24	B	605	CLA	C4B-CHC	2.82	1.47	1.39
25	a	420	PHO	C3B-C4B	2.83	1.49	1.43
24	C	510	CLA	C4B-CHC	2.83	1.47	1.39
24	C	513	CLA	C4B-CHC	2.83	1.47	1.39
24	b	608	CLA	C1B-CHB	2.83	1.47	1.39
24	C	502	CLA	C1B-CHB	2.83	1.47	1.39
24	C	510	CLA	C4C-C3C	2.83	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C4B-CHC	2.84	1.47	1.39
24	c	910	CLA	C1B-CHB	2.84	1.47	1.39
24	b	616	CLA	C4B-CHC	2.85	1.47	1.39
24	b	612	CLA	C1B-CHB	2.85	1.47	1.39
24	b	611	CLA	C1B-CHB	2.85	1.47	1.39
24	C	508	CLA	C4B-CHC	2.85	1.47	1.39
24	b	614	CLA	C4B-CHC	2.86	1.47	1.39
24	b	609	CLA	C4B-CHC	2.86	1.47	1.39
24	B	614	CLA	C1B-CHB	2.86	1.47	1.39
24	B	604	CLA	C4B-CHC	2.86	1.47	1.39
24	B	602	CLA	C4B-CHC	2.87	1.47	1.39
24	b	613	CLA	CHD-C4C	2.87	1.47	1.41
24	C	510	CLA	CHD-C4C	2.87	1.47	1.41
25	A	408	PHO	CHD-C4C	2.88	1.47	1.40
25	a	408	PHO	OBD-CAD	2.88	1.27	1.22
24	B	613	CLA	C1B-CHB	2.88	1.47	1.39
24	c	906	CLA	C4C-C3C	2.89	1.50	1.45
24	C	502	CLA	CHD-C4C	2.90	1.48	1.41
24	c	905	CLA	C1B-CHB	2.90	1.47	1.39
24	A	407	CLA	C1B-CHB	2.90	1.47	1.39
24	b	610	CLA	C1C-C2C	2.90	1.50	1.44
24	b	617	CLA	C1B-CHB	2.90	1.47	1.39
24	c	904	CLA	C4B-CHC	2.91	1.47	1.39
24	C	502	CLA	C4B-CHC	2.91	1.47	1.39
24	D	402	CLA	C1B-CHB	2.91	1.47	1.39
24	A	405	CLA	C4B-CHC	2.91	1.47	1.39
24	b	612	CLA	CHD-C4C	2.91	1.48	1.41
24	B	603	CLA	C1B-CHB	2.92	1.47	1.39
24	B	608	CLA	C4C-C3C	2.92	1.50	1.45
25	a	420	PHO	CHD-C4C	2.92	1.47	1.40
24	c	903	CLA	CHD-C4C	2.92	1.48	1.41
24	B	605	CLA	CHD-C4C	2.92	1.48	1.41
25	A	408	PHO	C3B-C4B	2.92	1.50	1.43
24	b	610	CLA	CHD-C4C	2.92	1.48	1.41
24	b	605	CLA	C4B-CHC	2.93	1.47	1.39
24	b	608	CLA	C1C-C2C	2.93	1.50	1.44
24	c	911	CLA	CHD-C4C	2.93	1.48	1.41
24	C	514	CLA	C1B-CHB	2.93	1.47	1.39
24	c	913	CLA	C4B-CHC	2.93	1.47	1.39
25	a	420	PHO	OBD-CAD	2.94	1.27	1.22
24	d	401	CLA	C1B-CHB	2.94	1.48	1.39
24	C	506	CLA	CHD-C4C	2.94	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C4B-CHC	2.95	1.48	1.39
24	c	908	CLA	C1B-CHB	2.95	1.48	1.39
24	b	609	CLA	CHD-C4C	2.95	1.48	1.41
24	c	903	CLA	C4B-CHC	2.95	1.48	1.39
24	B	608	CLA	CHD-C4C	2.95	1.48	1.41
24	c	907	CLA	C1B-CHB	2.95	1.48	1.39
24	b	608	CLA	C4B-CHC	2.96	1.48	1.39
24	C	509	CLA	C1B-CHB	2.96	1.48	1.39
25	A	409	PHO	CHD-C4C	2.96	1.47	1.40
24	B	612	CLA	C1B-CHB	2.96	1.48	1.39
24	c	906	CLA	C1B-CHB	2.96	1.48	1.39
24	c	912	CLA	C1B-CHB	2.96	1.48	1.39
24	a	407	CLA	C4B-CHC	2.96	1.48	1.39
24	B	612	CLA	CHD-C4C	2.97	1.48	1.41
24	c	910	CLA	C4B-CHC	2.97	1.48	1.39
24	C	506	CLA	C4B-CHC	2.97	1.48	1.39
24	b	609	CLA	C1B-CHB	2.97	1.48	1.39
24	b	606	CLA	C1B-CHB	2.97	1.48	1.39
24	b	614	CLA	C1B-CHB	2.98	1.48	1.39
24	B	615	CLA	CHD-C4C	2.98	1.48	1.41
24	b	608	CLA	C4C-C3C	2.98	1.50	1.45
24	B	609	CLA	CHD-C4C	2.98	1.48	1.41
24	C	505	CLA	CHD-C4C	2.98	1.48	1.41
24	c	910	CLA	CHD-C4C	2.99	1.48	1.41
24	d	403	CLA	C1B-CHB	2.99	1.48	1.39
24	C	511	CLA	CHD-C4C	2.99	1.48	1.41
24	c	908	CLA	CHD-C4C	2.99	1.48	1.41
24	A	410	CLA	C4B-CHC	2.99	1.48	1.39
24	c	903	CLA	C1B-CHB	2.99	1.48	1.39
24	B	611	CLA	CHD-C4C	2.99	1.48	1.41
24	C	509	CLA	CHD-C4C	3.00	1.48	1.41
25	A	409	PHO	C3B-C4B	3.00	1.50	1.43
24	c	911	CLA	C4B-CHC	3.00	1.48	1.39
24	B	617	CLA	C1B-CHB	3.00	1.48	1.39
24	B	610	CLA	C1B-CHB	3.00	1.48	1.39
24	b	620	CLA	C1B-CHB	3.01	1.48	1.39
24	c	904	CLA	CHD-C4C	3.01	1.48	1.41
24	C	510	CLA	C1B-CHB	3.01	1.48	1.39
24	b	613	CLA	C4B-CHC	3.01	1.48	1.39
24	b	618	CLA	CHD-C4C	3.02	1.48	1.41
24	A	406	CLA	CHD-C4C	3.02	1.48	1.41
24	b	613	CLA	C1B-CHB	3.03	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	410	CLA	CHD-C4C	3.03	1.48	1.41
24	B	606	CLA	C1B-CHB	3.03	1.48	1.39
24	A	405	CLA	C1B-CHB	3.03	1.48	1.39
24	c	912	CLA	CHD-C4C	3.04	1.48	1.41
25	a	408	PHO	CHC-C4B	3.04	1.48	1.40
24	b	608	CLA	CHD-C4C	3.05	1.48	1.41
37	D	406	LHG	O7-C7	3.05	1.43	1.34
24	a	407	CLA	CHD-C4C	3.06	1.48	1.41
24	B	612	CLA	C4B-CHC	3.06	1.48	1.39
24	c	907	CLA	CHD-C4C	3.06	1.48	1.41
24	C	503	CLA	C1B-CHB	3.06	1.48	1.39
24	C	504	CLA	CHD-C4C	3.07	1.48	1.41
24	C	503	CLA	CHD-C4C	3.07	1.48	1.41
24	b	616	CLA	C1B-CHB	3.07	1.48	1.39
24	C	507	CLA	CHD-C4C	3.07	1.48	1.41
24	C	508	CLA	CHD-C4C	3.07	1.48	1.41
24	C	512	CLA	C1B-CHB	3.08	1.48	1.39
24	b	614	CLA	CHD-C4C	3.08	1.48	1.41
24	C	512	CLA	CHD-C4C	3.09	1.48	1.41
24	b	607	CLA	CHD-C4C	3.10	1.48	1.41
24	A	407	CLA	C4B-CHC	3.12	1.48	1.39
24	B	605	CLA	C1B-CHB	3.13	1.48	1.39
24	C	511	CLA	C1B-CHB	3.13	1.48	1.39
24	C	505	CLA	C1B-CHB	3.16	1.48	1.39
24	d	402	CLA	OBD-CAD	3.16	1.27	1.22
24	B	602	CLA	CHD-C4C	3.16	1.48	1.41
24	b	612	CLA	C4B-CHC	3.17	1.48	1.39
24	D	401	CLA	C1B-CHB	3.18	1.48	1.39
24	b	605	CLA	CHD-C4C	3.19	1.48	1.41
24	C	507	CLA	C1B-CHB	3.20	1.48	1.39
24	A	407	CLA	CHD-C4C	3.21	1.48	1.41
24	B	611	CLA	C1B-CHB	3.22	1.48	1.39
24	a	406	CLA	CHD-C4C	3.23	1.48	1.41
24	c	902	CLA	C1B-CHB	3.23	1.48	1.39
25	A	409	PHO	CHC-C4B	3.23	1.48	1.40
24	B	605	CLA	C3D-C2D	3.25	1.47	1.40
24	B	615	CLA	C1B-CHB	3.26	1.48	1.39
24	b	615	CLA	C1B-CHB	3.26	1.48	1.39
24	B	616	CLA	OBD-CAD	3.26	1.27	1.22
24	C	511	CLA	C4B-CHC	3.27	1.48	1.39
25	a	408	PHO	CHD-C4C	3.28	1.48	1.40
24	b	618	CLA	C1B-CHB	3.30	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	914	CLA	CHD-C4C	3.31	1.49	1.41
38	e	102	HEM	FE-NC	3.31	2.08	1.95
25	A	408	PHO	C3D-C2D	3.32	1.47	1.38
38	E	103	HEM	FE-NC	3.33	2.08	1.95
24	B	611	CLA	OBD-CAD	3.34	1.27	1.22
25	A	408	PHO	CHC-C4B	3.34	1.48	1.40
24	c	906	CLA	C3D-C2D	3.37	1.48	1.40
25	a	420	PHO	CHC-C4B	3.38	1.48	1.40
24	c	911	CLA	C1B-CHB	3.39	1.49	1.39
37	D	407	LHG	O8-C23	3.40	1.43	1.33
24	C	506	CLA	C3D-C2D	3.44	1.48	1.40
37	d	407	LHG	O7-C7	3.44	1.44	1.34
38	V	201	HEM	FE-NC	3.45	2.09	1.95
24	a	406	CLA	C1B-CHB	3.46	1.49	1.39
24	B	605	CLA	OBD-CAD	3.46	1.27	1.22
25	a	408	PHO	C3D-C2D	3.46	1.48	1.38
24	A	406	CLA	OBD-CAD	3.48	1.27	1.22
38	v	202	HEM	FE-NC	3.48	2.09	1.95
37	D	408	LHG	O8-C23	3.49	1.43	1.33
37	d	408	LHG	O8-C23	3.49	1.43	1.33
24	a	406	CLA	O2A-CGA	3.49	1.43	1.33
27	a	411	SQD	O47-C7	3.52	1.44	1.34
24	b	607	CLA	C3D-C2D	3.53	1.48	1.40
24	b	616	CLA	C3D-C2D	3.53	1.48	1.40
34	b	624	LMG	O7-C10	3.54	1.44	1.34
36	C	518	DGD	O2G-C1B	3.54	1.44	1.34
24	b	618	CLA	C3D-C2D	3.56	1.48	1.40
24	B	608	CLA	C3D-C2D	3.56	1.48	1.40
36	c	916	DGD	O2G-C1B	3.56	1.44	1.34
24	d	402	CLA	CHC-C1C	3.59	1.46	1.35
37	L	101	LHG	O7-C7	3.59	1.45	1.34
25	A	409	PHO	CHB-C4A	3.59	1.47	1.40
24	C	511	CLA	OBD-CAD	3.59	1.27	1.22
24	b	611	CLA	C3D-C2D	3.60	1.48	1.40
34	J	101	LMG	O7-C10	3.60	1.45	1.34
24	b	609	CLA	C3D-C2D	3.61	1.48	1.40
36	C	517	DGD	O2G-C1B	3.61	1.45	1.34
37	D	407	LHG	O7-C7	3.61	1.45	1.34
24	A	406	CLA	O2A-CGA	3.62	1.44	1.33
24	A	406	CLA	CHC-C1C	3.62	1.46	1.35
27	A	412	SQD	O47-C7	3.62	1.45	1.34
36	c	918	DGD	O2G-C1B	3.62	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	O2A-CGA	3.62	1.44	1.33
24	b	613	CLA	O2A-CGA	3.63	1.44	1.33
36	C	519	DGD	O2G-C1B	3.63	1.45	1.34
34	j	101	LMG	O7-C10	3.63	1.45	1.34
24	B	606	CLA	CHC-C1C	3.64	1.46	1.35
24	A	405	CLA	OBD-CAD	3.64	1.27	1.22
25	a	408	PHO	CHB-C4A	3.64	1.47	1.40
25	A	409	PHO	OBD-CAD	3.64	1.29	1.22
24	b	607	CLA	OBD-CAD	3.65	1.27	1.22
24	B	607	CLA	C3D-C2D	3.65	1.48	1.40
37	d	408	LHG	O7-C7	3.66	1.45	1.34
36	c	917	DGD	O2G-C1B	3.67	1.45	1.34
24	B	609	CLA	CHC-C1C	3.67	1.46	1.35
24	c	907	CLA	CHC-C1C	3.68	1.46	1.35
24	B	607	CLA	CHC-C1C	3.69	1.46	1.35
24	C	511	CLA	O2A-CGA	3.69	1.44	1.33
24	b	608	CLA	C3D-C2D	3.69	1.49	1.40
36	C	517	DGD	O1G-C1A	3.70	1.44	1.33
24	c	902	CLA	OBD-CAD	3.70	1.28	1.22
24	c	914	CLA	C3D-C2D	3.71	1.49	1.40
25	A	409	PHO	O2A-CGA	3.71	1.44	1.33
34	c	919	LMG	O7-C10	3.72	1.45	1.34
24	B	614	CLA	O2A-CGA	3.72	1.44	1.33
37	d	409	LHG	O7-C7	3.72	1.45	1.34
36	H	102	DGD	O2G-C1B	3.72	1.45	1.34
24	b	613	CLA	C3D-C2D	3.72	1.49	1.40
24	C	503	CLA	OBD-CAD	3.73	1.28	1.22
24	C	512	CLA	C3D-C2D	3.73	1.49	1.40
24	B	613	CLA	O2A-CGA	3.73	1.44	1.33
34	a	412	LMG	O7-C10	3.73	1.45	1.34
24	b	619	CLA	CHC-C1C	3.73	1.47	1.35
24	d	402	CLA	C3D-C2D	3.73	1.49	1.40
34	J	101	LMG	O8-C28	3.73	1.44	1.33
24	D	402	CLA	C3D-C2D	3.74	1.49	1.40
24	A	407	CLA	O2A-CGA	3.74	1.44	1.33
36	h	102	DGD	O1G-C1A	3.75	1.44	1.33
24	C	509	CLA	O2A-CGA	3.75	1.44	1.33
24	b	608	CLA	OBD-CAD	3.75	1.28	1.22
34	C	520	LMG	O7-C10	3.75	1.45	1.34
24	B	605	CLA	O2A-CGA	3.75	1.44	1.33
25	A	408	PHO	OBD-CAD	3.75	1.29	1.22
24	b	617	CLA	O2A-CGA	3.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	CHC-C1C	3.76	1.47	1.35
34	B	622	LMG	O7-C10	3.76	1.45	1.34
24	c	909	CLA	CHC-C1C	3.76	1.47	1.35
24	C	503	CLA	O2A-CGA	3.76	1.44	1.33
37	l	101	LHG	O8-C23	3.76	1.44	1.33
24	C	509	CLA	CHC-C1C	3.76	1.47	1.35
36	c	916	DGD	O1G-C1A	3.77	1.44	1.33
37	D	406	LHG	O8-C23	3.77	1.44	1.33
24	B	615	CLA	C3D-C2D	3.77	1.49	1.40
25	a	420	PHO	C3D-C2D	3.77	1.49	1.38
34	j	101	LMG	O8-C28	3.78	1.44	1.33
36	C	518	DGD	O1G-C1A	3.78	1.44	1.33
24	a	406	CLA	CHC-C1C	3.78	1.47	1.35
24	C	509	CLA	OBD-CAD	3.78	1.28	1.22
27	a	402	SQD	O47-C7	3.78	1.45	1.34
24	C	502	CLA	CHC-C1C	3.78	1.47	1.35
24	b	615	CLA	CHC-C1C	3.78	1.47	1.35
24	B	611	CLA	CHC-C1C	3.78	1.47	1.35
24	C	510	CLA	OBD-CAD	3.78	1.28	1.22
24	c	904	CLA	OBD-CAD	3.79	1.28	1.22
37	L	101	LHG	O8-C23	3.79	1.44	1.33
34	z	101	LMG	O7-C10	3.79	1.45	1.34
36	C	519	DGD	O1G-C1A	3.79	1.44	1.33
37	E	101	LHG	O7-C7	3.79	1.45	1.34
24	b	608	CLA	O2A-CGA	3.80	1.44	1.33
24	b	620	CLA	OBD-CAD	3.80	1.28	1.22
24	C	506	CLA	O2A-CGA	3.80	1.44	1.33
24	d	401	CLA	CHC-C1C	3.80	1.47	1.35
36	H	102	DGD	O1G-C1A	3.80	1.44	1.33
27	B	621	SQD	O48-C23	3.81	1.44	1.33
24	C	510	CLA	CHC-C1C	3.81	1.47	1.35
24	c	911	CLA	C3D-C2D	3.81	1.49	1.40
24	B	604	CLA	C3D-C2D	3.83	1.49	1.40
24	C	504	CLA	CHC-C1C	3.83	1.47	1.35
24	B	614	CLA	OBD-CAD	3.83	1.28	1.22
24	C	504	CLA	O2A-CGA	3.84	1.44	1.33
24	b	614	CLA	C3D-C2D	3.84	1.49	1.40
24	c	911	CLA	O2A-CGA	3.84	1.44	1.33
37	D	408	LHG	O7-C7	3.84	1.45	1.34
24	c	906	CLA	CHC-C1C	3.84	1.47	1.35
24	c	904	CLA	C3D-C2D	3.84	1.49	1.40
24	C	507	CLA	CHC-C1C	3.85	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	O2A-CGA	3.85	1.44	1.33
24	b	612	CLA	C3D-C2D	3.85	1.49	1.40
24	B	617	CLA	CHC-C1C	3.85	1.47	1.35
24	C	514	CLA	OBD-CAD	3.85	1.28	1.22
24	B	608	CLA	CHC-C1C	3.85	1.47	1.35
24	C	503	CLA	CHC-C1C	3.86	1.47	1.35
24	B	605	CLA	CHC-C1C	3.86	1.47	1.35
24	c	902	CLA	CHC-C1C	3.86	1.47	1.35
24	c	913	CLA	OBD-CAD	3.86	1.28	1.22
37	e	101	LHG	O7-C7	3.86	1.45	1.34
24	c	902	CLA	C3D-C2D	3.86	1.49	1.40
24	b	614	CLA	O2A-CGA	3.86	1.45	1.33
37	l	101	LHG	O7-C7	3.87	1.45	1.34
24	B	603	CLA	C3D-C2D	3.87	1.49	1.40
24	c	913	CLA	C3D-C2D	3.87	1.49	1.40
24	C	511	CLA	CHC-C1C	3.87	1.47	1.35
24	c	908	CLA	C3D-C2D	3.88	1.49	1.40
24	a	409	CLA	CHC-C1C	3.88	1.47	1.35
24	a	407	CLA	C3D-C2D	3.88	1.49	1.40
24	a	409	CLA	O2A-CGA	3.88	1.45	1.33
24	C	502	CLA	C3D-C2D	3.88	1.49	1.40
24	C	505	CLA	C3D-C2D	3.88	1.49	1.40
24	c	908	CLA	CHC-C1C	3.88	1.47	1.35
36	c	917	DGD	O1G-C1A	3.88	1.45	1.33
36	c	918	DGD	O1G-C1A	3.88	1.45	1.33
24	b	606	CLA	C3D-C2D	3.88	1.49	1.40
24	C	512	CLA	CHC-C1C	3.88	1.47	1.35
24	c	912	CLA	C3D-C2D	3.89	1.49	1.40
24	C	504	CLA	C3D-C2D	3.89	1.49	1.40
24	a	406	CLA	C3D-C2D	3.89	1.49	1.40
24	A	410	CLA	CHC-C1C	3.89	1.47	1.35
24	B	617	CLA	C3D-C2D	3.89	1.49	1.40
24	b	615	CLA	O2A-CGA	3.90	1.45	1.33
24	c	907	CLA	O2A-CGA	3.90	1.45	1.33
24	B	615	CLA	CHC-C1C	3.90	1.47	1.35
24	C	514	CLA	CHC-C1C	3.90	1.47	1.35
24	b	615	CLA	C3D-C2D	3.91	1.49	1.40
24	c	907	CLA	OBD-CAD	3.91	1.28	1.22
24	C	513	CLA	OBD-CAD	3.91	1.28	1.22
24	d	403	CLA	CHC-C1C	3.92	1.47	1.35
24	B	603	CLA	OBD-CAD	3.92	1.28	1.22
24	b	617	CLA	C3D-C2D	3.92	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	CHC-C1C	3.92	1.47	1.35
24	b	610	CLA	C3D-C2D	3.93	1.49	1.40
24	B	611	CLA	O2A-CGA	3.93	1.45	1.33
24	D	402	CLA	OBD-CAD	3.93	1.28	1.22
24	c	905	CLA	CHC-C1C	3.93	1.47	1.35
24	d	403	CLA	O2A-CGA	3.93	1.45	1.33
24	b	620	CLA	CHC-C1C	3.93	1.47	1.35
24	B	616	CLA	CHC-C1C	3.93	1.47	1.35
24	d	401	CLA	O2A-CGA	3.94	1.45	1.33
24	B	604	CLA	O2A-CGA	3.94	1.45	1.33
37	d	407	LHG	O8-C23	3.94	1.45	1.33
24	A	405	CLA	C3D-C2D	3.94	1.49	1.40
25	A	409	PHO	C3D-C2D	3.94	1.49	1.38
34	c	920	LMG	O7-C10	3.94	1.46	1.34
24	b	610	CLA	CHC-C1C	3.94	1.47	1.35
25	A	408	PHO	CHB-C4A	3.94	1.47	1.40
24	d	403	CLA	C3D-C2D	3.95	1.49	1.40
24	c	905	CLA	O2A-CGA	3.95	1.45	1.33
24	C	514	CLA	C3D-C2D	3.95	1.49	1.40
24	D	401	CLA	OBD-CAD	3.95	1.28	1.22
24	C	506	CLA	CHC-C1C	3.96	1.47	1.35
24	A	407	CLA	C3D-C2D	3.96	1.49	1.40
24	B	614	CLA	C3D-C2D	3.96	1.49	1.40
24	C	508	CLA	C3D-C2D	3.96	1.49	1.40
24	b	610	CLA	OBD-CAD	3.96	1.28	1.22
24	c	904	CLA	O2A-CGA	3.96	1.45	1.33
24	B	612	CLA	C3D-C2D	3.96	1.49	1.40
24	D	401	CLA	C3D-C2D	3.96	1.49	1.40
24	C	508	CLA	CHC-C1C	3.97	1.47	1.35
24	b	617	CLA	CHC-C1C	3.97	1.47	1.35
24	c	903	CLA	O2A-CGA	3.97	1.45	1.33
24	B	616	CLA	O2A-CGA	3.97	1.45	1.33
24	b	614	CLA	CHC-C1C	3.97	1.47	1.35
36	h	102	DGD	O2G-C1B	3.97	1.46	1.34
24	b	615	CLA	OBD-CAD	3.97	1.28	1.22
27	L	102	SQD	O48-C23	3.97	1.45	1.33
24	C	507	CLA	OBD-CAD	3.98	1.28	1.22
24	c	903	CLA	C3D-C2D	3.99	1.49	1.40
24	B	612	CLA	O2A-CGA	3.99	1.45	1.33
24	B	608	CLA	O2A-CGA	3.99	1.45	1.33
27	L	102	SQD	O47-C7	3.99	1.46	1.34
24	B	612	CLA	CHC-C1C	4.00	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	620	CLA	C3D-C2D	4.00	1.49	1.40
24	C	507	CLA	C3D-C2D	4.00	1.49	1.40
24	A	405	CLA	O2A-CGA	4.00	1.45	1.33
24	b	617	CLA	OBD-CAD	4.01	1.28	1.22
24	b	609	CLA	CHC-C1C	4.01	1.47	1.35
34	a	412	LMG	O8-C28	4.01	1.45	1.33
27	A	416	SQD	O47-C7	4.02	1.46	1.34
24	b	605	CLA	CHC-C1C	4.02	1.47	1.35
24	D	401	CLA	O2A-CGA	4.02	1.45	1.33
24	B	611	CLA	C3D-C2D	4.02	1.49	1.40
24	B	606	CLA	C3D-C2D	4.02	1.49	1.40
24	c	902	CLA	O2A-CGA	4.02	1.45	1.33
24	c	907	CLA	C3D-C2D	4.02	1.49	1.40
24	c	912	CLA	CHC-C1C	4.02	1.47	1.35
24	B	617	CLA	O2A-CGA	4.02	1.45	1.33
34	Z	101	LMG	O7-C10	4.03	1.46	1.34
24	C	513	CLA	C3D-C2D	4.03	1.49	1.40
24	B	610	CLA	C3D-C2D	4.03	1.49	1.40
24	B	602	CLA	CHC-C1C	4.03	1.48	1.35
24	b	618	CLA	OBD-CAD	4.03	1.28	1.22
24	B	613	CLA	CHC-C1C	4.03	1.48	1.35
24	b	605	CLA	OBD-CAD	4.03	1.28	1.22
24	b	616	CLA	O2A-CGA	4.04	1.45	1.33
24	C	504	CLA	OBD-CAD	4.04	1.28	1.22
24	c	910	CLA	CHC-C1C	4.04	1.48	1.35
24	b	608	CLA	CHC-C1C	4.04	1.48	1.35
24	b	606	CLA	OBD-CAD	4.04	1.28	1.22
24	C	514	CLA	O2A-CGA	4.04	1.45	1.33
24	B	604	CLA	OBD-CAD	4.04	1.28	1.22
24	c	912	CLA	O2A-CGA	4.04	1.45	1.33
34	C	501	LMG	O7-C10	4.05	1.46	1.34
24	B	603	CLA	CHC-C1C	4.05	1.48	1.35
24	B	610	CLA	CHC-C1C	4.05	1.48	1.35
24	a	407	CLA	OBD-CAD	4.06	1.28	1.22
24	c	908	CLA	OBD-CAD	4.06	1.28	1.22
24	B	602	CLA	OBD-CAD	4.06	1.28	1.22
24	c	910	CLA	C3D-C2D	4.06	1.49	1.40
36	d	406	DGD	O2G-C1B	4.06	1.46	1.34
34	C	521	LMG	O7-C10	4.06	1.46	1.34
24	b	607	CLA	CHC-C1C	4.07	1.48	1.35
27	f	102	SQD	O48-C23	4.07	1.45	1.33
36	D	405	DGD	O2G-C1B	4.07	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	CLA	O2A-CGA	4.08	1.45	1.33
24	c	913	CLA	O2A-CGA	4.08	1.45	1.33
24	B	604	CLA	CHC-C1C	4.08	1.48	1.35
24	C	507	CLA	O2A-CGA	4.08	1.45	1.33
27	a	411	SQD	O48-C23	4.08	1.45	1.33
24	B	603	CLA	O2A-CGA	4.08	1.45	1.33
25	a	420	PHO	O2A-CGA	4.08	1.45	1.33
27	F	101	SQD	O48-C23	4.08	1.45	1.33
24	b	620	CLA	O2A-CGA	4.08	1.45	1.33
24	C	512	CLA	O2A-CGA	4.08	1.45	1.33
24	b	618	CLA	O2A-CGA	4.09	1.45	1.33
24	b	612	CLA	CHC-C1C	4.10	1.48	1.35
24	d	403	CLA	OBD-CAD	4.10	1.28	1.22
27	A	416	SQD	O48-C23	4.10	1.45	1.33
24	C	505	CLA	CHC-C1C	4.10	1.48	1.35
24	A	410	CLA	O2A-CGA	4.11	1.45	1.33
24	c	910	CLA	O2A-CGA	4.11	1.45	1.33
24	B	614	CLA	CHC-C1C	4.11	1.48	1.35
34	B	622	LMG	O8-C28	4.11	1.45	1.33
27	A	412	SQD	O48-C23	4.11	1.45	1.33
37	e	101	LHG	O8-C23	4.11	1.45	1.33
24	b	616	CLA	OBD-CAD	4.11	1.28	1.22
24	b	612	CLA	OBD-CAD	4.11	1.28	1.22
24	b	613	CLA	CHC-C1C	4.11	1.48	1.35
34	C	521	LMG	O8-C28	4.11	1.45	1.33
24	b	610	CLA	O2A-CGA	4.11	1.45	1.33
24	c	904	CLA	CHC-C1C	4.12	1.48	1.35
24	B	613	CLA	C3D-C2D	4.12	1.50	1.40
36	d	406	DGD	O1G-C1A	4.12	1.45	1.33
24	c	914	CLA	OBD-CAD	4.12	1.28	1.22
25	a	408	PHO	O2A-CGA	4.12	1.45	1.33
24	B	609	CLA	O2A-CGA	4.12	1.45	1.33
24	c	906	CLA	O2A-CGA	4.12	1.45	1.33
24	b	612	CLA	O2A-CGA	4.13	1.45	1.33
24	B	606	CLA	O2A-CGA	4.13	1.45	1.33
24	C	508	CLA	O2A-CGA	4.13	1.45	1.33
24	D	401	CLA	O2D-CGD	4.13	1.43	1.33
24	a	409	CLA	C3D-C2D	4.13	1.50	1.40
24	D	402	CLA	CHC-C1C	4.13	1.48	1.35
24	D	402	CLA	O2A-CGA	4.14	1.45	1.33
24	b	616	CLA	CHC-C1C	4.14	1.48	1.35
24	b	605	CLA	O2A-CGA	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	CLA	C3D-C2D	4.14	1.50	1.40
24	c	909	CLA	O2A-CGA	4.14	1.45	1.33
24	c	913	CLA	CHC-C1C	4.14	1.48	1.35
24	A	405	CLA	CHC-C1C	4.15	1.48	1.35
24	c	903	CLA	CHC-C1C	4.15	1.48	1.35
24	A	410	CLA	C3D-C2D	4.15	1.50	1.40
34	c	920	LMG	O8-C28	4.15	1.45	1.33
24	b	613	CLA	OBD-CAD	4.15	1.28	1.22
24	c	905	CLA	C3D-C2D	4.16	1.50	1.40
24	C	508	CLA	OBD-CAD	4.16	1.28	1.22
24	c	904	CLA	O2D-CGD	4.16	1.43	1.33
24	B	616	CLA	C3D-C2D	4.16	1.50	1.40
24	C	502	CLA	O2A-CGA	4.16	1.45	1.33
24	C	511	CLA	C3D-C2D	4.16	1.50	1.40
24	c	909	CLA	C3D-C2D	4.16	1.50	1.40
34	C	501	LMG	O8-C28	4.16	1.45	1.33
34	b	624	LMG	O8-C28	4.16	1.45	1.33
24	c	914	CLA	O2A-CGA	4.17	1.45	1.33
24	C	508	CLA	O2D-CGD	4.17	1.43	1.33
24	B	612	CLA	OBD-CAD	4.17	1.28	1.22
24	c	911	CLA	CHC-C1C	4.17	1.48	1.35
24	b	619	CLA	O2A-CGA	4.17	1.45	1.33
24	C	510	CLA	C3D-C2D	4.18	1.50	1.40
37	d	409	LHG	O8-C23	4.18	1.45	1.33
24	b	618	CLA	CHC-C1C	4.18	1.48	1.35
24	B	610	CLA	O2A-CGA	4.18	1.45	1.33
24	B	602	CLA	C3D-C2D	4.19	1.50	1.40
24	c	909	CLA	OBD-CAD	4.19	1.28	1.22
24	C	513	CLA	CHC-C1C	4.19	1.48	1.35
24	b	611	CLA	CHC-C1C	4.19	1.48	1.35
24	C	513	CLA	O2A-CGA	4.20	1.46	1.33
24	c	910	CLA	OBD-CAD	4.20	1.28	1.22
27	F	101	SQD	O47-C7	4.21	1.46	1.34
24	B	607	CLA	O2A-CGA	4.21	1.46	1.33
24	d	402	CLA	O2D-CGD	4.21	1.43	1.33
24	c	914	CLA	CHC-C1C	4.21	1.48	1.35
24	c	911	CLA	OBD-CAD	4.22	1.28	1.22
27	f	102	SQD	O47-C7	4.22	1.46	1.34
25	a	408	PHO	CHD-C1D	4.22	1.46	1.38
24	b	605	CLA	C3D-C2D	4.22	1.50	1.40
24	B	610	CLA	OBD-CAD	4.24	1.28	1.22
24	c	912	CLA	OBD-CAD	4.25	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	906	CLA	OBD-CAD	4.26	1.28	1.22
24	C	505	CLA	O2D-CGD	4.26	1.44	1.33
27	B	621	SQD	O47-C7	4.26	1.47	1.34
24	C	502	CLA	OBD-CAD	4.26	1.28	1.22
24	a	407	CLA	CHC-C1C	4.26	1.48	1.35
24	a	406	CLA	OBD-CAD	4.27	1.28	1.22
25	a	408	PHO	O2D-CGD	4.28	1.44	1.33
24	b	614	CLA	OBD-CAD	4.28	1.28	1.22
24	d	402	CLA	O2A-CGA	4.28	1.46	1.33
24	A	407	CLA	CHC-C1C	4.29	1.48	1.35
24	B	615	CLA	OBD-CAD	4.29	1.28	1.22
24	b	609	CLA	O2A-CGA	4.30	1.46	1.33
24	C	503	CLA	C3D-C2D	4.31	1.50	1.40
25	A	409	PHO	CHD-C1D	4.31	1.47	1.38
24	b	607	CLA	O2A-CGA	4.32	1.46	1.33
34	C	520	LMG	O8-C28	4.32	1.46	1.33
24	B	605	CLA	O2D-CGD	4.33	1.44	1.33
24	B	602	CLA	O2A-CGA	4.33	1.46	1.33
24	a	407	CLA	O2D-CGD	4.34	1.44	1.33
24	B	610	CLA	O2D-CGD	4.34	1.44	1.33
24	a	409	CLA	OBD-CAD	4.34	1.29	1.22
24	A	405	CLA	O2D-CGD	4.34	1.44	1.33
24	A	407	CLA	OBD-CAD	4.35	1.29	1.22
24	B	606	CLA	OBD-CAD	4.36	1.29	1.22
34	c	919	LMG	O8-C28	4.36	1.46	1.33
25	a	420	PHO	CHB-C4A	4.37	1.48	1.40
24	b	618	CLA	O2D-CGD	4.38	1.44	1.33
24	C	512	CLA	OBD-CAD	4.38	1.29	1.22
24	C	510	CLA	O2A-CGA	4.39	1.46	1.33
24	a	406	CLA	O2D-CGD	4.39	1.44	1.33
34	z	101	LMG	O8-C28	4.39	1.46	1.33
27	a	402	SQD	O48-C23	4.39	1.46	1.33
24	b	611	CLA	O2A-CGA	4.39	1.46	1.33
24	c	903	CLA	OBD-CAD	4.39	1.29	1.22
24	B	607	CLA	OBD-CAD	4.40	1.29	1.22
24	B	615	CLA	O2A-CGA	4.40	1.46	1.33
24	B	609	CLA	C3D-C2D	4.40	1.50	1.40
24	b	619	CLA	OBD-CAD	4.40	1.29	1.22
24	B	613	CLA	OBD-CAD	4.41	1.29	1.22
24	c	902	CLA	O2D-CGD	4.41	1.44	1.33
24	A	406	CLA	C3D-C2D	4.42	1.50	1.40
24	b	609	CLA	OBD-CAD	4.42	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	O2D-CGD	4.43	1.44	1.33
24	d	401	CLA	OBD-CAD	4.43	1.29	1.22
24	C	504	CLA	O2D-CGD	4.43	1.44	1.33
24	b	611	CLA	O2D-CGD	4.43	1.44	1.33
24	C	511	CLA	O2D-CGD	4.44	1.44	1.33
24	B	611	CLA	O2D-CGD	4.44	1.44	1.33
24	C	505	CLA	O2A-CGA	4.45	1.46	1.33
24	d	401	CLA	O2D-CGD	4.45	1.44	1.33
36	D	405	DGD	O1G-C1A	4.46	1.46	1.33
24	c	908	CLA	O2A-CGA	4.47	1.46	1.33
37	E	101	LHG	O8-C23	4.48	1.46	1.33
24	B	617	CLA	O2D-CGD	4.48	1.44	1.33
24	c	905	CLA	OBD-CAD	4.48	1.29	1.22
25	A	409	PHO	O2D-CGD	4.48	1.44	1.33
24	B	617	CLA	OBD-CAD	4.49	1.29	1.22
24	c	903	CLA	O2D-CGD	4.50	1.44	1.33
24	b	610	CLA	O2D-CGD	4.50	1.44	1.33
24	b	619	CLA	C3D-C2D	4.51	1.51	1.40
24	C	507	CLA	O2D-CGD	4.51	1.44	1.33
24	b	611	CLA	OBD-CAD	4.52	1.29	1.22
24	B	609	CLA	OBD-CAD	4.52	1.29	1.22
25	a	420	PHO	CHD-C1D	4.53	1.47	1.38
24	A	410	CLA	OBD-CAD	4.53	1.29	1.22
24	b	614	CLA	O2D-CGD	4.55	1.44	1.33
24	A	406	CLA	O2D-CGD	4.56	1.44	1.33
24	c	908	CLA	O2D-CGD	4.57	1.44	1.33
24	B	604	CLA	O2D-CGD	4.58	1.44	1.33
24	B	614	CLA	O2D-CGD	4.58	1.44	1.33
24	C	509	CLA	C3D-C2D	4.59	1.51	1.40
24	B	609	CLA	O2D-CGD	4.59	1.44	1.33
24	b	613	CLA	C3C-C2C	4.59	1.46	1.36
24	c	911	CLA	O2D-CGD	4.61	1.45	1.33
24	c	912	CLA	O2D-CGD	4.61	1.45	1.33
24	C	502	CLA	O2D-CGD	4.61	1.45	1.33
24	b	612	CLA	O2D-CGD	4.62	1.45	1.33
24	C	514	CLA	O2D-CGD	4.62	1.45	1.33
24	b	609	CLA	O2D-CGD	4.63	1.45	1.33
24	c	913	CLA	O2D-CGD	4.63	1.45	1.33
24	c	914	CLA	O2D-CGD	4.64	1.45	1.33
24	b	619	CLA	O2D-CGD	4.65	1.45	1.33
24	b	608	CLA	O2D-CGD	4.65	1.45	1.33
25	A	408	PHO	CHD-C1D	4.66	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	O2D-CGD	4.66	1.45	1.33
25	A	408	PHO	O2D-CGD	4.66	1.45	1.33
24	c	909	CLA	O2D-CGD	4.66	1.45	1.33
24	b	615	CLA	C3C-C2C	4.67	1.46	1.36
24	C	513	CLA	O2D-CGD	4.67	1.45	1.33
24	B	616	CLA	O2D-CGD	4.69	1.45	1.33
24	B	606	CLA	O2D-CGD	4.70	1.45	1.33
24	B	612	CLA	O2D-CGD	4.70	1.45	1.33
25	a	408	PHO	CHC-C1C	4.71	1.47	1.38
24	b	619	CLA	C3C-C2C	4.72	1.46	1.36
24	B	607	CLA	O2D-CGD	4.72	1.45	1.33
24	B	613	CLA	O2D-CGD	4.72	1.45	1.33
24	b	620	CLA	O2D-CGD	4.73	1.45	1.33
24	C	512	CLA	O2D-CGD	4.75	1.45	1.33
24	b	615	CLA	O2D-CGD	4.76	1.45	1.33
24	B	608	CLA	O2D-CGD	4.77	1.45	1.33
24	D	402	CLA	O2D-CGD	4.77	1.45	1.33
24	b	607	CLA	O2D-CGD	4.78	1.45	1.33
24	C	502	CLA	C3C-C2C	4.78	1.47	1.36
24	C	505	CLA	OBD-CAD	4.79	1.29	1.22
24	C	509	CLA	O2D-CGD	4.79	1.45	1.33
24	B	616	CLA	C3C-C2C	4.80	1.47	1.36
24	c	906	CLA	O2D-CGD	4.80	1.45	1.33
24	c	910	CLA	O2D-CGD	4.81	1.45	1.33
24	D	401	CLA	C3C-C2C	4.82	1.47	1.36
24	d	402	CLA	C3C-C2C	4.82	1.47	1.36
24	c	906	CLA	C3C-C2C	4.82	1.47	1.36
24	C	512	CLA	C3C-C2C	4.82	1.47	1.36
25	a	420	PHO	O2D-CGD	4.83	1.45	1.33
24	b	616	CLA	O2D-CGD	4.85	1.45	1.33
24	b	608	CLA	C3C-C2C	4.85	1.47	1.36
24	C	503	CLA	O2D-CGD	4.86	1.45	1.33
24	C	506	CLA	O2D-CGD	4.87	1.45	1.33
24	b	606	CLA	O2D-CGD	4.87	1.45	1.33
24	B	606	CLA	C3C-C2C	4.87	1.47	1.36
24	B	607	CLA	C3C-C2C	4.87	1.47	1.36
24	c	905	CLA	O2D-CGD	4.87	1.45	1.33
25	a	408	PHO	CHB-C1B	4.87	1.48	1.38
24	B	613	CLA	C3C-C2C	4.88	1.47	1.36
24	B	602	CLA	O2D-CGD	4.88	1.45	1.33
24	C	506	CLA	OBD-CAD	4.88	1.29	1.22
25	A	409	PHO	CHC-C1C	4.88	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	410	CLA	O2D-CGD	4.88	1.45	1.33
24	b	613	CLA	O2D-CGD	4.89	1.45	1.33
24	C	508	CLA	C3C-C2C	4.89	1.47	1.36
24	C	510	CLA	C3C-C2C	4.94	1.47	1.36
24	c	907	CLA	C3C-C2C	4.94	1.47	1.36
24	a	409	CLA	O2D-CGD	4.94	1.45	1.33
24	B	603	CLA	O2D-CGD	4.95	1.45	1.33
24	b	605	CLA	O2D-CGD	4.95	1.45	1.33
24	b	610	CLA	C3C-C2C	4.95	1.47	1.36
24	b	609	CLA	C3C-C2C	4.96	1.47	1.36
24	B	615	CLA	C3C-C2C	4.96	1.47	1.36
24	b	606	CLA	C3C-C2C	4.96	1.47	1.36
24	B	612	CLA	C3C-C2C	4.96	1.47	1.36
24	c	902	CLA	C3C-C2C	4.97	1.47	1.36
24	C	509	CLA	C3C-C2C	4.98	1.47	1.36
24	A	407	CLA	O2D-CGD	4.98	1.45	1.33
24	C	510	CLA	O2D-CGD	4.98	1.45	1.33
24	B	602	CLA	C3C-C2C	4.99	1.47	1.36
24	c	905	CLA	C3C-C2C	5.01	1.47	1.36
24	B	605	CLA	C3C-C2C	5.01	1.47	1.36
24	d	403	CLA	C3C-C2C	5.02	1.47	1.36
24	c	907	CLA	O2D-CGD	5.02	1.46	1.33
24	c	910	CLA	C3C-C2C	5.02	1.47	1.36
24	B	610	CLA	C3C-C2C	5.02	1.47	1.36
24	b	617	CLA	C3C-C2C	5.03	1.47	1.36
24	c	908	CLA	C3C-C2C	5.03	1.47	1.36
24	A	406	CLA	C3C-C2C	5.03	1.47	1.36
24	a	407	CLA	C3C-C2C	5.04	1.47	1.36
24	B	617	CLA	C3C-C2C	5.05	1.47	1.36
25	A	409	PHO	CHB-C1B	5.05	1.48	1.38
24	b	620	CLA	C3C-C2C	5.08	1.47	1.36
24	c	914	CLA	C3C-C2C	5.09	1.47	1.36
24	b	617	CLA	O2D-CGD	5.10	1.46	1.33
24	c	912	CLA	C3C-C2C	5.11	1.47	1.36
24	B	608	CLA	OBD-CAD	5.11	1.30	1.22
24	A	405	CLA	C3C-C2C	5.12	1.47	1.36
24	B	608	CLA	C3C-C2C	5.12	1.47	1.36
24	b	611	CLA	C3C-C2C	5.13	1.47	1.36
24	b	616	CLA	C3C-C2C	5.14	1.47	1.36
24	c	904	CLA	C3C-C2C	5.15	1.47	1.36
24	B	610	CLA	C3B-C2B	5.15	1.47	1.40
24	c	903	CLA	C3C-C2C	5.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C3C-C2C	5.19	1.47	1.36
25	a	408	PHO	C3C-C2C	5.20	1.48	1.36
24	C	505	CLA	C3C-C2C	5.20	1.48	1.36
24	C	503	CLA	C3C-C2C	5.22	1.48	1.36
24	a	409	CLA	C3C-C2C	5.23	1.48	1.36
24	A	410	CLA	C3C-C2C	5.24	1.48	1.36
24	c	911	CLA	C3C-C2C	5.24	1.48	1.36
24	c	909	CLA	C3C-C2C	5.26	1.48	1.36
24	c	913	CLA	C3C-C2C	5.26	1.48	1.36
24	a	406	CLA	C3C-C2C	5.28	1.48	1.36
25	A	408	PHO	CHC-C1C	5.29	1.49	1.38
24	b	607	CLA	C3C-C2C	5.30	1.48	1.36
25	A	408	PHO	CHB-C1B	5.30	1.49	1.38
24	C	514	CLA	C3C-C2C	5.30	1.48	1.36
24	C	506	CLA	C3C-C2C	5.31	1.48	1.36
24	d	401	CLA	C3C-C2C	5.32	1.48	1.36
24	B	614	CLA	C3C-C2C	5.34	1.48	1.36
24	B	604	CLA	C3C-C2C	5.35	1.48	1.36
24	b	614	CLA	C3C-C2C	5.35	1.48	1.36
25	a	420	PHO	CHC-C1C	5.36	1.49	1.38
24	C	513	CLA	C3C-C2C	5.36	1.48	1.36
24	C	511	CLA	C3C-C2C	5.38	1.48	1.36
24	B	609	CLA	C3C-C2C	5.38	1.48	1.36
25	a	420	PHO	C3C-C2C	5.41	1.48	1.36
24	D	402	CLA	C3C-C2C	5.41	1.48	1.36
24	b	612	CLA	C3C-C2C	5.41	1.48	1.36
24	C	507	CLA	C3C-C2C	5.42	1.48	1.36
24	c	903	CLA	C3B-C2B	5.43	1.47	1.40
24	b	618	CLA	C3C-C2C	5.44	1.48	1.36
24	c	906	CLA	C3B-C2B	5.45	1.47	1.40
24	C	504	CLA	C3C-C2C	5.46	1.48	1.36
24	B	602	CLA	C3B-C2B	5.56	1.47	1.40
24	A	407	CLA	C3C-C2C	5.56	1.48	1.36
24	A	407	CLA	C3B-C2B	5.61	1.47	1.40
24	b	605	CLA	C3C-C2C	5.62	1.48	1.36
25	a	408	PHO	C3B-C2B	5.62	1.48	1.36
25	A	409	PHO	C3C-C2C	5.63	1.48	1.36
24	a	409	CLA	C3B-C2B	5.64	1.47	1.40
24	b	613	CLA	C3B-C2B	5.66	1.47	1.40
24	B	611	CLA	C3C-C2C	5.67	1.49	1.36
24	D	402	CLA	C3B-C2B	5.69	1.47	1.40
24	b	616	CLA	C3B-C2B	5.76	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C3B-C2B	5.79	1.49	1.36
24	B	615	CLA	C3B-C2B	5.79	1.48	1.40
24	c	913	CLA	C3B-C2B	5.80	1.48	1.40
24	B	606	CLA	C3B-C2B	5.80	1.48	1.40
24	d	401	CLA	C3B-C2B	5.85	1.48	1.40
25	a	420	PHO	CHB-C1B	5.90	1.50	1.38
24	B	616	CLA	C3B-C2B	5.94	1.48	1.40
24	b	618	CLA	C3B-C2B	5.95	1.48	1.40
25	A	408	PHO	C3C-C2C	5.96	1.49	1.36
24	a	407	CLA	C3B-C2B	5.97	1.48	1.40
24	C	508	CLA	C3B-C2B	5.98	1.48	1.40
24	C	503	CLA	C3B-C2B	6.00	1.48	1.40
24	C	506	CLA	C3B-C2B	6.01	1.48	1.40
24	b	609	CLA	C3B-C2B	6.02	1.48	1.40
24	c	904	CLA	C3B-C2B	6.04	1.48	1.40
25	A	409	PHO	C3B-C2B	6.06	1.49	1.36
24	c	914	CLA	C3B-C2B	6.07	1.48	1.40
24	b	605	CLA	C3B-C2B	6.11	1.48	1.40
24	c	908	CLA	C3B-C2B	6.11	1.48	1.40
24	A	405	CLA	C3B-C2B	6.12	1.48	1.40
24	c	905	CLA	C3B-C2B	6.13	1.48	1.40
25	a	420	PHO	C3B-C2B	6.13	1.49	1.36
24	d	402	CLA	C3B-C2B	6.13	1.48	1.40
24	b	610	CLA	C3B-C2B	6.14	1.48	1.40
24	C	505	CLA	C3B-C2B	6.16	1.48	1.40
24	c	911	CLA	C3B-C2B	6.21	1.48	1.40
24	D	401	CLA	C3B-C2B	6.24	1.48	1.40
24	b	611	CLA	C3B-C2B	6.24	1.48	1.40
24	C	513	CLA	C3B-C2B	6.25	1.48	1.40
24	b	612	CLA	C3B-C2B	6.27	1.48	1.40
24	C	504	CLA	C3B-C2B	6.32	1.48	1.40
24	A	410	CLA	C3B-C2B	6.32	1.48	1.40
24	B	608	CLA	C3B-C2B	6.32	1.48	1.40
24	c	907	CLA	C3B-C2B	6.32	1.48	1.40
24	B	611	CLA	C3B-C2B	6.34	1.48	1.40
24	B	603	CLA	C3B-C2B	6.34	1.48	1.40
24	C	512	CLA	C3B-C2B	6.35	1.48	1.40
24	C	507	CLA	C3B-C2B	6.40	1.48	1.40
24	b	607	CLA	C3B-C2B	6.40	1.48	1.40
24	b	606	CLA	C3B-C2B	6.46	1.48	1.40
24	c	912	CLA	C3B-C2B	6.50	1.48	1.40
24	C	509	CLA	C3B-C2B	6.52	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	C3B-C2B	6.54	1.48	1.40
24	B	612	CLA	C3B-C2B	6.55	1.48	1.40
24	c	902	CLA	C3B-C2B	6.56	1.49	1.40
24	b	615	CLA	C3B-C2B	6.57	1.49	1.40
24	B	607	CLA	C3B-C2B	6.65	1.49	1.40
24	b	617	CLA	C3B-C2B	6.67	1.49	1.40
24	b	614	CLA	C3B-C2B	6.68	1.49	1.40
24	d	403	CLA	C3B-C2B	6.71	1.49	1.40
24	B	609	CLA	C3B-C2B	6.72	1.49	1.40
24	C	502	CLA	C3B-C2B	6.74	1.49	1.40
24	c	909	CLA	C3B-C2B	6.76	1.49	1.40
24	b	619	CLA	C3B-C2B	6.76	1.49	1.40
24	B	605	CLA	C3B-C2B	6.84	1.49	1.40
24	B	613	CLA	C3B-C2B	6.88	1.49	1.40
24	b	608	CLA	C3B-C2B	6.90	1.49	1.40
24	C	511	CLA	C3B-C2B	6.91	1.49	1.40
24	C	514	CLA	C3B-C2B	6.95	1.49	1.40
24	C	510	CLA	C3B-C2B	6.97	1.49	1.40
24	B	604	CLA	C3B-C2B	6.98	1.49	1.40
24	c	910	CLA	C3B-C2B	7.04	1.49	1.40
24	B	617	CLA	C3B-C2B	7.13	1.49	1.40
24	a	406	CLA	C3B-C2B	7.14	1.49	1.40
24	b	620	CLA	C3B-C2B	7.14	1.49	1.40
24	B	614	CLA	C3B-C2B	7.39	1.50	1.40

All (1989) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	CHD-C4C-C3C	-6.46	114.96	124.94
24	b	611	CLA	CHD-C4C-C3C	-6.41	115.04	124.94
24	C	513	CLA	CHD-C4C-C3C	-6.38	115.08	124.94
24	B	615	CLA	CHD-C4C-C3C	-6.35	115.12	124.94
24	B	617	CLA	CHD-C4C-C3C	-6.22	115.32	124.94
24	b	605	CLA	CHD-C4C-C3C	-6.15	115.43	124.94
24	b	615	CLA	CHD-C4C-C3C	-6.10	115.51	124.94
24	B	604	CLA	CHD-C4C-C3C	-6.08	115.55	124.94
24	B	605	CLA	CHD-C4C-C3C	-6.05	115.58	124.94
24	B	603	CLA	CHD-C4C-C3C	-6.05	115.59	124.94
24	b	606	CLA	CHD-C4C-C3C	-6.03	115.62	124.94
24	B	610	CLA	CHD-C4C-C3C	-5.99	115.68	124.94
24	b	618	CLA	CHD-C4C-C3C	-5.97	115.71	124.94
24	B	616	CLA	CHD-C4C-C3C	-5.94	115.76	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	CHD-C4C-C3C	-5.94	115.76	124.94
24	A	410	CLA	CHD-C4C-C3C	-5.87	115.87	124.94
24	A	406	CLA	CHD-C4C-C3C	-5.86	115.88	124.94
24	c	913	CLA	CHD-C4C-C3C	-5.81	115.95	124.94
24	C	508	CLA	CHD-C4C-C3C	-5.81	115.96	124.94
24	b	616	CLA	CHD-C4C-C3C	-5.78	116.00	124.94
24	c	903	CLA	CHD-C4C-C3C	-5.76	116.03	124.94
24	a	407	CLA	CHD-C4C-C3C	-5.75	116.05	124.94
24	b	613	CLA	CHD-C4C-C3C	-5.74	116.07	124.94
24	C	511	CLA	CHD-C4C-C3C	-5.72	116.10	124.94
24	b	617	CLA	CHD-C4C-C3C	-5.70	116.13	124.94
24	c	902	CLA	CHD-C4C-C3C	-5.68	116.15	124.94
24	d	403	CLA	CHD-C4C-C3C	-5.67	116.17	124.94
24	C	512	CLA	CHD-C4C-C3C	-5.67	116.17	124.94
24	c	911	CLA	CHD-C4C-C3C	-5.65	116.20	124.94
24	b	610	CLA	CHD-C4C-C3C	-5.64	116.22	124.94
24	C	504	CLA	CHD-C4C-C3C	-5.64	116.22	124.94
24	D	402	CLA	CHD-C4C-C3C	-5.63	116.23	124.94
24	c	912	CLA	CHD-C4C-C3C	-5.63	116.24	124.94
24	c	910	CLA	CHD-C4C-C3C	-5.61	116.27	124.94
24	A	407	CLA	CHD-C4C-C3C	-5.60	116.29	124.94
24	B	606	CLA	CHD-C4C-C3C	-5.59	116.30	124.94
24	b	620	CLA	CHD-C4C-C3C	-5.55	116.36	124.94
24	c	904	CLA	CHD-C4C-C3C	-5.53	116.39	124.94
24	B	612	CLA	CHD-C4C-C3C	-5.49	116.46	124.94
24	C	503	CLA	CHD-C4C-C3C	-5.49	116.46	124.94
24	c	908	CLA	CHD-C4C-C3C	-5.49	116.46	124.94
24	b	612	CLA	CHD-C4C-C3C	-5.48	116.46	124.94
24	B	602	CLA	CHD-C4C-C3C	-5.46	116.50	124.94
24	C	509	CLA	CHD-C4C-C3C	-5.46	116.50	124.94
24	A	405	CLA	CHD-C4C-C3C	-5.43	116.54	124.94
24	B	611	CLA	CHD-C4C-C3C	-5.40	116.59	124.94
24	c	914	CLA	CHD-C4C-C3C	-5.39	116.61	124.94
24	C	514	CLA	CHD-C4C-C3C	-5.38	116.62	124.94
24	c	905	CLA	CHD-C4C-C3C	-5.36	116.65	124.94
24	B	614	CLA	CHD-C4C-C3C	-5.35	116.67	124.94
26	K	102	BCR	C33-C5-C6	-5.34	119.36	124.61
24	b	614	CLA	CHD-C4C-C3C	-5.33	116.71	124.94
24	C	502	CLA	CHD-C4C-C3C	-5.32	116.72	124.94
24	C	506	CLA	CHD-C4C-C3C	-5.30	116.75	124.94
24	B	609	CLA	CHD-C4C-C3C	-5.29	116.77	124.94
24	B	613	CLA	CHD-C4C-C3C	-5.29	116.77	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	906	CLA	CHD-C4C-C3C	-5.28	116.79	124.94
24	c	909	CLA	CHD-C4C-C3C	-5.26	116.81	124.94
24	c	907	CLA	CHD-C4C-C3C	-5.23	116.86	124.94
24	C	510	CLA	CHD-C4C-C3C	-5.22	116.88	124.94
26	y	101	BCR	C33-C5-C6	-5.19	119.50	124.61
24	d	401	CLA	CHD-C4C-C3C	-5.18	116.93	124.94
24	d	402	CLA	CHD-C4C-C3C	-5.13	117.02	124.94
25	a	408	PHO	C3D-C2D-C1D	-5.11	97.57	105.77
24	B	607	CLA	CHD-C4C-C3C	-5.08	117.09	124.94
24	C	505	CLA	CHD-C4C-C3C	-5.07	117.10	124.94
24	b	608	CLA	CHD-C4C-C3C	-4.99	117.22	124.94
26	t	101	BCR	C33-C5-C6	-4.99	119.71	124.61
24	b	607	CLA	CHD-C4C-C3C	-4.93	117.32	124.94
26	K	103	BCR	C7-C8-C9	-4.93	118.70	126.22
25	A	408	PHO	C3D-C2D-C1D	-4.92	97.86	105.77
26	d	404	BCR	C28-C27-C26	-4.92	106.05	113.87
38	e	102	HEM	CBA-CAA-C2A	-4.90	103.75	112.53
24	C	507	CLA	CHD-C4C-C3C	-4.90	117.37	124.94
24	b	619	CLA	CHD-C4C-C3C	-4.87	117.41	124.94
25	a	420	PHO	C3D-C2D-C1D	-4.83	98.02	105.77
31	a	417	PL9	C32-C33-C34	-4.77	117.38	127.76
24	D	401	CLA	CHD-C4C-C3C	-4.74	117.62	124.94
27	A	412	SQD	C45-O47-C7	-4.73	106.55	117.89
25	a	420	PHO	C4C-C3C-C2C	-4.72	101.54	106.81
26	D	403	BCR	C7-C8-C9	-4.68	119.08	126.22
26	T	102	BCR	C33-C5-C6	-4.62	120.06	124.61
31	A	419	PL9	C27-C28-C29	-4.55	117.86	127.76
38	V	201	HEM	C3B-CAB-CBB	-4.54	117.49	124.46
26	h	101	BCR	C38-C26-C25	-4.53	120.15	124.61
31	a	417	PL9	C37-C38-C39	-4.53	117.92	127.76
26	B	620	BCR	C38-C26-C25	-4.52	120.16	124.61
31	A	419	PL9	C37-C38-C39	-4.51	117.96	127.76
26	b	621	BCR	C33-C5-C6	-4.46	120.23	124.61
26	C	516	BCR	C7-C8-C9	-4.43	119.47	126.22
25	A	409	PHO	C3D-C2D-C1D	-4.40	98.71	105.77
24	c	902	CLA	O2D-CGD-O1D	-4.37	114.77	123.79
24	a	406	CLA	CHD-C4C-C3C	-4.36	118.20	124.94
24	B	608	CLA	CHD-C4C-C3C	-4.32	118.27	124.94
25	A	408	PHO	O1D-CGD-CBD	-4.30	118.47	124.62
26	D	403	BCR	C28-C27-C26	-4.29	107.06	113.87
26	B	618	BCR	C33-C5-C6	-4.26	120.42	124.61
24	B	615	CLA	C1D-CHD-C4C	-4.22	116.21	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	101	BCR	C38-C26-C25	-4.22	120.46	124.61
26	y	101	BCR	C15-C14-C13	-4.20	121.13	127.20
26	D	403	BCR	C24-C23-C22	-4.19	119.83	126.22
26	D	403	BCR	C38-C26-C25	-4.17	120.51	124.61
25	A	408	PHO	C4C-C3C-C2C	-4.11	102.22	106.81
27	F	101	SQD	C1-C2-C3	-4.11	101.88	109.97
25	a	420	PHO	O2D-CGD-O1D	-4.09	115.35	123.79
31	a	417	PL9	C27-C28-C29	-4.08	118.88	127.76
24	a	406	CLA	C1C-C2C-C3C	-4.08	102.03	106.91
26	C	515	BCR	C38-C26-C25	-4.03	120.65	124.61
24	b	618	CLA	O2D-CGD-O1D	-4.02	115.48	123.79
27	F	101	SQD	C44-O6-C1	-4.02	105.38	113.82
24	A	406	CLA	C1C-C2C-C3C	-4.01	102.11	106.91
27	A	412	SQD	C1-O5-C5	-4.01	105.96	113.75
26	c	915	BCR	C33-C5-C6	-4.00	120.68	124.61
24	B	617	CLA	C1D-CHD-C4C	-3.99	116.56	122.60
24	B	615	CLA	C1C-C2C-C3C	-3.97	102.16	106.91
24	C	507	CLA	C1C-C2C-C3C	-3.96	102.17	106.91
24	c	904	CLA	C1D-CHD-C4C	-3.96	116.61	122.60
27	A	412	SQD	C1-C2-C3	-3.95	102.18	109.97
26	c	915	BCR	C7-C8-C9	-3.94	120.21	126.22
24	a	407	CLA	C1D-CHD-C4C	-3.94	116.64	122.60
24	C	509	CLA	O2D-CGD-O1D	-3.93	115.68	123.79
24	B	607	CLA	C1C-C2C-C3C	-3.92	102.22	106.91
24	B	615	CLA	O2D-CGD-O1D	-3.91	115.72	123.79
26	C	515	BCR	C7-C8-C9	-3.91	120.26	126.22
31	a	417	PL9	C22-C23-C24	-3.90	119.29	127.76
26	K	102	BCR	C38-C26-C25	-3.88	120.79	124.61
26	b	623	BCR	C38-C26-C25	-3.88	120.80	124.61
26	b	623	BCR	C3-C4-C5	-3.87	107.72	113.87
26	d	404	BCR	C33-C5-C6	-3.86	120.81	124.61
24	B	606	CLA	O2D-CGD-O1D	-3.86	115.83	123.79
38	E	103	HEM	CBA-CAA-C2A	-3.85	105.62	112.53
24	d	401	CLA	C1C-C2C-C3C	-3.85	102.30	106.91
24	b	609	CLA	O2D-CGD-O1D	-3.85	115.84	123.79
24	B	609	CLA	C1C-C2C-C3C	-3.83	102.32	106.91
24	B	605	CLA	C1C-C2C-C3C	-3.83	102.33	106.91
24	b	607	CLA	O2D-CGD-O1D	-3.79	115.95	123.79
24	b	606	CLA	CAA-C2A-C3A	-3.78	102.34	113.22
26	d	404	BCR	C7-C8-C9	-3.76	120.48	126.22
24	d	402	CLA	O2D-CGD-O1D	-3.75	116.04	123.79
24	B	608	CLA	C1C-C2C-C3C	-3.75	102.42	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	411	SQD	C1-O5-C5	-3.74	106.48	113.75
38	E	103	HEM	CBD-CAD-C3D	-3.73	102.69	113.55
24	A	405	CLA	CAA-C2A-C3A	-3.73	102.50	113.22
25	A	409	PHO	C4C-C3C-C2C	-3.73	102.65	106.81
27	a	411	SQD	C45-O47-C7	-3.71	108.99	117.89
24	C	506	CLA	C3B-CAB-CBB	-3.70	118.75	126.32
24	B	604	CLA	C1D-CHD-C4C	-3.69	117.01	122.60
24	C	509	CLA	C1C-C2C-C3C	-3.69	102.50	106.91
26	c	915	BCR	C38-C26-C25	-3.68	120.99	124.61
24	C	502	CLA	CBC-CAC-C3C	-3.68	101.16	112.39
25	a	408	PHO	C4C-C3C-C2C	-3.67	102.72	106.81
24	a	409	CLA	CAA-C2A-C3A	-3.66	102.69	113.22
24	b	607	CLA	CAA-C2A-C3A	-3.64	102.75	113.22
31	A	419	PL9	C22-C23-C24	-3.64	119.86	127.76
24	b	609	CLA	C1D-CHD-C4C	-3.63	117.10	122.60
24	A	410	CLA	C1C-C2C-C3C	-3.63	102.56	106.91
24	A	407	CLA	CBC-CAC-C3C	-3.62	101.35	112.39
27	F	101	SQD	C1-O5-C5	-3.61	106.73	113.75
24	C	502	CLA	C1C-C2C-C3C	-3.60	102.60	106.91
24	b	608	CLA	C1C-C2C-C3C	-3.60	102.61	106.91
24	B	603	CLA	C3B-CAB-CBB	-3.59	118.97	126.32
26	k	101	BCR	C33-C5-C6	-3.59	121.08	124.61
24	c	907	CLA	C1C-C2C-C3C	-3.59	102.62	106.91
24	A	406	CLA	C1D-CHD-C4C	-3.59	117.17	122.60
24	c	908	CLA	C1C-C2C-C3C	-3.57	102.64	106.91
24	b	610	CLA	C1C-C2C-C3C	-3.57	102.64	106.91
24	c	905	CLA	C1C-C2C-C3C	-3.57	102.64	106.91
24	d	403	CLA	C1C-C2C-C3C	-3.56	102.65	106.91
24	b	611	CLA	CAA-C2A-C3A	-3.56	102.97	113.22
24	B	611	CLA	CHC-C1C-C2C	-3.54	117.04	126.35
24	B	604	CLA	CAA-C2A-C3A	-3.54	103.04	113.22
24	a	406	CLA	CHC-C1C-C2C	-3.54	117.04	126.35
26	d	404	BCR	C38-C26-C25	-3.54	121.13	124.61
26	k	102	BCR	C20-C21-C22	-3.54	122.09	127.20
24	c	908	CLA	O1D-CGD-CBD	-3.53	119.56	124.62
24	C	508	CLA	C1D-CHD-C4C	-3.52	117.27	122.60
24	B	617	CLA	O2D-CGD-O1D	-3.52	116.52	123.79
24	C	505	CLA	C1C-C2C-C3C	-3.52	102.70	106.91
24	C	512	CLA	C1D-CHD-C4C	-3.51	117.28	122.60
24	b	617	CLA	C1C-C2C-C3C	-3.51	102.71	106.91
24	c	902	CLA	C1C-C2C-C3C	-3.51	102.71	106.91
26	a	410	BCR	C7-C8-C9	-3.51	120.87	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	619	CLA	CHC-C1C-C2C	-3.49	117.17	126.35
24	B	611	CLA	C1D-CHD-C4C	-3.49	117.32	122.60
24	a	406	CLA	CAA-C2A-C3A	-3.48	103.21	113.22
24	A	406	CLA	CAA-C2A-C3A	-3.47	103.23	113.22
31	a	417	PL9	C17-C18-C19	-3.47	120.21	127.76
24	B	606	CLA	C1D-CHD-C4C	-3.47	117.35	122.60
31	A	419	PL9	C32-C33-C34	-3.47	120.23	127.76
26	K	103	BCR	C20-C21-C22	-3.47	122.19	127.20
24	B	607	CLA	C3B-CAB-CBB	-3.46	119.24	126.32
24	b	608	CLA	O1D-CGD-CBD	-3.46	119.66	124.62
24	C	505	CLA	O2D-CGD-O1D	-3.46	116.65	123.79
24	c	910	CLA	O2D-CGD-O1D	-3.46	116.65	123.79
24	A	407	CLA	C1D-CHD-C4C	-3.46	117.37	122.60
24	B	608	CLA	CAA-C2A-C3A	-3.46	103.28	113.22
24	b	616	CLA	C4C-C3C-C2C	-3.46	101.33	106.94
24	c	913	CLA	C1C-C2C-C3C	-3.45	102.78	106.91
24	C	513	CLA	C1D-CHD-C4C	-3.45	117.38	122.60
31	a	417	PL9	C42-C43-C44	-3.45	120.27	127.76
24	a	409	CLA	C1C-C2C-C3C	-3.45	102.79	106.91
24	c	913	CLA	C3B-CAB-CBB	-3.44	119.27	126.32
26	k	101	BCR	C15-C14-C13	-3.44	122.23	127.20
24	B	607	CLA	O1D-CGD-CBD	-3.44	119.69	124.62
24	b	610	CLA	O2D-CGD-O1D	-3.44	116.70	123.79
24	b	607	CLA	O2A-CGA-O1A	-3.43	114.64	123.49
24	b	606	CLA	C4C-C3C-C2C	-3.42	101.39	106.94
24	B	606	CLA	C1C-C2C-C3C	-3.42	102.81	106.91
24	B	614	CLA	C1C-C2C-C3C	-3.42	102.81	106.91
24	C	508	CLA	C1C-C2C-C3C	-3.42	102.81	106.91
31	A	419	PL9	C7-C8-C9	-3.42	120.90	126.70
24	B	603	CLA	CAA-C2A-C3A	-3.42	103.39	113.22
26	d	404	BCR	C3-C4-C5	-3.41	108.45	113.87
24	b	609	CLA	C1C-C2C-C3C	-3.41	102.83	106.91
24	b	605	CLA	C1C-C2C-C3C	-3.41	102.83	106.91
24	D	401	CLA	C3B-CAB-CBB	-3.40	119.36	126.32
24	B	616	CLA	C3B-CAB-CBB	-3.40	119.36	126.32
24	C	504	CLA	C1D-CHD-C4C	-3.39	117.47	122.60
24	d	401	CLA	CHC-C1C-C2C	-3.39	117.44	126.35
24	C	507	CLA	CHC-C1C-C2C	-3.39	117.45	126.35
24	A	405	CLA	C1C-C2C-C3C	-3.39	102.86	106.91
31	D	404	PL9	C7-C8-C9	-3.39	120.96	126.70
24	B	604	CLA	O2D-CGD-O1D	-3.38	116.82	123.79
24	B	610	CLA	C1D-CHD-C4C	-3.37	117.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	C3B-CAB-CBB	-3.37	119.42	126.32
24	D	401	CLA	C1C-C2C-C3C	-3.36	102.89	106.91
31	d	405	PL9	C27-C28-C29	-3.36	120.46	127.76
26	C	516	BCR	C33-C5-C6	-3.36	121.31	124.61
24	c	911	CLA	C1D-CHD-C4C	-3.35	117.53	122.60
26	b	622	BCR	C28-C27-C26	-3.35	108.55	113.87
24	B	604	CLA	O2A-CGA-O1A	-3.35	114.85	123.49
24	c	908	CLA	O2D-CGD-O1D	-3.35	116.88	123.79
24	b	607	CLA	C1D-CHD-C4C	-3.34	117.54	122.60
24	a	409	CLA	C1D-CHD-C4C	-3.34	117.54	122.60
24	b	612	CLA	C1C-C2C-C3C	-3.34	102.92	106.91
26	k	102	BCR	C24-C23-C22	-3.34	121.13	126.22
24	c	903	CLA	O2D-CGD-O1D	-3.33	116.91	123.79
24	c	908	CLA	C1D-CHD-C4C	-3.33	117.56	122.60
24	a	407	CLA	O2D-CGD-O1D	-3.33	116.92	123.79
37	D	406	LHG	O8-C23-O10	-3.33	114.91	123.49
31	D	404	PL9	C27-C28-C29	-3.32	120.53	127.76
24	C	506	CLA	O2D-CGD-O1D	-3.32	116.93	123.79
38	v	202	HEM	C3B-CAB-CBB	-3.32	119.36	124.46
24	c	910	CLA	C1C-C2C-C3C	-3.32	102.94	106.91
24	B	611	CLA	C4C-C3C-C2C	-3.32	101.56	106.94
24	B	617	CLA	C4C-C3C-C2C	-3.31	101.58	106.94
35	V	202	HTG	C1-C2-C3	-3.30	103.38	110.69
24	A	406	CLA	O2A-CGA-O1A	-3.30	114.98	123.49
24	b	611	CLA	C1C-C2C-C3C	-3.30	102.97	106.91
24	B	615	CLA	C3B-CAB-CBB	-3.29	119.58	126.32
24	b	614	CLA	C1C-C2C-C3C	-3.29	102.97	106.91
24	A	406	CLA	CBC-CAC-C3C	-3.29	102.36	112.39
26	b	622	BCR	C38-C26-C25	-3.28	121.39	124.61
24	C	503	CLA	C1C-C2C-C3C	-3.27	103.00	106.91
24	D	402	CLA	C3B-CAB-CBB	-3.27	119.63	126.32
24	C	510	CLA	C1C-C2C-C3C	-3.26	103.00	106.91
24	B	603	CLA	C1C-C2C-C3C	-3.26	103.01	106.91
24	c	907	CLA	CHC-C1C-C2C	-3.26	117.78	126.35
24	B	608	CLA	C3B-CAB-CBB	-3.26	119.65	126.32
24	b	607	CLA	C5-C3-C2	-3.26	114.88	121.05
24	b	620	CLA	C1D-CHD-C4C	-3.25	117.68	122.60
24	c	914	CLA	C1C-C2C-C3C	-3.25	103.02	106.91
24	C	506	CLA	C1C-C2C-C3C	-3.25	103.03	106.91
24	B	602	CLA	C1C-C2C-C3C	-3.24	103.03	106.91
24	c	904	CLA	C1C-C2C-C3C	-3.24	103.03	106.91
24	c	906	CLA	CHC-C1C-C2C	-3.24	117.84	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	602	CLA	C1D-CHD-C4C	-3.23	117.72	122.60
24	b	606	CLA	C1D-CHD-C4C	-3.23	117.72	122.60
24	B	606	CLA	C1C-NC-C4C	-3.22	102.35	106.27
31	d	405	PL9	C7-C8-C9	-3.22	121.24	126.70
24	b	618	CLA	C1D-CHD-C4C	-3.22	117.73	122.60
24	b	620	CLA	C4C-C3C-C2C	-3.21	101.73	106.94
24	C	511	CLA	O2D-CGD-O1D	-3.21	117.15	123.79
31	D	404	PL9	C42-C43-C44	-3.20	120.79	127.76
24	C	511	CLA	C1C-C2C-C3C	-3.20	103.08	106.91
24	c	906	CLA	O2D-CGD-O1D	-3.20	117.18	123.79
24	C	513	CLA	C1C-C2C-C3C	-3.19	103.09	106.91
24	b	618	CLA	C4C-C3C-C2C	-3.19	101.76	106.94
24	C	514	CLA	C1D-CHD-C4C	-3.19	117.78	122.60
24	b	616	CLA	O2D-CGD-O1D	-3.19	117.21	123.79
24	c	910	CLA	C1D-CHD-C4C	-3.19	117.78	122.60
24	C	502	CLA	O2D-CGD-O1D	-3.19	117.21	123.79
24	A	406	CLA	CHC-C1C-C2C	-3.18	117.98	126.35
24	d	403	CLA	CHC-C1C-C2C	-3.18	117.98	126.35
24	D	401	CLA	CHC-C1C-C2C	-3.18	117.99	126.35
24	b	615	CLA	C1D-CHD-C4C	-3.18	117.80	122.60
24	b	615	CLA	C4C-C3C-C2C	-3.16	101.81	106.94
24	c	909	CLA	CHC-C1C-C2C	-3.16	118.04	126.35
24	c	907	CLA	CBC-CAC-C3C	-3.16	102.75	112.39
31	a	417	PL9	C7-C3-C2	-3.15	120.81	123.42
27	A	412	SQD	C44-O6-C1	-3.14	107.21	113.82
24	A	405	CLA	C1D-CHD-C4C	-3.14	117.85	122.60
26	y	101	BCR	C40-C30-C25	-3.14	105.38	110.30
24	C	510	CLA	O2D-CGD-O1D	-3.14	117.31	123.79
24	c	903	CLA	C1C-C2C-C3C	-3.14	103.16	106.91
24	b	605	CLA	C1D-CHD-C4C	-3.13	117.87	122.60
24	B	604	CLA	C1C-C2C-C3C	-3.13	103.17	106.91
24	c	906	CLA	C1C-C2C-C3C	-3.13	103.17	106.91
24	c	907	CLA	C1D-CHD-C4C	-3.13	117.87	122.60
24	d	402	CLA	CHC-C1C-C2C	-3.12	118.13	126.35
31	a	417	PL9	C7-C8-C9	-3.12	121.41	126.70
31	D	404	PL9	C7-C3-C2	-3.12	120.83	123.42
29	C	522	LMT	C2'-C3'-C4'	-3.11	102.77	109.60
25	a	420	PHO	CHD-C1D-C2D	-3.11	118.58	125.61
25	A	409	PHO	CHD-C1D-C2D	-3.10	118.59	125.61
24	C	509	CLA	CHC-C1C-C2C	-3.10	118.19	126.35
24	b	615	CLA	C3B-CAB-CBB	-3.10	119.98	126.32
24	D	401	CLA	O2D-CGD-O1D	-3.10	117.39	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	C1D-CHD-C4C	-3.09	117.92	122.60
24	B	612	CLA	C1C-C2C-C3C	-3.09	103.21	106.91
24	b	614	CLA	C1D-CHD-C4C	-3.09	117.92	122.60
24	c	909	CLA	C4C-C3C-C2C	-3.09	101.93	106.94
24	b	612	CLA	C1D-CHD-C4C	-3.09	117.93	122.60
24	C	504	CLA	C4C-C3C-C2C	-3.09	101.93	106.94
26	A	411	BCR	C33-C5-C6	-3.08	121.58	124.61
24	b	611	CLA	C4C-C3C-C2C	-3.08	101.94	106.94
26	D	403	BCR	C15-C14-C13	-3.08	122.75	127.20
24	B	605	CLA	C1D-CHD-C4C	-3.08	117.94	122.60
24	c	911	CLA	C1C-C2C-C3C	-3.08	103.23	106.91
24	b	619	CLA	C1C-C2C-C3C	-3.08	103.23	106.91
24	D	402	CLA	C4C-C3C-C2C	-3.08	101.95	106.94
24	B	606	CLA	C4C-C3C-C2C	-3.07	101.96	106.94
24	b	619	CLA	O2D-CGD-O1D	-3.07	117.45	123.79
24	d	401	CLA	C2A-C1A-CHA	-3.07	118.24	123.89
24	A	406	CLA	O1D-CGD-CBD	-3.07	120.23	124.62
31	A	419	PL9	C42-C43-C44	-3.06	121.11	127.76
24	C	512	CLA	C1C-C2C-C3C	-3.06	103.25	106.91
24	d	402	CLA	C4C-C3C-C2C	-3.05	101.99	106.94
24	c	912	CLA	C1D-CHD-C4C	-3.05	117.99	122.60
31	A	419	PL9	C7-C3-C2	-3.05	120.89	123.42
24	C	509	CLA	C2A-C1A-CHA	-3.04	118.28	123.89
24	B	613	CLA	O2D-CGD-O1D	-3.04	117.50	123.79
24	C	514	CLA	C1C-C2C-C3C	-3.04	103.27	106.91
24	B	612	CLA	CHC-C1C-C2C	-3.03	118.37	126.35
24	B	611	CLA	CAA-C2A-C3A	-3.03	104.49	113.22
24	C	503	CLA	C1D-CHD-C4C	-3.03	118.01	122.60
24	c	902	CLA	CHC-C1C-C2C	-3.03	118.38	126.35
25	a	420	PHO	CHC-C1C-C2C	-3.02	118.77	125.61
24	b	610	CLA	C1D-CHD-C4C	-3.02	118.03	122.60
24	B	610	CLA	C1C-C2C-C3C	-3.02	103.30	106.91
24	B	608	CLA	CHC-C1C-C2C	-3.02	118.41	126.35
24	C	511	CLA	C1D-CHD-C4C	-3.02	118.03	122.60
24	b	614	CLA	O1D-CGD-CBD	-3.02	120.30	124.62
24	b	614	CLA	CHC-C1C-C2C	-3.02	118.42	126.35
25	a	408	PHO	C4D-ND-C1D	-3.01	101.52	107.05
24	b	615	CLA	CHC-C1C-C2C	-3.01	118.42	126.35
24	a	406	CLA	C1D-CHD-C4C	-3.01	118.04	122.60
24	a	406	CLA	CAA-C2A-C1A	-3.01	101.85	112.47
24	c	909	CLA	C1C-C2C-C3C	-3.01	103.31	106.91
24	B	616	CLA	C1C-C2C-C3C	-3.01	103.31	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	615	CLA	CHC-C1C-C2C	-3.01	118.44	126.35
24	a	406	CLA	O2A-CGA-O1A	-3.00	115.74	123.49
24	B	606	CLA	CHC-C1C-C2C	-3.00	118.45	126.35
27	a	411	SQD	O47-C7-O49	-3.00	115.61	123.67
24	C	507	CLA	O2D-CGD-O1D	-3.00	117.60	123.79
24	c	908	CLA	CHC-C1C-C2C	-3.00	118.47	126.35
24	d	402	CLA	C1C-C2C-C3C	-3.00	103.32	106.91
26	k	101	BCR	C38-C26-C25	-3.00	121.66	124.61
24	C	510	CLA	CHC-C1C-C2C	-3.00	118.47	126.35
24	A	407	CLA	CAA-C2A-C3A	-3.00	104.60	113.22
24	d	401	CLA	CAA-C2A-C3A	-3.00	104.60	113.22
24	B	605	CLA	O2A-CGA-O1A	-2.99	115.77	123.49
24	B	602	CLA	CHC-C1C-C2C	-2.99	118.49	126.35
26	D	403	BCR	C33-C5-C6	-2.99	121.67	124.61
24	b	607	CLA	C1C-C2C-C3C	-2.99	103.33	106.91
24	B	602	CLA	O1D-CGD-CBD	-2.99	120.34	124.62
24	a	407	CLA	CBC-CAC-C3C	-2.98	103.28	112.39
24	C	512	CLA	CHC-C1C-C2C	-2.98	118.50	126.35
24	C	514	CLA	CHC-C1C-C2C	-2.98	118.52	126.35
24	b	612	CLA	CHC-C1C-C2C	-2.98	118.52	126.35
24	a	406	CLA	C2A-C1A-CHA	-2.98	118.40	123.89
24	C	506	CLA	CHC-C1C-C2C	-2.98	118.53	126.35
24	c	913	CLA	C1D-CHD-C4C	-2.98	118.10	122.60
24	C	502	CLA	CHC-C1C-C2C	-2.97	118.53	126.35
24	C	507	CLA	CBC-CAC-C3C	-2.97	103.32	112.39
24	b	617	CLA	C1D-CHD-C4C	-2.97	118.10	122.60
24	b	605	CLA	CHC-C1C-C2C	-2.97	118.53	126.35
24	c	905	CLA	O1D-CGD-CBD	-2.97	120.37	124.62
24	c	912	CLA	C4C-C3C-C2C	-2.97	102.13	106.94
24	d	401	CLA	C1D-CHD-C4C	-2.96	118.12	122.60
24	B	605	CLA	CHC-C1C-C2C	-2.96	118.56	126.35
36	C	519	DGD	O3G-C3G-C2G	-2.96	103.95	110.99
24	C	508	CLA	CHC-C1C-C2C	-2.96	118.57	126.35
24	b	620	CLA	CHC-C1C-C2C	-2.96	118.57	126.35
26	k	102	BCR	C33-C5-C6	-2.95	121.70	124.61
24	b	608	CLA	CHC-C1C-C2C	-2.95	118.58	126.35
26	H	101	BCR	C37-C22-C21	-2.95	118.54	122.90
34	a	412	LMG	C8-O7-C10	-2.95	110.81	117.89
24	B	612	CLA	C1D-CHD-C4C	-2.95	118.13	122.60
24	c	906	CLA	C4C-C3C-C2C	-2.95	102.16	106.94
26	K	103	BCR	C38-C26-C25	-2.95	121.71	124.61
24	a	409	CLA	CHC-C1C-C2C	-2.95	118.60	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	408	PHO	CHC-C1C-C2C	-2.95	118.95	125.61
24	B	603	CLA	CHC-C1C-C2C	-2.94	118.61	126.35
31	d	405	PL9	C42-C43-C44	-2.94	121.36	127.76
36	C	517	DGD	O3G-C3G-C2G	-2.94	103.99	110.99
24	C	505	CLA	C1D-CHD-C4C	-2.94	118.15	122.60
24	B	613	CLA	C1C-C2C-C3C	-2.94	103.39	106.91
26	h	101	BCR	C7-C8-C9	-2.94	121.74	126.22
25	A	408	PHO	CHC-C1C-C2C	-2.93	118.97	125.61
24	B	616	CLA	O2D-CGD-O1D	-2.93	117.74	123.79
31	d	405	PL9	C31-C32-C33	-2.93	104.02	111.69
24	C	503	CLA	O2D-CGD-O1D	-2.93	117.75	123.79
24	A	410	CLA	C3B-CAB-CBB	-2.92	120.34	126.32
24	d	403	CLA	C1D-CHD-C4C	-2.92	118.18	122.60
24	B	609	CLA	C1D-CHD-C4C	-2.92	118.18	122.60
24	D	401	CLA	C4C-C3C-C2C	-2.92	102.20	106.94
24	B	603	CLA	O1D-CGD-CBD	-2.92	120.44	124.62
26	C	515	BCR	C33-C5-C6	-2.92	121.74	124.61
25	A	409	PHO	CHC-C1C-C2C	-2.92	119.01	125.61
24	b	618	CLA	C2A-C1A-CHA	-2.92	118.52	123.89
24	C	509	CLA	C1D-CHD-C4C	-2.91	118.19	122.60
24	b	617	CLA	C4C-C3C-C2C	-2.91	102.22	106.94
24	b	616	CLA	C1D-CHD-C4C	-2.91	118.20	122.60
24	C	513	CLA	O1D-CGD-CBD	-2.91	120.45	124.62
24	b	613	CLA	C1C-C2C-C3C	-2.91	103.43	106.91
26	H	101	BCR	C16-C17-C18	-2.91	123.00	127.20
24	B	607	CLA	CHC-C1C-C2C	-2.91	118.70	126.35
24	C	512	CLA	C4C-C3C-C2C	-2.91	102.22	106.94
24	b	611	CLA	C4B-CHC-C1C	-2.91	123.02	129.26
24	c	914	CLA	C1D-CHD-C4C	-2.90	118.21	122.60
24	b	612	CLA	O2A-CGA-O1A	-2.90	116.00	123.49
24	b	615	CLA	C1C-C2C-C3C	-2.90	103.44	106.91
24	b	610	CLA	O2A-CGA-O1A	-2.90	116.01	123.49
36	H	102	DGD	O1G-C1A-O1A	-2.90	116.01	123.49
24	b	619	CLA	C4B-CHC-C1C	-2.90	123.03	129.26
24	B	603	CLA	C1D-CHD-C4C	-2.89	118.22	122.60
24	B	604	CLA	C4C-C3C-C2C	-2.89	102.25	106.94
25	A	408	PHO	C4D-ND-C1D	-2.89	101.75	107.05
24	A	410	CLA	C1D-CHD-C4C	-2.89	118.23	122.60
24	B	611	CLA	OBD-CAD-C3D	-2.89	122.46	128.35
24	b	618	CLA	C1C-C2C-C3C	-2.88	103.46	106.91
24	B	614	CLA	C4C-C3C-C2C	-2.88	102.27	106.94
24	A	405	CLA	CAA-C2A-C1A	-2.88	102.31	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	O2A-CGA-O1A	-2.88	116.06	123.49
24	C	508	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
24	c	904	CLA	C3B-CAB-CBB	-2.88	120.43	126.32
26	B	620	BCR	C24-C23-C22	-2.88	121.83	126.22
24	B	607	CLA	C1D-CHD-C4C	-2.88	118.25	122.60
24	A	405	CLA	C4C-C3C-C2C	-2.87	102.28	106.94
24	a	409	CLA	C3B-CAB-CBB	-2.87	120.44	126.32
24	b	611	CLA	C1C-NC-C4C	-2.87	102.78	106.27
24	C	503	CLA	OBD-CAD-C3D	-2.87	122.50	128.35
24	a	407	CLA	CAA-C2A-C3A	-2.87	104.97	113.22
24	b	616	CLA	OBD-CAD-C3D	-2.87	122.50	128.35
24	c	912	CLA	CHC-C1C-C2C	-2.87	118.81	126.35
24	C	514	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
24	c	906	CLA	C1D-CHD-C4C	-2.87	118.27	122.60
24	b	609	CLA	OBD-CAD-C3D	-2.86	122.51	128.35
24	C	503	CLA	CHC-C1C-C2C	-2.86	118.82	126.35
24	B	617	CLA	CHC-C1C-C2C	-2.86	118.83	126.35
24	C	514	CLA	C4C-C3C-C2C	-2.86	102.30	106.94
24	b	618	CLA	CHC-C1C-C2C	-2.86	118.83	126.35
24	B	613	CLA	C2A-C1A-CHA	-2.86	118.62	123.89
26	b	621	BCR	C7-C8-C9	-2.86	121.86	126.22
24	b	615	CLA	O2D-CGD-O1D	-2.85	117.90	123.79
24	b	611	CLA	CHC-C1C-C2C	-2.85	118.85	126.35
35	V	202	HTG	O5-C1-C2	-2.85	106.32	110.19
24	C	507	CLA	C1D-CHD-C4C	-2.85	118.29	122.60
24	c	903	CLA	C3B-CAB-CBB	-2.84	120.50	126.32
24	b	605	CLA	O2D-CGD-O1D	-2.84	117.93	123.79
24	C	506	CLA	C1D-CHD-C4C	-2.84	118.31	122.60
24	c	906	CLA	C1C-NC-C4C	-2.84	102.82	106.27
24	C	504	CLA	C1C-C2C-C3C	-2.83	103.52	106.91
24	C	502	CLA	C1D-CHD-C4C	-2.83	118.31	122.60
24	b	607	CLA	CHC-C1C-C2C	-2.83	118.91	126.35
24	C	503	CLA	O2A-CGA-O1A	-2.83	116.19	123.49
24	B	610	CLA	CHC-C1C-C2C	-2.83	118.91	126.35
24	b	606	CLA	O2D-CGD-O1D	-2.83	117.95	123.79
24	C	506	CLA	C4C-C3C-C2C	-2.83	102.36	106.94
24	A	406	CLA	C3B-CAB-CBB	-2.83	120.53	126.32
25	A	409	PHO	C4D-ND-C1D	-2.82	101.87	107.05
24	A	405	CLA	CHC-C1C-C2C	-2.82	118.93	126.35
34	C	521	LMG	C8-O7-C10	-2.82	111.12	117.89
24	C	509	CLA	O2A-CGA-O1A	-2.82	116.22	123.49
24	B	614	CLA	CHC-C1C-C2C	-2.82	118.94	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	c	916	DGD	O5D-C6D-C5D	-2.81	103.98	109.08
24	c	914	CLA	CAA-C2A-C3A	-2.81	105.13	113.22
24	B	613	CLA	C4C-C3C-C2C	-2.81	102.38	106.94
26	c	915	BCR	C3-C4-C5	-2.81	109.41	113.87
24	c	912	CLA	C3B-CAB-CBB	-2.81	120.58	126.32
24	d	401	CLA	CBC-CAC-C3C	-2.80	103.83	112.39
24	B	616	CLA	C11-C10-C8	-2.80	106.19	115.49
26	C	516	BCR	C15-C14-C13	-2.80	123.15	127.20
24	c	911	CLA	CHC-C1C-C2C	-2.80	118.98	126.35
24	b	612	CLA	O2D-CGD-O1D	-2.80	118.01	123.79
24	A	407	CLA	CHC-C1C-C2C	-2.80	118.99	126.35
24	D	402	CLA	CHC-C1C-C2C	-2.80	118.99	126.35
24	c	904	CLA	CHC-C1C-C2C	-2.80	118.99	126.35
24	B	603	CLA	C4C-C3C-C2C	-2.80	102.41	106.94
24	c	911	CLA	O1D-CGD-CBD	-2.80	120.61	124.62
24	b	619	CLA	C4C-C3C-C2C	-2.79	102.41	106.94
24	c	907	CLA	CAA-C2A-C3A	-2.79	105.19	113.22
24	a	407	CLA	C4C-C3C-C2C	-2.79	102.42	106.94
24	D	402	CLA	C1C-C2C-C3C	-2.79	103.58	106.91
24	B	616	CLA	CHC-C1C-C2C	-2.78	119.03	126.35
24	d	401	CLA	C3B-CAB-CBB	-2.78	120.62	126.32
24	A	405	CLA	C1C-NC-C4C	-2.78	102.89	106.27
24	C	510	CLA	C1D-CHD-C4C	-2.78	118.40	122.60
24	b	614	CLA	C4C-C3C-C2C	-2.78	102.44	106.94
24	c	903	CLA	C4C-C3C-C2C	-2.77	102.45	106.94
24	c	903	CLA	C1D-CHD-C4C	-2.77	118.41	122.60
24	A	410	CLA	CHC-C1C-C2C	-2.77	119.07	126.35
24	b	619	CLA	C1D-CHD-C4C	-2.77	118.42	122.60
24	B	613	CLA	O1D-CGD-CBD	-2.76	120.66	124.62
24	C	504	CLA	CHC-C1C-C2C	-2.76	119.08	126.35
26	d	404	BCR	C16-C17-C18	-2.76	123.21	127.20
24	b	610	CLA	CAA-C2A-C3A	-2.76	105.28	113.22
24	a	407	CLA	C1C-C2C-C3C	-2.76	103.61	106.91
24	c	909	CLA	O2D-CGD-O1D	-2.75	118.11	123.79
27	A	416	SQD	O48-C23-O10	-2.75	116.39	123.49
24	c	908	CLA	C4C-C3C-C2C	-2.75	102.48	106.94
24	B	616	CLA	C4C-C3C-C2C	-2.75	102.48	106.94
24	c	905	CLA	CHC-C1C-C2C	-2.75	119.12	126.35
24	c	905	CLA	O2D-CGD-O1D	-2.75	118.12	123.79
24	b	613	CLA	O2D-CGD-O1D	-2.75	118.12	123.79
24	C	513	CLA	CHC-C1C-C2C	-2.75	119.13	126.35
24	b	606	CLA	CHC-C1C-C2C	-2.75	119.13	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	C1C-NC-C4C	-2.74	102.93	106.27
24	b	610	CLA	CBC-CAC-C3C	-2.74	104.02	112.39
24	C	503	CLA	C4C-C3C-C2C	-2.74	102.49	106.94
24	a	409	CLA	O2D-CGD-O1D	-2.74	118.13	123.79
24	a	409	CLA	C4C-C3C-C2C	-2.74	102.50	106.94
37	D	408	LHG	O8-C23-O10	-2.74	116.43	123.49
24	B	615	CLA	C2A-C1A-CHA	-2.73	118.85	123.89
24	c	903	CLA	CHC-C1C-C2C	-2.73	119.16	126.35
24	C	512	CLA	C3B-CAB-CBB	-2.73	120.73	126.32
24	b	618	CLA	OBD-CAD-C3D	-2.72	122.80	128.35
24	B	611	CLA	C1C-C2C-C3C	-2.72	103.66	106.91
24	c	902	CLA	C1D-CHD-C4C	-2.72	118.49	122.60
24	C	507	CLA	CAA-C2A-C3A	-2.72	105.41	113.22
26	T	102	BCR	C7-C6-C5	-2.72	115.15	121.37
24	c	907	CLA	O2D-CGD-O1D	-2.71	118.19	123.79
24	c	910	CLA	CHC-C1C-C2C	-2.71	119.23	126.35
24	c	911	CLA	C4C-C3C-C2C	-2.71	102.55	106.94
31	d	405	PL9	C32-C33-C34	-2.71	121.88	127.76
24	A	407	CLA	C1C-C2C-C3C	-2.70	103.68	106.91
24	b	607	CLA	C4C-C3C-C2C	-2.70	102.56	106.94
24	B	606	CLA	O2A-CGA-O1A	-2.70	116.52	123.49
24	c	902	CLA	C4C-C3C-C2C	-2.70	102.56	106.94
24	b	618	CLA	C3B-CAB-CBB	-2.70	120.80	126.32
24	B	607	CLA	C1C-NC-C4C	-2.70	102.99	106.27
24	B	609	CLA	CHC-C1C-C2C	-2.70	119.26	126.35
24	d	402	CLA	CAA-C2A-C3A	-2.70	105.47	113.22
26	h	101	BCR	C24-C23-C22	-2.69	122.11	126.22
24	B	610	CLA	O2D-CGD-O1D	-2.69	118.23	123.79
26	d	404	BCR	C21-C20-C19	-2.69	114.92	123.13
24	B	609	CLA	O2D-CGD-O1D	-2.69	118.23	123.79
24	B	615	CLA	CBC-CAC-C3C	-2.69	104.18	112.39
24	A	407	CLA	C4C-C3C-C2C	-2.69	102.58	106.94
24	d	402	CLA	C1C-NC-C4C	-2.69	103.00	106.27
24	b	620	CLA	O2D-CGD-O1D	-2.69	118.24	123.79
24	a	407	CLA	CHC-C1C-C2C	-2.69	119.28	126.35
24	B	614	CLA	O2A-CGA-O1A	-2.69	116.56	123.49
24	a	409	CLA	CBC-CAC-C3C	-2.69	104.19	112.39
24	c	914	CLA	CHC-C1C-C2C	-2.69	119.29	126.35
24	B	609	CLA	C4C-C3C-C2C	-2.68	102.59	106.94
24	c	908	CLA	C3B-CAB-CBB	-2.68	120.83	126.32
31	d	405	PL9	C37-C38-C39	-2.68	121.94	127.76
26	y	101	BCR	C28-C27-C26	-2.68	109.62	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	CHC-C1C-C2C	-2.68	119.31	126.35
24	C	513	CLA	C4C-C3C-C2C	-2.68	102.60	106.94
24	b	613	CLA	C4C-C3C-C2C	-2.67	102.60	106.94
24	D	401	CLA	O2A-CGA-O1A	-2.67	116.60	123.49
24	B	610	CLA	C4C-C3C-C2C	-2.67	102.61	106.94
24	C	510	CLA	C4C-C3C-C2C	-2.67	102.62	106.94
24	d	402	CLA	C2A-C1A-CHA	-2.67	118.98	123.89
25	a	420	PHO	C4-C3-C2	-2.67	118.27	123.50
25	A	408	PHO	C3A-C2A-C1A	-2.66	98.47	101.84
34	c	920	LMG	C8-O7-C10	-2.66	111.50	117.89
24	b	610	CLA	C3B-CAB-CBB	-2.66	120.88	126.32
24	b	608	CLA	O2D-CGD-O1D	-2.66	118.30	123.79
24	b	611	CLA	O1D-CGD-CBD	-2.66	120.81	124.62
24	C	508	CLA	C4C-C3C-C2C	-2.66	102.63	106.94
24	c	914	CLA	C2A-C1A-CHA	-2.66	118.99	123.89
26	T	102	BCR	C21-C20-C19	-2.66	115.03	123.13
24	b	616	CLA	C2A-C1A-CHA	-2.66	119.00	123.89
24	b	609	CLA	C4C-C3C-C2C	-2.65	102.64	106.94
31	D	404	PL9	C22-C23-C24	-2.65	121.99	127.76
24	B	616	CLA	CBC-CAC-C3C	-2.65	104.30	112.39
24	c	913	CLA	CHC-C1C-C2C	-2.65	119.38	126.35
24	c	902	CLA	C3B-CAB-CBB	-2.65	120.89	126.32
26	y	101	BCR	C38-C26-C25	-2.65	122.00	124.61
24	c	909	CLA	C1D-CHD-C4C	-2.65	118.59	122.60
27	L	102	SQD	C1-C2-C3	-2.65	104.75	109.97
31	D	404	PL9	C36-C37-C38	-2.65	104.76	111.69
24	c	913	CLA	CBC-CAC-C3C	-2.64	104.32	112.39
24	C	511	CLA	C4C-C3C-C2C	-2.64	102.66	106.94
24	B	606	CLA	C2A-C1A-CHA	-2.64	119.02	123.89
31	D	404	PL9	C12-C13-C14	-2.64	122.02	127.76
34	a	412	LMG	C7-O1-C1	-2.64	108.28	113.82
24	b	609	CLA	CHC-C1C-C2C	-2.64	119.41	126.35
24	A	410	CLA	CAA-C2A-C3A	-2.64	105.63	113.22
34	J	101	LMG	O8-C28-O10	-2.64	116.69	123.49
26	t	101	BCR	C15-C16-C17	-2.64	117.56	123.39
24	C	511	CLA	CHC-C1C-C2C	-2.63	119.42	126.35
24	b	617	CLA	CHC-C1C-C2C	-2.63	119.43	126.35
24	a	407	CLA	OBD-CAD-C3D	-2.63	122.98	128.35
24	C	508	CLA	C3B-CAB-CBB	-2.63	120.93	126.32
24	B	607	CLA	CAA-C2A-C3A	-2.63	105.66	113.22
24	B	604	CLA	CHC-C1C-C2C	-2.63	119.44	126.35
26	k	101	BCR	C24-C23-C22	-2.63	122.21	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	C4B-CHC-C1C	-2.62	123.62	129.26
24	b	613	CLA	C2A-C1A-CHA	-2.62	119.05	123.89
24	b	620	CLA	C1C-C2C-C3C	-2.62	103.77	106.91
24	c	904	CLA	C4C-C3C-C2C	-2.62	102.69	106.94
38	e	102	HEM	CBD-CAD-C3D	-2.62	105.93	113.55
24	c	913	CLA	O1D-CGD-CBD	-2.62	120.87	124.62
24	b	611	CLA	C1D-CHD-C4C	-2.62	118.64	122.60
24	C	509	CLA	C3B-CAB-CBB	-2.62	120.96	126.32
26	t	101	BCR	C7-C6-C5	-2.62	115.38	121.37
24	B	602	CLA	C4C-C3C-C2C	-2.62	102.70	106.94
24	B	617	CLA	OBD-CAD-C3D	-2.61	123.02	128.35
26	a	410	BCR	C3-C4-C5	-2.61	109.73	113.87
24	A	405	CLA	C2A-C1A-CHA	-2.60	119.09	123.89
25	a	408	PHO	C1C-C2C-C3C	-2.60	103.39	106.50
24	B	602	CLA	O2D-CGD-O1D	-2.60	118.42	123.79
24	B	613	CLA	CHC-C1C-C2C	-2.60	119.52	126.35
24	c	912	CLA	C1C-C2C-C3C	-2.60	103.80	106.91
24	d	403	CLA	C4C-C3C-C2C	-2.60	102.73	106.94
24	b	612	CLA	C4C-C3C-C2C	-2.59	102.73	106.94
26	B	619	BCR	C28-C27-C26	-2.59	109.75	113.87
24	c	911	CLA	C4-C3-C2	-2.59	118.42	123.50
24	B	612	CLA	O1D-CGD-CBD	-2.59	120.91	124.62
24	d	402	CLA	C1D-CHD-C4C	-2.59	118.69	122.60
24	D	401	CLA	C1C-NC-C4C	-2.59	103.12	106.27
27	a	411	SQD	C44-O6-C1	-2.59	108.38	113.82
24	C	505	CLA	CBC-CAC-C3C	-2.58	104.51	112.39
31	A	419	PL9	C16-C17-C18	-2.58	104.92	111.69
24	B	612	CLA	C4C-C3C-C2C	-2.58	102.75	106.94
34	Z	101	LMG	C8-O7-C10	-2.58	111.70	117.89
24	c	904	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
24	d	401	CLA	O2A-CGA-O1A	-2.58	116.83	123.49
24	B	609	CLA	C3B-CAB-CBB	-2.58	121.04	126.32
25	A	409	PHO	C1C-C2C-C3C	-2.58	103.42	106.50
31	D	404	PL9	C37-C38-C39	-2.58	122.16	127.76
24	C	503	CLA	C3B-CAB-CBB	-2.57	121.05	126.32
24	b	611	CLA	C3B-CAB-CBB	-2.57	121.05	126.32
26	y	101	BCR	C10-C11-C12	-2.57	115.29	123.13
24	A	410	CLA	CBC-CAC-C3C	-2.57	104.54	112.39
25	a	420	PHO	C4D-ND-C1D	-2.57	102.34	107.05
24	B	605	CLA	C4B-CHC-C1C	-2.56	123.76	129.26
34	B	622	LMG	O8-C28-O10	-2.56	116.89	123.49
24	a	406	CLA	O2D-CGD-O1D	-2.56	118.51	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	C5-C3-C2	-2.55	116.21	121.05
36	h	102	DGD	O1G-C1A-O1A	-2.55	116.92	123.49
25	a	408	PHO	O1D-CGD-CBD	-2.54	120.97	124.62
24	B	617	CLA	O1D-CGD-CBD	-2.54	120.98	124.62
24	d	402	CLA	O2A-CGA-O1A	-2.54	116.94	123.49
26	k	101	BCR	C7-C8-C9	-2.54	122.34	126.22
31	a	417	PL9	C37-C36-C34	-2.54	104.44	112.71
24	b	617	CLA	C1C-NC-C4C	-2.54	103.18	106.27
36	c	916	DGD	C2G-O2G-C1B	-2.54	111.80	117.89
24	C	504	CLA	O2D-CGD-O1D	-2.54	118.55	123.79
24	C	514	CLA	C2A-C1A-CHA	-2.53	119.22	123.89
24	c	905	CLA	C4C-C3C-C2C	-2.53	102.84	106.94
24	b	609	CLA	O2A-CGA-O1A	-2.53	116.97	123.49
24	B	612	CLA	C2A-C1A-CHA	-2.53	119.23	123.89
24	B	611	CLA	O2D-CGD-O1D	-2.52	118.58	123.79
24	c	902	CLA	C4B-CHC-C1C	-2.52	123.86	129.26
24	b	610	CLA	CHC-C1C-C2C	-2.52	119.73	126.35
24	C	509	CLA	C4C-C3C-C2C	-2.51	102.86	106.94
31	A	419	PL9	C30-C29-C28	-2.51	118.57	123.50
31	A	419	PL9	C25-C24-C23	-2.51	118.57	123.50
24	B	609	CLA	CAA-C2A-C3A	-2.51	106.00	113.22
26	K	103	BCR	C15-C14-C13	-2.51	123.57	127.20
24	c	907	CLA	O2A-CGA-O1A	-2.51	117.02	123.49
26	B	619	BCR	C37-C22-C21	-2.51	119.20	122.90
24	b	607	CLA	C2A-C1A-CHA	-2.51	119.27	123.89
24	c	914	CLA	C4C-C3C-C2C	-2.51	102.88	106.94
24	b	617	CLA	O2A-CGA-O1A	-2.50	117.03	123.49
24	c	903	CLA	O2A-CGA-O1A	-2.50	117.03	123.49
24	d	401	CLA	CMA-C3A-C2A	-2.50	103.27	114.35
24	c	913	CLA	O2D-CGD-O1D	-2.50	118.62	123.79
24	b	610	CLA	O1D-CGD-CBD	-2.50	121.04	124.62
24	b	609	CLA	C2A-C1A-CHA	-2.50	119.28	123.89
24	D	402	CLA	C2A-C1A-CHA	-2.49	119.29	123.89
26	b	623	BCR	C15-C14-C13	-2.49	123.59	127.20
24	c	910	CLA	OBD-CAD-C3D	-2.49	123.27	128.35
26	K	102	BCR	C24-C23-C22	-2.49	122.42	126.22
27	B	621	SQD	C1-C2-C3	-2.49	105.07	109.97
24	c	913	CLA	CBA-CAA-C2A	-2.49	106.71	113.73
37	L	101	LHG	O8-C23-O10	-2.49	117.08	123.49
25	A	408	PHO	C4-C3-C2	-2.48	118.62	123.50
24	c	910	CLA	C4C-C3C-C2C	-2.48	102.91	106.94
26	B	620	BCR	C39-C30-C25	-2.48	106.42	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	O2A-CGA-O1A	-2.48	117.09	123.49
38	e	102	HEM	C1D-CHD-C4C	-2.47	121.69	125.82
24	b	608	CLA	C4C-C3C-C2C	-2.47	102.94	106.94
26	a	410	BCR	C38-C26-C25	-2.47	122.18	124.61
24	C	508	CLA	CBC-CAC-C3C	-2.46	104.87	112.39
26	H	101	BCR	C7-C8-C9	-2.46	122.46	126.22
26	d	404	BCR	C24-C23-C22	-2.46	122.47	126.22
24	b	620	CLA	O1D-CGD-CBD	-2.46	121.10	124.62
24	a	406	CLA	CMA-C3A-C2A	-2.46	103.47	114.35
24	a	409	CLA	OBD-CAD-C3D	-2.46	123.34	128.35
26	K	102	BCR	C16-C17-C18	-2.46	123.65	127.20
26	C	516	BCR	C3-C4-C5	-2.45	109.97	113.87
24	b	609	CLA	C3B-CAB-CBB	-2.45	121.30	126.32
24	c	909	CLA	CAA-C2A-C3A	-2.45	106.17	113.22
24	B	608	CLA	O2D-CGD-O1D	-2.45	118.73	123.79
26	K	103	BCR	C33-C5-C6	-2.45	122.20	124.61
24	b	615	CLA	O2A-CGA-O1A	-2.45	117.17	123.49
24	c	913	CLA	C4C-C3C-C2C	-2.45	102.97	106.94
26	D	403	BCR	C10-C11-C12	-2.45	115.67	123.13
25	A	408	PHO	CHD-C1D-C2D	-2.45	120.07	125.61
24	c	903	CLA	C2A-C1A-CHA	-2.44	119.38	123.89
24	b	618	CLA	CAA-C2A-C3A	-2.44	106.19	113.22
25	a	408	PHO	CHD-C1D-C2D	-2.44	120.08	125.61
24	b	613	CLA	CHC-C1C-C2C	-2.44	119.92	126.35
24	d	403	CLA	C1C-NC-C4C	-2.44	103.30	106.27
24	C	508	CLA	O1D-CGD-CBD	-2.44	121.12	124.62
24	b	620	CLA	OBD-CAD-C3D	-2.44	123.38	128.35
24	A	407	CLA	C2A-C1A-CHA	-2.44	119.39	123.89
24	D	402	CLA	C1D-CHD-C4C	-2.44	118.91	122.60
24	C	514	CLA	C3B-CAB-CBB	-2.44	121.33	126.32
24	B	607	CLA	C4C-C3C-C2C	-2.44	102.99	106.94
24	A	407	CLA	O1D-CGD-CBD	-2.44	121.13	124.62
37	l	101	LHG	C6-C5-C4	-2.44	106.37	112.07
24	b	608	CLA	C4B-CHC-C1C	-2.43	124.03	129.26
24	b	607	CLA	OBD-CAD-C3D	-2.43	123.39	128.35
24	C	503	CLA	C4-C3-C2	-2.43	118.72	123.50
26	t	101	BCR	C21-C20-C19	-2.43	115.71	123.13
24	B	607	CLA	C4A-NA-C1A	-2.43	103.21	106.36
25	a	408	PHO	CBA-CAA-C2A	-2.43	106.87	113.73
26	d	404	BCR	C15-C14-C13	-2.43	123.69	127.20
34	z	101	LMG	C7-O1-C1	-2.43	108.72	113.82
24	b	612	CLA	C2A-C1A-CHA	-2.43	119.41	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	h	101	BCR	C10-C11-C12	-2.43	115.73	123.13
24	b	608	CLA	C1C-NC-C4C	-2.43	103.32	106.27
24	B	610	CLA	CBC-CAC-C3C	-2.43	104.99	112.39
24	B	608	CLA	C2A-C1A-CHA	-2.42	119.43	123.89
24	b	605	CLA	C4C-C3C-C2C	-2.42	103.01	106.94
26	B	620	BCR	C3-C4-C5	-2.42	110.03	113.87
24	b	606	CLA	O1D-CGD-CBD	-2.42	121.15	124.62
24	B	608	CLA	C4C-C3C-C2C	-2.42	103.02	106.94
24	b	617	CLA	C3B-CAB-CBB	-2.42	121.37	126.32
24	b	616	CLA	O2A-CGA-O1A	-2.41	117.26	123.49
24	B	605	CLA	C4C-C3C-C2C	-2.41	103.03	106.94
26	y	101	BCR	C21-C20-C19	-2.41	115.77	123.13
26	c	915	BCR	C15-C14-C13	-2.41	123.71	127.20
24	c	906	CLA	C3B-CAB-CBB	-2.41	121.38	126.32
24	B	615	CLA	CAA-C2A-C3A	-2.41	106.28	113.22
24	c	912	CLA	O2D-CGD-O1D	-2.41	118.82	123.79
24	c	904	CLA	OBD-CAD-C3D	-2.40	123.45	128.35
26	y	101	BCR	C35-C13-C14	-2.40	119.35	122.90
24	C	510	CLA	OBD-CAD-C3D	-2.40	123.46	128.35
24	B	603	CLA	CAA-CBA-CGA	-2.40	106.30	113.32
24	C	505	CLA	C4C-C3C-C2C	-2.40	103.05	106.94
24	B	607	CLA	C2A-C1A-CHA	-2.40	119.47	123.89
37	d	408	LHG	O8-C23-O10	-2.40	117.31	123.49
24	c	907	CLA	OBD-CAD-C3D	-2.39	123.47	128.35
31	A	419	PL9	C17-C18-C19	-2.39	122.56	127.76
24	A	406	CLA	CMA-C3A-C2A	-2.39	103.77	114.35
24	b	614	CLA	CAA-C2A-C3A	-2.39	106.34	113.22
29	B	623	LMT	O1B-C4'-C5'	-2.39	103.04	109.32
24	C	511	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
24	C	503	CLA	C2A-C1A-CHA	-2.39	119.49	123.89
24	b	609	CLA	CAA-C2A-C3A	-2.39	106.35	113.22
38	E	103	HEM	C1D-CHD-C4C	-2.39	121.83	125.82
24	c	904	CLA	C1C-NC-C4C	-2.39	103.37	106.27
24	a	407	CLA	C2A-C1A-CHA	-2.39	119.49	123.89
26	y	101	BCR	C16-C17-C18	-2.39	123.75	127.20
24	c	914	CLA	C3B-CAB-CBB	-2.39	121.44	126.32
26	d	404	BCR	C40-C30-C25	-2.38	106.56	110.30
34	j	101	LMG	O8-C28-O10	-2.38	117.34	123.49
24	B	604	CLA	C2A-C1A-CHA	-2.38	119.49	123.89
24	a	407	CLA	C3B-CAB-CBB	-2.38	121.44	126.32
24	c	909	CLA	C4-C3-C2	-2.38	118.82	123.50
34	C	520	LMG	C8-O7-C10	-2.38	112.17	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	C4B-CHC-C1C	-2.38	124.14	129.26
24	d	401	CLA	O2D-CGD-O1D	-2.38	118.87	123.79
27	A	412	SQD	O47-C7-O49	-2.38	117.28	123.67
24	c	905	CLA	C2A-C1A-CHA	-2.38	119.50	123.89
26	B	618	BCR	C37-C22-C21	-2.38	119.39	122.90
26	B	618	BCR	C7-C8-C9	-2.38	122.59	126.22
31	d	405	PL9	C36-C37-C38	-2.38	105.47	111.69
27	A	412	SQD	O48-C23-O10	-2.38	117.36	123.49
24	b	618	CLA	C4B-CHC-C1C	-2.37	124.16	129.26
25	a	408	PHO	C4D-CHA-C1A	-2.37	119.79	125.06
25	A	409	PHO	C4D-CHA-C1A	-2.37	119.79	125.06
24	b	618	CLA	O2A-CGA-O1A	-2.37	117.38	123.49
24	b	606	CLA	C1C-C2C-C3C	-2.37	104.08	106.91
31	D	404	PL9	C25-C24-C23	-2.37	118.86	123.50
24	b	616	CLA	CHC-C1C-C2C	-2.37	120.13	126.35
24	C	505	CLA	C2A-C1A-CHA	-2.37	119.53	123.89
26	k	101	BCR	C35-C13-C14	-2.36	119.41	122.90
24	b	616	CLA	C1C-C2C-C3C	-2.36	104.09	106.91
34	z	101	LMG	C8-O7-C10	-2.36	112.23	117.89
24	C	513	CLA	C4B-CHC-C1C	-2.36	124.19	129.26
26	T	102	BCR	C11-C10-C9	-2.36	123.80	127.20
24	B	603	CLA	C4B-CHC-C1C	-2.35	124.21	129.26
24	C	504	CLA	C3B-CAB-CBB	-2.35	121.51	126.32
24	d	403	CLA	C4B-CHC-C1C	-2.35	124.22	129.26
24	b	618	CLA	C1C-NC-C4C	-2.34	103.42	106.27
24	B	613	CLA	C4B-CHC-C1C	-2.34	124.23	129.26
26	B	619	BCR	C33-C5-C6	-2.34	122.31	124.61
38	V	201	HEM	C3B-C4B-NB	-2.34	107.15	111.63
24	B	613	CLA	C1C-NC-C4C	-2.34	103.42	106.27
24	d	402	CLA	C4A-NA-C1A	-2.34	103.33	106.36
24	a	407	CLA	O2A-CGA-O1A	-2.34	117.45	123.49
24	b	615	CLA	C2A-C1A-CHA	-2.34	119.58	123.89
24	b	619	CLA	C1C-NC-C4C	-2.34	103.43	106.27
24	B	608	CLA	OBD-CAD-C3D	-2.34	123.59	128.35
24	C	509	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
24	B	613	CLA	C1D-CHD-C4C	-2.33	119.07	122.60
24	b	606	CLA	C1C-NC-C4C	-2.33	103.43	106.27
24	D	401	CLA	C4B-CHC-C1C	-2.33	124.26	129.26
24	B	606	CLA	OBD-CAD-C3D	-2.33	123.61	128.35
24	b	618	CLA	C4-C3-C2	-2.33	118.94	123.50
24	b	613	CLA	C1D-CHD-C4C	-2.32	119.08	122.60
24	B	617	CLA	C2A-C1A-CHA	-2.32	119.61	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	411	SQD	C1-C2-C3	-2.32	105.41	109.97
24	B	604	CLA	CBC-CAC-C3C	-2.32	105.32	112.39
24	c	905	CLA	C4-C3-C2	-2.31	118.96	123.50
24	c	908	CLA	C1C-NC-C4C	-2.31	103.46	106.27
25	A	409	PHO	O2D-CGD-O1D	-2.31	119.02	123.79
24	c	904	CLA	O2A-CGA-O1A	-2.31	117.53	123.49
24	c	902	CLA	CBC-CAC-C3C	-2.31	105.34	112.39
24	b	605	CLA	O1D-CGD-CBD	-2.31	121.31	124.62
24	d	403	CLA	C3B-CAB-CBB	-2.31	121.59	126.32
26	B	618	BCR	C34-C9-C10	-2.31	119.49	122.90
24	c	907	CLA	C4C-C3C-C2C	-2.31	103.20	106.94
24	c	905	CLA	C1D-CHD-C4C	-2.30	119.11	122.60
24	c	906	CLA	O1D-CGD-CBD	-2.30	121.32	124.62
24	c	911	CLA	O2A-CGA-O1A	-2.30	117.55	123.49
31	a	417	PL9	C30-C29-C28	-2.30	118.98	123.50
24	b	610	CLA	C4C-C3C-C2C	-2.30	103.21	106.94
31	D	404	PL9	C40-C39-C38	-2.30	118.99	123.50
24	B	610	CLA	O2A-CGA-O1A	-2.30	117.56	123.49
38	v	202	HEM	CBA-CAA-C2A	-2.30	108.41	112.53
24	C	505	CLA	CAA-C2A-C3A	-2.30	106.62	113.22
26	t	101	BCR	C29-C28-C27	-2.30	105.75	111.53
24	d	401	CLA	C4C-C3C-C2C	-2.29	103.22	106.94
24	b	608	CLA	C1D-CHD-C4C	-2.29	119.14	122.60
24	C	502	CLA	C2A-C1A-CHA	-2.29	119.67	123.89
24	B	615	CLA	OBD-CAD-C3D	-2.28	123.70	128.35
24	b	611	CLA	O2D-CGD-O1D	-2.28	119.08	123.79
26	D	403	BCR	C29-C28-C27	-2.28	105.79	111.53
24	B	617	CLA	C4-C3-C2	-2.28	119.03	123.50
24	b	614	CLA	O2A-CGA-O1A	-2.28	117.61	123.49
29	B	623	LMT	C1-O1'-C1'	-2.28	109.96	113.94
24	B	617	CLA	C4B-CHC-C1C	-2.28	124.37	129.26
26	b	623	BCR	C10-C11-C12	-2.28	116.19	123.13
31	A	419	PL9	C12-C13-C14	-2.27	122.82	127.76
24	B	610	CLA	C2A-C1A-CHA	-2.27	119.70	123.89
24	B	611	CLA	CAA-CBA-CGA	-2.27	106.66	113.32
24	b	605	CLA	C2A-C1A-CHA	-2.27	119.70	123.89
24	C	513	CLA	OBD-CAD-C3D	-2.27	123.72	128.35
24	B	603	CLA	O2D-CGD-O1D	-2.27	119.10	123.79
24	c	912	CLA	C2A-C1A-CHA	-2.27	119.71	123.89
24	C	502	CLA	C4C-C3C-C2C	-2.27	103.26	106.94
26	k	101	BCR	C21-C20-C19	-2.27	116.22	123.13
36	C	517	DGD	C2G-O2G-C1B	-2.26	112.46	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	C1C-C2C-C3C	-2.26	104.20	106.91
24	B	612	CLA	O2A-CGA-O1A	-2.26	117.65	123.49
24	B	615	CLA	C4C-C3C-C2C	-2.26	103.28	106.94
24	b	613	CLA	C4A-NA-C1A	-2.26	103.43	106.36
27	L	102	SQD	C44-O6-C1	-2.26	109.07	113.82
24	C	504	CLA	C2A-C1A-CHA	-2.26	119.73	123.89
24	c	909	CLA	C2A-C1A-CHA	-2.26	119.73	123.89
26	b	623	BCR	C16-C15-C14	-2.26	118.40	123.39
24	B	605	CLA	O1D-CGD-CBD	-2.26	121.39	124.62
24	C	512	CLA	O2D-CGD-O1D	-2.26	119.13	123.79
24	C	502	CLA	O2A-CGA-O1A	-2.25	117.67	123.49
24	B	605	CLA	O2D-CGD-O1D	-2.25	119.14	123.79
26	D	403	BCR	C16-C17-C18	-2.25	123.94	127.20
24	C	503	CLA	CBC-CAC-C3C	-2.25	105.52	112.39
26	d	404	BCR	C27-C26-C25	-2.25	119.91	122.78
31	A	419	PL9	C35-C34-C33	-2.25	119.09	123.50
24	C	510	CLA	C4-C3-C2	-2.25	119.09	123.50
24	B	602	CLA	C3B-CAB-CBB	-2.25	121.72	126.32
24	c	905	CLA	CAA-C2A-C3A	-2.25	106.75	113.22
24	b	609	CLA	C1C-NC-C4C	-2.25	103.54	106.27
24	C	511	CLA	C2A-C1A-CHA	-2.25	119.75	123.89
24	b	606	CLA	O2A-CGA-O1A	-2.24	117.71	123.49
36	c	918	DGD	O1G-C1A-O1A	-2.24	117.71	123.49
24	B	603	CLA	CBC-CAC-C3C	-2.24	105.55	112.39
24	C	513	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
31	a	417	PL9	C35-C34-C33	-2.24	119.11	123.50
24	B	608	CLA	C4B-CHC-C1C	-2.24	124.45	129.26
26	d	404	BCR	C30-C25-C26	-2.24	119.38	122.66
31	d	405	PL9	C12-C13-C14	-2.24	122.90	127.76
24	c	902	CLA	OBD-CAD-C3D	-2.23	123.79	128.35
24	c	907	CLA	CGD-CBD-CAD	-2.23	103.05	110.62
27	f	102	SQD	O47-C7-O49	-2.23	117.67	123.67
24	a	409	CLA	CMA-C3A-C2A	-2.23	104.47	114.35
24	B	610	CLA	CGD-CBD-CAD	-2.23	103.07	110.62
27	L	102	SQD	C45-O47-C7	-2.23	112.54	117.89
26	T	102	BCR	C3-C4-C5	-2.23	110.33	113.87
24	b	612	CLA	OBD-CAD-C3D	-2.23	123.81	128.35
24	c	910	CLA	C2A-C1A-CHA	-2.23	119.78	123.89
26	K	102	BCR	C10-C11-C12	-2.23	116.34	123.13
24	C	512	CLA	C1C-NC-C4C	-2.22	103.56	106.27
24	b	613	CLA	CMA-C3A-C2A	-2.22	104.52	114.35
24	C	513	CLA	CBC-CAC-C3C	-2.22	105.61	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	CAA-C2A-C3A	-2.22	106.84	113.22
24	B	606	CLA	CAA-C2A-C3A	-2.21	106.85	113.22
24	B	609	CLA	O2A-CGA-O1A	-2.21	117.78	123.49
24	d	403	CLA	O2D-CGD-O1D	-2.21	119.22	123.79
24	A	407	CLA	CMA-C3A-C2A	-2.21	104.56	114.35
37	E	101	LHG	C5-O7-C7	-2.21	112.58	117.89
36	c	916	DGD	C3G-C2G-C1G	-2.21	106.90	112.07
24	B	603	CLA	C2A-C1A-CHA	-2.21	119.81	123.89
24	C	510	CLA	C3B-CAB-CBB	-2.21	121.80	126.32
24	d	403	CLA	C2A-C1A-CHA	-2.21	119.82	123.89
24	B	605	CLA	C1C-NC-C4C	-2.21	103.59	106.27
31	a	417	PL9	C40-C39-C38	-2.20	119.17	123.50
24	C	508	CLA	O2A-CGA-O1A	-2.20	117.81	123.49
26	b	623	BCR	C21-C20-C19	-2.20	116.41	123.13
24	C	507	CLA	C2A-C1A-CHA	-2.20	119.83	123.89
24	B	608	CLA	C1D-CHD-C4C	-2.20	119.28	122.60
24	b	606	CLA	C2A-C1A-CHA	-2.19	119.84	123.89
24	B	616	CLA	C4A-NA-C1A	-2.19	103.52	106.36
24	b	619	CLA	C4-C3-C2	-2.19	119.20	123.50
24	b	620	CLA	C4B-CHC-C1C	-2.19	124.55	129.26
24	c	907	CLA	C1C-NC-C4C	-2.19	103.60	106.27
24	A	407	CLA	O2A-CGA-O1A	-2.19	117.84	123.49
26	c	915	BCR	C39-C30-C25	-2.19	106.87	110.30
24	A	406	CLA	C4-C3-C2	-2.19	119.21	123.50
24	b	608	CLA	O2A-CGA-O1A	-2.19	117.85	123.49
26	A	411	BCR	C37-C22-C21	-2.19	119.67	122.90
27	L	102	SQD	O47-C7-O49	-2.19	117.81	123.67
24	A	410	CLA	CMA-C3A-C2A	-2.18	104.68	114.35
24	B	602	CLA	C2A-C1A-CHA	-2.18	119.87	123.89
38	v	202	HEM	C3B-C4B-NB	-2.18	107.46	111.63
34	C	501	LMG	C8-O7-C10	-2.17	112.67	117.89
26	b	623	BCR	C7-C8-C9	-2.17	122.90	126.22
24	C	506	CLA	C1C-NC-C4C	-2.17	103.63	106.27
24	A	410	CLA	C4B-CHC-C1C	-2.17	124.60	129.26
24	C	507	CLA	C4C-C3C-C2C	-2.17	103.42	106.94
37	L	101	LHG	C6-C5-C4	-2.17	107.00	112.07
24	C	514	CLA	CAA-C2A-C3A	-2.17	106.99	113.22
24	b	620	CLA	C1C-NC-C4C	-2.17	103.63	106.27
24	B	605	CLA	C2A-C1A-CHA	-2.17	119.90	123.89
26	c	915	BCR	C15-C16-C17	-2.16	118.61	123.39
24	c	902	CLA	C2A-C1A-CHA	-2.16	119.90	123.89
24	b	617	CLA	C2A-C1A-CHA	-2.16	119.90	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409	PHO	C4-C3-C2	-2.16	119.26	123.50
24	A	410	CLA	O2A-CGA-O1A	-2.16	117.91	123.49
24	C	502	CLA	OBD-CAD-C3D	-2.16	123.95	128.35
26	c	915	BCR	C37-C22-C21	-2.16	119.71	122.90
24	B	603	CLA	OBD-CAD-C3D	-2.16	123.95	128.35
24	c	909	CLA	C1C-NC-C4C	-2.16	103.64	106.27
31	D	404	PL9	C15-C14-C13	-2.16	119.27	123.50
24	A	407	CLA	O2D-CGD-O1D	-2.16	119.34	123.79
24	b	614	CLA	C1C-NC-C4C	-2.16	103.65	106.27
36	C	518	DGD	C2G-O2G-C1B	-2.15	112.72	117.89
31	A	419	PL9	C40-C39-C38	-2.15	119.27	123.50
24	b	605	CLA	CBC-CAC-C3C	-2.15	105.81	112.39
24	C	505	CLA	C3B-CAB-CBB	-2.15	121.91	126.32
24	b	610	CLA	C2A-C1A-CHA	-2.15	119.92	123.89
24	C	502	CLA	O1D-CGD-CBD	-2.15	121.54	124.62
24	C	508	CLA	C1C-NC-C4C	-2.15	103.65	106.27
24	B	616	CLA	C2A-C1A-CHA	-2.15	119.92	123.89
24	C	510	CLA	C2A-C1A-CHA	-2.15	119.92	123.89
24	c	902	CLA	C1C-NC-C4C	-2.15	103.65	106.27
37	l	101	LHG	O7-C7-O9	-2.15	117.89	123.67
24	c	912	CLA	O2A-CGA-O1A	-2.15	117.94	123.49
37	d	409	LHG	O7-C7-O9	-2.15	117.90	123.67
24	C	502	CLA	C1C-NC-C4C	-2.14	103.66	106.27
24	B	615	CLA	O2A-CGA-O1A	-2.14	117.96	123.49
24	b	617	CLA	C6-C7-C8	-2.14	108.39	115.49
26	y	101	BCR	C37-C22-C21	-2.14	119.74	122.90
24	B	606	CLA	C3B-CAB-CBB	-2.14	121.94	126.32
24	A	405	CLA	C4A-NA-C1A	-2.14	103.59	106.36
24	b	619	CLA	O2A-CGA-O1A	-2.14	117.98	123.49
37	d	407	LHG	O8-C23-O10	-2.14	117.98	123.49
24	C	509	CLA	C1C-NC-C4C	-2.14	103.67	106.27
24	B	616	CLA	OBD-CAD-C3D	-2.13	124.00	128.35
24	a	406	CLA	C4B-CHC-C1C	-2.13	124.68	129.26
34	b	624	LMG	O8-C28-O10	-2.13	117.99	123.49
24	D	401	CLA	C2A-C1A-CHA	-2.13	119.96	123.89
24	a	406	CLA	C5-C3-C2	-2.13	117.01	121.05
26	B	618	BCR	C21-C20-C19	-2.13	116.65	123.13
24	a	407	CLA	CMA-C3A-C2A	-2.13	104.94	114.35
24	d	403	CLA	CAA-C2A-C3A	-2.13	107.10	113.22
38	V	201	HEM	CBA-CAA-C2A	-2.12	108.72	112.53
24	B	607	CLA	C4B-CHC-C1C	-2.12	124.70	129.26
24	c	906	CLA	C4B-CHC-C1C	-2.12	124.70	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	C6-C7-C8	-2.12	108.46	115.49
24	b	614	CLA	C2A-C1A-CHA	-2.12	119.98	123.89
24	b	612	CLA	C3B-CAB-CBB	-2.12	121.98	126.32
24	C	502	CLA	C4B-CHC-C1C	-2.12	124.72	129.26
24	C	503	CLA	C1C-NC-C4C	-2.12	103.69	106.27
27	F	101	SQD	O47-C7-O49	-2.12	117.99	123.67
24	C	506	CLA	O1D-CGD-CBD	-2.11	121.59	124.62
24	b	611	CLA	OBD-CAD-C3D	-2.11	124.04	128.35
24	A	406	CLA	C4B-CHC-C1C	-2.11	124.72	129.26
24	A	407	CLA	C4-C3-C2	-2.11	119.36	123.50
24	c	905	CLA	O2A-CGA-O1A	-2.11	118.04	123.49
37	D	407	LHG	O8-C23-O10	-2.11	118.04	123.49
24	b	613	CLA	C4-C3-C2	-2.11	119.36	123.50
24	C	504	CLA	O2A-CGA-O1A	-2.11	118.05	123.49
24	B	602	CLA	CBC-CAC-C3C	-2.11	105.95	112.39
26	k	101	BCR	C28-C27-C26	-2.11	110.52	113.87
24	d	401	CLA	O1D-CGD-CBD	-2.11	121.60	124.62
24	c	914	CLA	O2A-CGA-O1A	-2.10	118.06	123.49
24	A	410	CLA	C4C-C3C-C2C	-2.10	103.53	106.94
24	C	508	CLA	C4B-CHC-C1C	-2.10	124.74	129.26
24	C	513	CLA	CBA-CAA-C2A	-2.10	107.80	113.73
24	d	403	CLA	O2A-CGA-O1A	-2.10	118.07	123.49
24	D	402	CLA	C4-C3-C2	-2.10	119.38	123.50
26	K	102	BCR	C15-C14-C13	-2.10	124.16	127.20
24	b	606	CLA	CMA-C3A-C2A	-2.10	105.07	114.35
24	C	509	CLA	C4B-CHC-C1C	-2.10	124.76	129.26
24	b	619	CLA	CBC-CAC-C3C	-2.10	106.00	112.39
24	b	614	CLA	C11-C12-C13	-2.09	108.54	115.49
24	b	612	CLA	C11-C10-C8	-2.09	108.54	115.49
24	C	510	CLA	C16-C15-C13	-2.09	108.56	115.49
24	c	911	CLA	C2A-C1A-CHA	-2.09	120.04	123.89
36	C	517	DGD	O1G-C1G-C2G	-2.09	103.07	108.69
26	A	411	BCR	C8-C7-C6	-2.09	121.05	127.32
38	e	102	HEM	C3B-CAB-CBB	-2.09	121.25	124.46
25	a	408	PHO	O2D-CGD-O1D	-2.09	119.48	123.79
34	B	622	LMG	C9-C8-C7	-2.09	107.19	112.07
26	k	101	BCR	C16-C17-C18	-2.09	124.18	127.20
24	C	506	CLA	O2A-CGA-O1A	-2.09	118.11	123.49
24	b	615	CLA	C4B-CHC-C1C	-2.08	124.78	129.26
24	B	607	CLA	O2D-CGD-O1D	-2.08	119.49	123.79
24	B	607	CLA	O2A-CGA-O1A	-2.08	118.11	123.49
24	b	612	CLA	C4B-CHC-C1C	-2.08	124.79	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	OBD-CAD-C3D	-2.08	124.10	128.35
24	C	502	CLA	C3B-CAB-CBB	-2.08	122.06	126.32
24	b	617	CLA	OBD-CAD-C3D	-2.08	124.11	128.35
26	H	101	BCR	C20-C21-C22	-2.08	124.19	127.20
24	b	615	CLA	OBD-CAD-C3D	-2.08	124.11	128.35
36	h	102	DGD	C3E-C4E-C5E	-2.08	106.58	110.20
24	D	401	CLA	CBC-CAC-C3C	-2.08	106.05	112.39
24	B	612	CLA	C4-C3-C2	-2.07	119.43	123.50
31	D	404	PL9	C20-C19-C18	-2.07	119.43	123.50
24	C	509	CLA	C4A-NA-C1A	-2.07	103.67	106.36
24	B	603	CLA	O2A-CGA-O1A	-2.07	118.14	123.49
26	A	411	BCR	C16-C17-C18	-2.07	124.20	127.20
24	D	402	CLA	CAA-C2A-C3A	-2.07	107.26	113.22
36	C	519	DGD	O1G-C1A-O1A	-2.07	118.15	123.49
24	B	614	CLA	C2A-C1A-CHA	-2.07	120.08	123.89
36	c	917	DGD	C2G-O2G-C1B	-2.07	112.93	117.89
24	C	510	CLA	C1C-NC-C4C	-2.07	103.75	106.27
27	a	402	SQD	O48-C23-O10	-2.07	118.16	123.49
24	B	607	CLA	CBC-CAC-C3C	-2.07	106.08	112.39
24	D	402	CLA	OBD-CAD-C3D	-2.07	124.14	128.35
24	b	607	CLA	C4A-NA-C1A	-2.06	103.68	106.36
24	D	402	CLA	O1D-CGD-CBD	-2.06	121.66	124.62
24	b	614	CLA	CAA-CBA-CGA	-2.06	107.28	113.32
25	A	408	PHO	CHD-C4C-C3C	-2.06	120.48	124.58
24	b	617	CLA	O2D-CGD-O1D	-2.06	119.53	123.79
38	e	102	HEM	C3B-C4B-NB	-2.06	107.69	111.63
24	B	614	CLA	C4B-CHC-C1C	-2.06	124.83	129.26
27	A	416	SQD	O6-C44-C45	-2.06	106.09	110.99
24	d	401	CLA	C4B-CHC-C1C	-2.06	124.84	129.26
25	A	408	PHO	O2D-CGD-O1D	-2.06	119.54	123.79
24	a	406	CLA	C4C-C3C-C2C	-2.06	103.61	106.94
29	m	103	LMT	O6'-C6'-C5'	-2.05	104.54	111.33
26	T	102	BCR	C37-C22-C21	-2.05	119.87	122.90
26	H	101	BCR	C24-C23-C22	-2.05	123.09	126.22
34	Z	101	LMG	C7-O1-C1	-2.05	109.51	113.82
24	C	514	CLA	OBD-CAD-C3D	-2.05	124.17	128.35
24	B	602	CLA	CAA-C2A-C3A	-2.05	107.33	113.22
25	a	420	PHO	C4D-CHA-C1A	-2.05	120.51	125.06
25	A	408	PHO	C1C-C2C-C3C	-2.05	104.05	106.50
24	C	511	CLA	C4-C3-C2	-2.05	119.48	123.50
26	B	619	BCR	C15-C16-C17	-2.05	118.87	123.39
26	C	516	BCR	C32-C1-C6	-2.04	107.10	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	906	CLA	OBD-CAD-C3D	-2.04	124.19	128.35
37	D	406	LHG	O7-C7-O9	-2.04	118.19	123.67
25	A	408	PHO	C4D-CHA-C1A	-2.04	120.52	125.06
31	D	404	PL9	C17-C18-C19	-2.04	123.33	127.76
34	C	520	LMG	O1-C1-C2	-2.04	105.47	108.04
26	T	102	BCR	C7-C8-C9	-2.04	123.11	126.22
24	b	611	CLA	C2A-C1A-CHA	-2.04	120.13	123.89
24	c	907	CLA	C4B-CHC-C1C	-2.04	124.89	129.26
24	C	514	CLA	C4B-CHC-C1C	-2.03	124.89	129.26
24	C	505	CLA	OBD-CAD-C3D	-2.03	124.21	128.35
26	B	619	BCR	C32-C1-C6	-2.03	107.12	110.30
31	d	405	PL9	C40-C39-C38	-2.03	119.51	123.50
24	B	612	CLA	O2D-CGD-O1D	-2.03	119.60	123.79
24	B	612	CLA	CBC-CAC-C3C	-2.03	106.19	112.39
24	a	409	CLA	C1C-NC-C4C	-2.03	103.80	106.27
34	b	624	LMG	C8-O7-C10	-2.03	113.02	117.89
24	b	605	CLA	C4B-CHC-C1C	-2.03	124.90	129.26
31	a	417	PL9	C16-C14-C13	-2.03	117.20	121.05
24	B	603	CLA	C1C-NC-C4C	-2.03	103.80	106.27
24	C	507	CLA	CGD-CBD-CAD	-2.03	103.75	110.62
36	C	517	DGD	C3G-C2G-C1G	-2.03	107.33	112.07
24	C	512	CLA	C11-C10-C8	-2.03	108.77	115.49
24	C	510	CLA	C11-C12-C13	-2.02	108.77	115.49
24	D	401	CLA	CAA-C2A-C3A	-2.02	107.39	113.22
35	B	624	HTG	O2-C2-C3	-2.02	105.78	110.34
24	b	616	CLA	O1D-CGD-CBD	-2.02	121.72	124.62
34	c	920	LMG	O8-C28-O10	-2.02	118.27	123.49
24	D	402	CLA	O2D-CGD-O1D	-2.02	119.62	123.79
24	B	617	CLA	CBC-CAC-C3C	-2.02	106.22	112.39
36	C	517	DGD	O1G-C1A-O1A	-2.02	118.28	123.49
24	C	514	CLA	C4-C3-C2	-2.02	119.54	123.50
36	C	518	DGD	O6D-C1D-O3G	-2.02	105.20	110.05
24	c	908	CLA	O2A-CGA-O1A	-2.02	118.29	123.49
24	B	611	CLA	O2A-CGA-O1A	-2.02	118.29	123.49
24	C	505	CLA	O1D-CGD-CBD	-2.02	121.73	124.62
31	A	419	PL9	C37-C36-C34	-2.01	106.15	112.71
26	b	622	BCR	C11-C10-C9	-2.01	124.29	127.20
34	z	101	LMG	C1-C2-C3	-2.01	106.01	109.97
24	b	620	CLA	C2A-C1A-CHA	-2.01	120.18	123.89
24	B	617	CLA	C1C-NC-C4C	-2.01	103.82	106.27
24	B	609	CLA	C2A-C1A-CHA	-2.01	120.19	123.89
26	k	102	BCR	C37-C22-C21	-2.01	119.94	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	404	BCR	C10-C11-C12	-2.01	117.01	123.13
31	d	405	PL9	C22-C23-C24	-2.01	123.40	127.76
24	C	505	CLA	C5-C3-C2	-2.01	117.25	121.05
24	a	409	CLA	O2A-CGA-O1A	-2.00	118.32	123.49
24	B	608	CLA	C1C-NC-C4C	-2.00	103.83	106.27
24	c	904	CLA	C2A-C1A-CHA	-2.00	120.20	123.89
24	b	610	CLA	CMB-C2B-C3B	2.00	129.00	125.09
24	C	510	CLA	CMB-C2B-C3B	2.00	129.00	125.09
26	T	102	BCR	C2-C1-C6	2.00	113.53	110.36
24	C	507	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	b	617	CLA	CED-O2D-CGD	2.01	120.70	115.99
34	Z	101	LMG	C1-C2-C3	2.01	113.94	109.97
24	B	610	CLA	C4-C3-C5	2.01	118.48	115.41
24	B	615	CLA	CAC-C3C-C4C	2.01	127.75	124.83
24	c	903	CLA	C4-C3-C5	2.01	118.48	115.41
24	c	913	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	a	409	CLA	CED-O2D-CGD	2.02	120.72	115.99
24	c	906	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	b	614	CLA	CED-O2D-CGD	2.02	120.72	115.99
24	a	409	CLA	CMB-C2B-C3B	2.02	129.04	125.09
25	a	408	PHO	C4D-C3D-CAD	2.02	109.15	105.51
24	B	617	CLA	CMB-C2B-C3B	2.03	129.05	125.09
26	D	403	BCR	C37-C22-C23	2.03	121.47	118.10
31	D	404	PL9	C45-C44-C46	2.03	118.50	115.41
29	f	103	LMT	O5'-C5'-C4'	2.03	114.03	109.75
24	A	410	CLA	CAC-C3C-C4C	2.03	127.78	124.83
24	a	406	CLA	CMC-C2C-C1C	2.03	128.16	125.02
24	A	407	CLA	O2A-CGA-CBA	2.03	118.09	111.90
26	K	102	BCR	C37-C22-C23	2.03	121.48	118.10
29	a	401	LMT	O1'-C1'-C2'	2.04	110.61	108.04
24	d	401	CLA	CED-O2D-CGD	2.04	120.77	115.99
26	y	101	BCR	C37-C22-C23	2.04	121.49	118.10
24	b	608	CLA	CMB-C2B-C3B	2.04	129.07	125.09
34	C	501	LMG	O6-C5-C4	2.04	113.51	109.68
24	A	406	CLA	CAC-C3C-C4C	2.04	127.79	124.83
34	j	101	LMG	O7-C10-C11	2.04	115.96	111.53
24	b	606	CLA	CMB-C2B-C3B	2.04	129.08	125.09
26	K	103	BCR	C2-C1-C6	2.04	113.60	110.36
34	C	520	LMG	O6-C5-C6	2.04	111.52	106.36
36	H	102	DGD	O6E-C5E-C6E	2.04	111.52	106.36
31	D	404	PL9	C51-C49-C50	2.05	119.67	114.64
24	B	611	CLA	CHC-C1C-NC	2.05	127.53	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	907	CLA	CAA-CBA-CGA	2.05	119.33	113.32
26	H	101	BCR	C29-C30-C25	2.05	113.62	110.36
24	c	914	CLA	CHB-C4A-NA	2.06	127.36	124.51
36	c	916	DGD	O6E-C5E-C4E	2.06	113.55	109.68
36	C	517	DGD	O1G-C1A-C2A	2.06	118.17	111.90
25	a	420	PHO	CMB-C2B-C1B	2.06	128.41	125.06
24	b	614	CLA	CMC-C2C-C1C	2.06	128.21	125.02
26	T	102	BCR	C37-C22-C23	2.06	121.53	118.10
24	d	401	CLA	CMB-C2B-C1B	2.06	131.78	128.36
36	D	405	DGD	C1E-O6E-C5E	2.07	117.75	113.75
31	D	404	PL9	C30-C29-C31	2.07	118.57	115.41
25	A	409	PHO	C4D-C3D-CAD	2.07	109.23	105.51
34	C	521	LMG	O8-C28-C29	2.07	118.21	111.90
34	z	101	LMG	C9-O8-C28	2.07	122.64	116.85
24	c	909	CLA	CMB-C2B-C3B	2.07	129.14	125.09
24	B	616	CLA	C4-C3-C5	2.08	118.58	115.41
24	C	510	CLA	O2A-CGA-CBA	2.08	118.23	111.90
36	C	518	DGD	C6D-C5D-C4D	2.09	116.75	112.03
24	c	905	CLA	C6-C5-C3	2.09	117.06	112.48
24	B	616	CLA	O2A-CGA-CBA	2.09	118.26	111.90
34	j	101	LMG	O8-C28-C29	2.09	118.26	111.90
25	a	420	PHO	C4D-C3D-CAD	2.09	109.27	105.51
24	D	401	CLA	CED-O2D-CGD	2.09	120.89	115.99
24	B	614	CLA	CMC-C2C-C1C	2.09	128.26	125.02
24	B	603	CLA	CHB-C4A-NA	2.09	127.41	124.51
26	d	404	BCR	C35-C13-C12	2.09	121.58	118.10
24	b	611	CLA	CAC-C3C-C4C	2.10	127.87	124.83
24	c	902	CLA	O2A-CGA-CBA	2.10	118.30	111.90
24	c	914	CLA	CED-O2D-CGD	2.10	120.92	115.99
35	b	603	HTG	O5-C1-C2	2.10	113.04	110.19
25	A	409	PHO	CMC-C2C-C1C	2.11	128.49	125.06
24	c	905	CLA	CMB-C2B-C3B	2.11	129.22	125.09
24	B	614	CLA	C6-C5-C3	2.11	117.12	112.48
36	h	102	DGD	O5D-C1E-C2E	2.12	110.71	108.04
24	c	905	CLA	O2A-CGA-CBA	2.12	118.35	111.90
24	b	618	CLA	CHB-C4A-NA	2.12	127.44	124.51
34	Z	101	LMG	C9-O8-C28	2.12	122.50	117.14
34	Z	101	LMG	O1-C1-C2	2.12	110.72	108.04
24	b	613	CLA	C4-C3-C5	2.12	118.64	115.41
26	B	618	BCR	C37-C22-C23	2.12	121.62	118.10
24	B	605	CLA	CMB-C2B-C3B	2.12	129.24	125.09
24	C	512	CLA	CED-O2D-CGD	2.12	120.97	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	404	BCR	C37-C22-C23	2.12	121.63	118.10
24	d	403	CLA	O2A-CGA-CBA	2.12	118.37	111.90
24	C	512	CLA	CMB-C2B-C3B	2.13	129.25	125.09
25	a	420	PHO	C2C-C1C-NC	2.13	112.92	109.73
24	a	407	CLA	CMB-C2B-C3B	2.13	129.25	125.09
24	B	616	CLA	CED-O2D-CGD	2.13	120.98	115.99
24	B	616	CLA	C3D-CAD-CBD	2.13	110.61	107.60
24	B	609	CLA	C4-C3-C5	2.13	118.66	115.41
24	B	615	CLA	CMB-C2B-C3B	2.14	129.27	125.09
24	b	605	CLA	CAC-C3C-C2C	2.14	131.26	127.51
25	a	420	PHO	C2A-C1A-NA	2.14	114.83	112.08
26	k	102	BCR	C29-C30-C25	2.14	113.76	110.36
24	b	613	CLA	C6-C5-C3	2.15	117.20	112.48
24	b	610	CLA	CAC-C3C-C4C	2.15	127.95	124.83
24	A	405	CLA	CMB-C2B-C3B	2.15	129.29	125.09
31	d	405	PL9	C30-C29-C31	2.15	118.69	115.41
35	b	603	HTG	C1-O5-C5	2.15	116.84	112.74
24	b	612	CLA	C4-C3-C5	2.16	118.70	115.41
24	c	909	CLA	O2A-CGA-CBA	2.16	118.47	111.90
24	A	406	CLA	O2A-CGA-CBA	2.16	118.47	111.90
29	C	522	LMT	O5'-C5'-C4'	2.16	114.31	109.75
31	a	417	PL9	C45-C44-C46	2.16	118.71	115.41
36	D	405	DGD	O5D-C1E-C2E	2.16	110.77	108.04
24	b	619	CLA	CMC-C2C-C1C	2.17	128.37	125.02
29	f	103	LMT	O1B-C1B-C2B	2.17	113.38	108.10
34	C	501	LMG	O8-C28-C29	2.17	118.50	111.90
31	a	417	PL9	C51-C49-C50	2.17	119.97	114.64
37	d	408	LHG	O8-C23-C24	2.17	118.51	111.90
24	b	619	CLA	CMB-C2B-C3B	2.17	129.33	125.09
24	B	604	CLA	CAC-C3C-C4C	2.17	127.98	124.83
24	b	607	CLA	CHB-C4A-NA	2.17	127.51	124.51
24	B	606	CLA	CMC-C2C-C1C	2.17	128.38	125.02
27	A	412	SQD	C3-C4-C5	2.17	113.99	110.20
27	a	411	SQD	O7-S-C6	2.18	108.78	106.94
26	k	102	BCR	C36-C18-C19	2.18	121.72	118.10
24	B	604	CLA	C6-C5-C3	2.18	117.28	112.48
24	d	402	CLA	C3D-CAD-CBD	2.19	110.69	107.60
24	C	509	CLA	CMB-C2B-C3B	2.19	129.38	125.09
24	B	603	CLA	CMC-C2C-C1C	2.19	128.41	125.02
35	O	303	HTG	C1'-S1-C1	2.19	103.32	100.30
26	D	403	BCR	C30-C25-C24	2.19	121.97	115.82
24	c	908	CLA	CHB-C4A-NA	2.20	127.55	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t	101	BCR	C31-C1-C6	2.20	113.75	110.30
24	B	608	CLA	CMB-C2B-C3B	2.20	129.39	125.09
34	Z	101	LMG	C1-O6-C5	2.20	118.02	113.75
24	d	401	CLA	CAA-CBA-CGA	2.21	119.78	113.32
25	A	409	PHO	O2A-CGA-CBA	2.21	118.62	111.90
29	M	101	LMT	O5B-C5B-C6B	2.21	111.93	106.36
34	C	501	LMG	O1-C1-C2	2.21	110.83	108.04
35	b	627	HTG	C1-C2-C3	2.21	115.59	110.69
24	B	605	CLA	C4-C3-C5	2.22	118.80	115.41
24	B	614	CLA	CMB-C2B-C3B	2.22	129.43	125.09
24	A	410	CLA	CHB-C4A-NA	2.22	127.59	124.51
27	a	402	SQD	C3-C4-C5	2.23	114.08	110.20
24	D	401	CLA	C4-C3-C5	2.23	118.81	115.41
27	A	416	SQD	O5-C5-C4	2.23	113.86	109.68
24	B	612	CLA	CHB-C4A-NA	2.23	127.60	124.51
29	a	401	LMT	C1'-O5'-C5'	2.23	118.08	113.75
24	a	409	CLA	CAC-C3C-C4C	2.23	128.07	124.83
24	D	402	CLA	O2A-CGA-CBA	2.23	118.70	111.90
24	C	512	CLA	CMC-C2C-C1C	2.23	128.47	125.02
35	b	626	HTG	O5-C1-C2	2.24	113.23	110.19
24	B	602	CLA	CMC-C2C-C1C	2.24	128.49	125.02
36	C	518	DGD	O6E-C5E-C6E	2.24	112.02	106.36
34	C	521	LMG	C9-O8-C28	2.24	123.12	116.85
24	C	507	CLA	O2A-CGA-CBA	2.24	118.74	111.90
29	E	102	LMT	O1'-C1'-C2'	2.25	110.89	108.04
24	B	613	CLA	CMB-C2B-C3B	2.26	129.50	125.09
38	e	102	HEM	CAD-CBD-CGD	2.26	122.22	113.02
24	C	509	CLA	CAC-C3C-C4C	2.26	128.11	124.83
24	c	908	CLA	C4-C3-C5	2.26	118.86	115.41
26	C	515	BCR	C2-C1-C6	2.27	113.95	110.36
24	B	609	CLA	CAC-C3C-C4C	2.27	128.13	124.83
24	d	403	CLA	CMB-C2B-C3B	2.28	129.54	125.09
24	d	401	CLA	O2A-CGA-CBA	2.28	118.84	111.90
24	b	614	CLA	CHB-C4A-NA	2.28	127.66	124.51
24	C	508	CLA	C4-C3-C5	2.28	118.89	115.41
24	C	513	CLA	CHB-C4A-NA	2.28	127.67	124.51
25	a	408	PHO	CBD-CHA-C1A	2.28	131.74	126.36
24	b	605	CLA	CMB-C2B-C3B	2.28	129.56	125.09
24	C	508	CLA	CAC-C3C-C4C	2.29	128.15	124.83
36	D	405	DGD	O6D-C5D-C6D	2.29	111.29	106.61
24	B	603	CLA	CMB-C2B-C3B	2.29	129.57	125.09
26	k	102	BCR	C2-C1-C6	2.29	113.99	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	621	SQD	C3-C4-C5	2.29	114.20	110.20
24	C	504	CLA	O2A-CGA-CBA	2.30	118.91	111.90
26	D	403	BCR	C38-C26-C27	2.30	117.80	113.43
24	b	619	CLA	O2A-CGA-CBA	2.30	118.92	111.90
24	D	401	CLA	CMC-C2C-C1C	2.31	128.59	125.02
37	e	101	LHG	O8-C23-C24	2.31	118.93	111.90
24	C	513	CLA	CMB-C2B-C3B	2.31	129.60	125.09
24	B	617	CLA	C4-C3-C5	2.31	118.93	115.41
26	h	101	BCR	C7-C6-C5	2.31	126.66	121.37
24	C	509	CLA	CMC-C2C-C1C	2.31	128.60	125.02
26	B	618	BCR	C29-C30-C25	2.32	114.03	110.36
24	a	406	CLA	CMB-C2B-C3B	2.32	129.63	125.09
24	c	907	CLA	CMB-C2B-C3B	2.32	129.63	125.09
25	A	408	PHO	C2C-C1C-NC	2.32	113.21	109.73
24	A	406	CLA	CAA-CBA-CGA	2.32	120.12	113.32
24	D	402	CLA	CAC-C3C-C4C	2.33	128.21	124.83
24	C	503	CLA	C3D-CAD-CBD	2.33	110.89	107.60
27	f	102	SQD	C3-C4-C5	2.33	114.26	110.20
24	B	608	CLA	O2A-CGA-CBA	2.33	119.01	111.90
24	b	612	CLA	CMB-C2B-C3B	2.34	129.66	125.09
36	c	917	DGD	O3G-C1D-C2D	2.34	111.00	108.04
29	f	103	LMT	O5B-C5B-C4B	2.34	114.08	109.68
25	A	409	PHO	C2A-C1A-NA	2.34	115.08	112.08
35	B	634	HTG	O5-C5-C4	2.34	114.08	109.68
38	E	103	HEM	CAD-CBD-CGD	2.35	122.60	113.02
25	a	420	PHO	C2B-C1B-NB	2.36	113.26	109.73
31	A	419	PL9	C8-C7-C3	2.36	118.97	111.60
24	B	614	CLA	CAC-C3C-C4C	2.36	128.25	124.83
24	B	611	CLA	C3D-CAD-CBD	2.36	110.94	107.60
24	C	504	CLA	CMC-C2C-C1C	2.36	128.68	125.02
25	a	408	PHO	C2B-C1B-NB	2.36	113.27	109.73
24	C	506	CLA	O2A-CGA-CBA	2.37	119.11	111.90
25	a	408	PHO	C2A-C1A-NA	2.38	115.13	112.08
24	b	612	CLA	CAC-C3C-C4C	2.38	128.29	124.83
35	C	524	HTG	O5-C5-C4	2.39	114.17	109.68
24	b	618	CLA	C4-C3-C5	2.39	119.06	115.41
24	C	511	CLA	CMB-C2B-C3B	2.39	129.77	125.09
35	c	923	HTG	O5-C5-C4	2.39	114.17	109.68
38	E	103	HEM	CHC-C4B-NB	2.40	130.29	124.52
27	A	412	SQD	O7-S-C6	2.40	108.96	106.94
24	b	612	CLA	CMC-C2C-C1C	2.40	128.74	125.02
36	C	518	DGD	O1G-C1A-C2A	2.40	119.22	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409	PHO	CAC-C3C-C4C	2.41	127.97	125.16
24	a	407	CLA	C4-C3-C5	2.41	119.09	115.41
24	a	407	CLA	CMC-C2C-C1C	2.42	128.76	125.02
24	C	507	CLA	CMC-C2C-C1C	2.42	128.76	125.02
24	B	607	CLA	O2A-CGA-CBA	2.42	119.26	111.90
24	B	608	CLA	CMC-C2C-C1C	2.42	128.76	125.02
24	C	502	CLA	CMB-C2B-C3B	2.42	129.82	125.09
24	C	504	CLA	CMB-C2B-C3B	2.42	129.82	125.09
24	C	502	CLA	O2A-CGA-CBA	2.42	119.28	111.90
24	C	506	CLA	CMC-C2C-C1C	2.42	128.77	125.02
24	C	509	CLA	O2A-CGA-CBA	2.43	119.29	111.90
35	B	634	HTG	C1-O5-C5	2.44	117.39	112.74
27	A	416	SQD	C3-C4-C5	2.44	114.45	110.20
29	a	401	LMT	O5'-C5'-C4'	2.45	114.92	109.75
31	A	419	PL9	C40-C39-C41	2.45	119.15	115.41
24	b	615	CLA	O2A-CGA-CBA	2.45	119.37	111.90
24	a	409	CLA	CMC-C2C-C1C	2.45	128.82	125.02
24	B	603	CLA	O2A-CGA-CBA	2.46	119.39	111.90
24	C	503	CLA	CMC-C2C-C1C	2.46	128.82	125.02
24	C	514	CLA	O2A-CGA-CBA	2.46	119.39	111.90
24	b	617	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	a	408	PHO	CMC-C2C-C1C	2.47	129.07	125.06
36	C	519	DGD	O2G-C1B-C2B	2.47	116.90	111.53
37	l	101	LHG	O8-C23-C24	2.47	119.43	111.90
29	b	601	LMT	O5'-C1'-C2'	2.47	115.35	110.28
38	e	102	HEM	CMD-C2D-C3D	2.47	125.29	114.35
35	C	524	HTG	O5-C1-C2	2.47	113.55	110.19
29	m	104	LMT	O5'-C5'-C4'	2.48	114.98	109.75
27	a	411	SQD	O48-C23-C24	2.48	119.44	111.90
24	B	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	T	102	BCR	C1-C6-C7	2.49	122.78	115.82
24	b	607	CLA	CMC-C2C-C1C	2.49	128.87	125.02
24	B	604	CLA	CMC-C2C-C1C	2.50	128.89	125.02
24	C	508	CLA	O2A-CGA-CBA	2.50	119.52	111.90
24	C	502	CLA	C4-C3-C5	2.50	119.23	115.41
36	C	519	DGD	O1G-C1A-C2A	2.50	119.53	111.90
24	b	620	CLA	C4-C3-C5	2.51	119.24	115.41
25	a	420	PHO	O2A-CGA-CBA	2.51	119.55	111.90
24	d	403	CLA	C4-C3-C5	2.51	119.24	115.41
31	a	417	PL9	C53-C6-C1	2.52	120.96	114.94
24	C	508	CLA	CMC-C2C-C1C	2.52	128.92	125.02
24	B	605	CLA	CMC-C2C-C1C	2.52	128.93	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	CMB-C2B-C3B	2.53	130.04	125.09
31	D	404	PL9	C25-C24-C26	2.53	119.27	115.41
24	a	409	CLA	O2A-CGA-CBA	2.53	119.62	111.90
24	b	613	CLA	O2A-CGA-CBA	2.54	119.64	111.90
25	A	408	PHO	CAC-C3C-C4C	2.54	128.13	125.16
24	C	503	CLA	O2A-CGA-CBA	2.54	119.64	111.90
24	c	902	CLA	CAC-C3C-C4C	2.55	128.53	124.83
24	b	606	CLA	CMC-C2C-C1C	2.55	128.96	125.02
25	a	408	PHO	C3C-C4C-NC	2.55	114.36	110.24
31	A	419	PL9	C30-C29-C31	2.55	119.30	115.41
26	a	410	BCR	C2-C1-C6	2.55	114.40	110.36
24	b	606	CLA	O2A-CGA-CBA	2.55	119.67	111.90
24	c	913	CLA	CED-O2D-CGD	2.55	121.98	115.99
24	A	405	CLA	O2A-CGA-CBA	2.56	119.70	111.90
24	c	911	CLA	O2A-CGA-CBA	2.56	119.70	111.90
25	A	408	PHO	C4D-C3D-CAD	2.57	110.13	105.51
25	A	408	PHO	C2B-C1B-NB	2.57	113.59	109.73
24	b	607	CLA	CMB-C2B-C3B	2.57	130.12	125.09
24	b	618	CLA	CMC-C2C-C1C	2.58	129.00	125.02
24	B	609	CLA	CHB-C4A-NA	2.58	128.07	124.51
24	C	513	CLA	O2A-CGA-CBA	2.58	119.75	111.90
34	Z	101	LMG	O6-C5-C4	2.58	114.52	109.68
37	d	409	LHG	O8-C23-C24	2.58	119.76	111.90
34	a	412	LMG	O8-C28-C29	2.58	119.77	111.90
24	B	612	CLA	O2A-CGA-CBA	2.58	119.77	111.90
25	A	408	PHO	C4-C3-C5	2.59	119.36	115.41
24	B	614	CLA	CHB-C4A-NA	2.59	128.09	124.51
36	d	406	DGD	O1G-C1A-C2A	2.59	119.79	111.90
36	H	102	DGD	O1G-C1A-C2A	2.59	119.79	111.90
24	C	514	CLA	CAC-C3C-C4C	2.59	128.59	124.83
24	b	608	CLA	C4-C3-C5	2.60	119.37	115.41
24	c	913	CLA	O2A-CGA-CBA	2.60	119.81	111.90
25	A	409	PHO	C3C-C4C-NC	2.60	114.44	110.24
26	t	101	BCR	C1-C6-C7	2.60	123.10	115.82
24	c	906	CLA	CMC-C2C-C1C	2.60	129.04	125.02
24	C	514	CLA	CMB-C2B-C3B	2.60	130.18	125.09
25	A	408	PHO	C3C-C4C-NC	2.60	114.44	110.24
24	B	607	CLA	CMB-C2B-C3B	2.60	130.18	125.09
24	B	617	CLA	O2A-CGA-CBA	2.61	119.84	111.90
24	b	609	CLA	O2A-CGA-CBA	2.61	119.84	111.90
31	d	405	PL9	C20-C19-C21	2.61	119.39	115.41
36	c	918	DGD	O1G-C1A-C2A	2.61	119.85	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	616	CLA	CMC-C2C-C1C	2.61	129.06	125.02
24	c	910	CLA	O2A-CGA-CBA	2.61	119.86	111.90
29	A	417	LMT	C1'-O5'-C5'	2.62	118.82	113.75
24	d	401	CLA	CAC-C3C-C4C	2.62	128.63	124.83
24	C	507	CLA	CAC-C3C-C4C	2.62	128.63	124.83
24	c	905	CLA	CAC-C3C-C4C	2.62	128.64	124.83
24	b	613	CLA	C3B-C4B-NB	2.63	112.61	109.21
24	C	510	CLA	CMC-C2C-C1C	2.63	129.09	125.02
38	E	103	HEM	CMD-C2D-C3D	2.63	125.97	114.35
24	B	614	CLA	CED-O2D-CGD	2.63	122.16	115.99
36	D	405	DGD	C3D-C4D-C5D	2.63	114.78	110.20
31	d	405	PL9	C35-C34-C36	2.63	119.43	115.41
24	C	505	CLA	CAC-C3C-C4C	2.64	128.66	124.83
24	B	603	CLA	C4-C3-C5	2.64	119.44	115.41
29	m	103	LMT	C1'-C2'-C3'	2.64	115.18	109.97
38	V	201	HEM	CMD-C2D-C3D	2.65	126.07	114.35
24	c	911	CLA	CAC-C3C-C4C	2.65	128.68	124.83
24	D	401	CLA	CAC-C3C-C4C	2.66	128.69	124.83
25	A	408	PHO	C2A-C1A-NA	2.66	115.48	112.08
27	a	402	SQD	O5-C5-C4	2.66	114.67	109.68
24	B	602	CLA	C4-C3-C5	2.66	119.47	115.41
24	B	602	CLA	CAC-C3C-C4C	2.66	128.69	124.83
37	D	408	LHG	O8-C23-C24	2.67	120.02	111.90
38	v	202	HEM	CMD-C2D-C3D	2.67	126.15	114.35
24	B	610	CLA	CMB-C2B-C1B	2.67	132.78	128.36
26	D	403	BCR	C29-C30-C25	2.67	114.59	110.36
38	e	102	HEM	C2D-C3D-C4D	2.67	106.03	101.50
27	F	101	SQD	O48-C23-C24	2.67	120.04	111.90
27	A	416	SQD	O9-S-C6	2.67	109.19	106.94
36	d	406	DGD	C1E-O6E-C5E	2.68	118.94	113.75
24	c	903	CLA	CMC-C2C-C1C	2.68	129.16	125.02
25	A	409	PHO	C2C-C1C-NC	2.68	113.75	109.73
24	B	606	CLA	O2A-CGA-CBA	2.68	120.06	111.90
34	J	101	LMG	O8-C28-C29	2.68	120.06	111.90
34	c	920	LMG	O6-C5-C4	2.68	114.71	109.68
24	c	908	CLA	CMC-C2C-C1C	2.68	129.17	125.02
24	c	904	CLA	O2A-CGA-CBA	2.69	120.09	111.90
24	B	605	CLA	O2A-CGA-CBA	2.69	120.09	111.90
24	A	406	CLA	CED-O2D-CGD	2.69	122.30	115.99
24	C	513	CLA	CMC-C2C-C1C	2.69	129.18	125.02
24	A	410	CLA	O2A-CGA-CBA	2.70	120.12	111.90
24	c	903	CLA	CAC-C3C-C4C	2.70	128.75	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	O2A-CGA-CBA	2.71	120.14	111.90
24	B	608	CLA	CAC-C3C-C4C	2.71	128.76	124.83
24	c	908	CLA	CAC-C3C-C4C	2.71	128.76	124.83
24	A	407	CLA	CED-O2D-CGD	2.71	122.35	115.99
34	b	624	LMG	O7-C10-C11	2.71	117.42	111.53
24	B	608	CLA	C4-C3-C5	2.72	119.56	115.41
24	c	910	CLA	C4-C3-C5	2.72	119.56	115.41
24	B	613	CLA	C4-C3-C5	2.72	119.57	115.41
24	c	912	CLA	CAC-C3C-C4C	2.73	128.79	124.83
24	b	617	CLA	C4-C3-C5	2.73	119.57	115.41
24	b	614	CLA	CAC-C3C-C4C	2.73	128.79	124.83
36	D	405	DGD	C4D-C3D-C2D	2.73	115.88	110.79
24	B	610	CLA	CAC-C3C-C4C	2.73	128.79	124.83
26	B	619	BCR	C2-C1-C6	2.73	114.69	110.36
24	a	407	CLA	C3B-C4B-NB	2.73	112.74	109.21
26	b	623	BCR	C2-C1-C6	2.74	114.69	110.36
25	A	409	PHO	C2B-C1B-NB	2.74	113.84	109.73
24	C	504	CLA	CAC-C3C-C4C	2.74	128.81	124.83
24	c	910	CLA	CMB-C2B-C3B	2.75	130.46	125.09
24	A	406	CLA	CHB-C4A-NA	2.75	128.31	124.51
31	d	405	PL9	C40-C39-C41	2.75	119.61	115.41
35	B	626	HTG	O5-C1-C2	2.75	113.93	110.19
29	m	102	LMT	O5'-C5'-C4'	2.76	115.57	109.75
34	c	920	LMG	O8-C28-C29	2.76	120.30	111.90
24	c	910	CLA	CAC-C3C-C4C	2.76	128.83	124.83
24	c	914	CLA	C4-C3-C5	2.76	119.62	115.41
24	b	606	CLA	C4-C3-C5	2.76	119.62	115.41
24	c	911	CLA	CMC-C2C-C1C	2.76	129.30	125.02
25	a	420	PHO	C3C-C4C-NC	2.77	114.71	110.24
27	f	102	SQD	O48-C23-C24	2.77	120.34	111.90
27	L	102	SQD	O48-C23-C24	2.77	120.35	111.90
24	a	409	CLA	C4-C3-C5	2.77	119.64	115.41
24	b	608	CLA	O2A-CGA-CBA	2.78	120.36	111.90
24	c	902	CLA	CMC-C2C-C1C	2.78	129.33	125.02
24	B	612	CLA	CMC-C2C-C1C	2.79	129.33	125.02
36	H	102	DGD	O2G-C1B-C2B	2.79	117.58	111.53
36	D	405	DGD	O1G-C1A-C2A	2.79	120.40	111.90
24	B	610	CLA	C6-C5-C3	2.79	118.61	112.48
24	B	606	CLA	C4-C3-C5	2.79	119.67	115.41
24	b	618	CLA	CAC-C3C-C4C	2.79	128.89	124.83
34	z	101	LMG	O8-C28-C29	2.80	120.42	111.90
26	b	623	BCR	C37-C22-C23	2.80	122.75	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	CAC-C3C-C4C	2.80	128.90	124.83
24	A	405	CLA	CAC-C3C-C4C	2.80	128.90	124.83
24	b	617	CLA	CAC-C3C-C4C	2.80	128.90	124.83
24	B	616	CLA	CAC-C3C-C4C	2.81	128.90	124.83
24	c	912	CLA	C4-C3-C5	2.81	119.69	115.41
24	b	605	CLA	O2A-CGA-CBA	2.81	120.46	111.90
24	b	616	CLA	O2A-CGA-CBA	2.81	120.47	111.90
31	A	419	PL9	C45-C44-C46	2.81	119.70	115.41
24	b	620	CLA	O2A-CGA-CBA	2.81	120.47	111.90
24	C	510	CLA	C4-C3-C5	2.82	119.71	115.41
24	b	610	CLA	O2A-CGA-CBA	2.82	120.48	111.90
31	a	417	PL9	C40-C39-C41	2.82	119.71	115.41
27	F	101	SQD	C3-C4-C5	2.82	115.11	110.20
31	d	405	PL9	C45-C44-C46	2.82	119.71	115.41
24	c	912	CLA	CMB-C2B-C3B	2.82	130.61	125.09
24	b	611	CLA	CAA-CBA-CGA	2.82	121.58	113.32
36	h	102	DGD	O2G-C1B-C2B	2.83	117.68	111.53
24	C	511	CLA	CMC-C2C-C1C	2.83	129.40	125.02
24	B	616	CLA	CMC-C2C-C1C	2.83	129.40	125.02
24	B	609	CLA	CMC-C2C-C1C	2.84	129.41	125.02
25	a	408	PHO	C2C-C1C-NC	2.84	113.98	109.73
31	A	419	PL9	C53-C6-C1	2.84	121.72	114.94
34	J	101	LMG	O7-C10-C11	2.84	117.70	111.53
24	C	513	CLA	C4-C3-C5	2.85	119.76	115.41
24	d	403	CLA	CAC-C3C-C4C	2.85	128.97	124.83
24	c	903	CLA	O2A-CGA-CBA	2.86	120.60	111.90
24	c	908	CLA	O2A-CGA-CBA	2.86	120.62	111.90
24	B	607	CLA	CAC-C3C-C4C	2.87	128.99	124.83
24	A	405	CLA	CMC-C2C-C1C	2.87	129.46	125.02
24	c	912	CLA	O2A-CGA-CBA	2.87	120.64	111.90
24	d	403	CLA	CMC-C2C-C1C	2.87	129.46	125.02
27	a	402	SQD	O6-C1-C2	2.88	111.67	108.04
31	A	419	PL9	C35-C34-C36	2.88	119.81	115.41
24	C	507	CLA	C4-C3-C5	2.88	119.81	115.41
29	C	522	LMT	C1B-O5B-C5B	2.88	119.34	113.75
24	A	406	CLA	CMB-C2B-C3B	2.88	130.73	125.09
37	L	101	LHG	O8-C23-C24	2.88	120.69	111.90
24	C	511	CLA	C4-C3-C5	2.89	119.81	115.41
31	d	405	PL9	C15-C14-C16	2.89	119.82	115.41
24	B	615	CLA	O2A-CGA-CBA	2.89	120.71	111.90
24	c	903	CLA	C3B-C4B-NB	2.89	112.95	109.21
24	b	620	CLA	CMB-C2B-C3B	2.90	130.76	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	O2A-CGA-CBA	2.90	120.73	111.90
38	v	202	HEM	C2D-C3D-C4D	2.90	106.42	101.50
29	A	417	LMT	O5'-C5'-C4'	2.90	115.87	109.75
24	B	604	CLA	CMB-C2B-C3B	2.90	130.77	125.09
24	b	615	CLA	CMC-C2C-C1C	2.90	129.51	125.02
24	c	907	CLA	CMC-C2C-C1C	2.91	129.52	125.02
24	b	611	CLA	CMC-C2C-C1C	2.91	129.52	125.02
31	A	419	PL9	C25-C24-C26	2.91	119.86	115.41
29	f	103	LMT	C1B-O5B-C5B	2.91	119.40	113.75
26	d	404	BCR	C38-C26-C27	2.91	118.95	113.43
37	L	101	LHG	O7-C7-C8	2.92	117.87	111.53
24	b	614	CLA	C4-C3-C5	2.92	119.86	115.41
37	d	407	LHG	O8-C23-C24	2.92	120.79	111.90
24	b	605	CLA	C3B-C4B-NB	2.92	112.98	109.21
27	B	621	SQD	O48-C23-C24	2.92	120.79	111.90
24	a	409	CLA	CHB-C4A-NA	2.92	128.55	124.51
24	c	907	CLA	C4-C3-C5	2.92	119.87	115.41
31	D	404	PL9	C53-C6-C1	2.92	121.92	114.94
24	B	609	CLA	O2A-CGA-CBA	2.93	120.83	111.90
31	a	417	PL9	C20-C19-C21	2.93	119.89	115.41
37	D	406	LHG	O7-C7-C8	2.94	117.91	111.53
24	a	407	CLA	O2A-CGA-CBA	2.94	120.87	111.90
24	c	914	CLA	CAC-C3C-C4C	2.95	129.11	124.83
31	d	405	PL9	C53-C6-C1	2.95	121.98	114.94
36	h	102	DGD	O1G-C1A-C2A	2.95	120.89	111.90
26	b	622	BCR	C29-C30-C25	2.95	115.04	110.36
25	a	408	PHO	CAC-C3C-C4C	2.96	128.61	125.16
24	c	904	CLA	CAC-C3C-C4C	2.96	129.13	124.83
24	b	611	CLA	C4-C3-C5	2.96	119.93	115.41
24	c	904	CLA	CMC-C2C-C1C	2.97	129.62	125.02
25	a	408	PHO	CMB-C2B-C1B	2.97	129.90	125.06
24	C	506	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	c	913	CLA	CMC-C2C-C1C	2.97	129.62	125.02
24	b	607	CLA	CAC-C3C-C4C	2.98	129.15	124.83
24	b	617	CLA	O2A-CGA-CBA	2.98	120.98	111.90
31	a	417	PL9	C25-C24-C26	2.98	119.96	115.41
24	c	905	CLA	C4-C3-C5	2.99	119.97	115.41
24	B	611	CLA	CAC-C3C-C4C	2.99	129.17	124.83
24	b	616	CLA	CAC-C3C-C4C	2.99	129.17	124.83
24	d	402	CLA	C4-C3-C5	2.99	119.98	115.41
24	D	401	CLA	O2A-CGA-CBA	2.99	121.02	111.90
24	a	406	CLA	C4-C3-C5	3.00	119.99	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	904	CLA	C4-C3-C5	3.00	120.00	115.41
24	C	508	CLA	C3B-C4B-NB	3.01	113.10	109.21
34	a	412	LMG	O1-C1-C2	3.01	111.84	108.04
24	B	615	CLA	C4-C3-C5	3.01	120.01	115.41
24	B	606	CLA	C3B-C4B-NB	3.02	113.11	109.21
24	C	502	CLA	CAC-C3C-C4C	3.02	129.22	124.83
24	C	503	CLA	C4-C3-C5	3.02	120.02	115.41
24	c	913	CLA	C4-C3-C5	3.02	120.02	115.41
31	D	404	PL9	C20-C19-C21	3.02	120.03	115.41
38	E	103	HEM	C2D-C3D-C4D	3.02	106.63	101.50
24	b	609	CLA	C3B-C4B-NB	3.03	113.12	109.21
24	c	907	CLA	CAC-C3C-C4C	3.03	129.22	124.83
24	c	914	CLA	O2A-CGA-CBA	3.03	121.14	111.90
27	a	402	SQD	O9-S-C6	3.04	109.51	106.94
31	D	404	PL9	C40-C39-C41	3.06	120.08	115.41
24	B	614	CLA	O2D-CGD-CBD	3.06	115.50	111.30
24	B	611	CLA	C4-C3-C5	3.06	120.08	115.41
24	C	506	CLA	CAC-C3C-C4C	3.06	129.28	124.83
24	B	611	CLA	O2A-CGA-CBA	3.06	121.24	111.90
24	A	405	CLA	O2D-CGD-CBD	3.07	115.50	111.30
24	A	406	CLA	CMC-C2C-C1C	3.07	129.78	125.02
24	b	614	CLA	O2A-CGA-CBA	3.08	121.28	111.90
24	B	614	CLA	O2A-CGA-CBA	3.09	121.31	111.90
24	c	911	CLA	C4-C3-C5	3.09	120.13	115.41
29	m	104	LMT	C1'-O5'-C5'	3.10	119.75	113.75
27	f	102	SQD	O5-C5-C4	3.10	115.50	109.68
24	C	505	CLA	CMC-C2C-C1C	3.11	129.83	125.02
24	c	914	CLA	C3B-C4B-NB	3.11	113.23	109.21
24	B	612	CLA	CAC-C3C-C4C	3.11	129.35	124.83
24	C	513	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	b	617	CLA	CMC-C2C-C1C	3.12	129.84	125.02
24	B	603	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	c	913	CLA	C3B-C4B-NB	3.13	113.25	109.21
31	A	419	PL9	C10-C9-C11	3.13	120.19	115.41
34	z	101	LMG	O1-C1-C2	3.13	112.00	108.04
24	B	616	CLA	C3B-C4B-NB	3.14	113.26	109.21
24	B	606	CLA	CAC-C3C-C4C	3.14	129.39	124.83
24	c	914	CLA	CMC-C2C-C1C	3.15	129.89	125.02
24	C	512	CLA	CAC-C3C-C4C	3.15	129.41	124.83
37	d	408	LHG	O7-C7-C8	3.15	118.38	111.53
24	B	610	CLA	O2A-CGA-CBA	3.16	121.53	111.90
24	b	616	CLA	C3B-C4B-NB	3.16	113.30	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	411	SQD	O9-S-C6	3.16	109.61	106.94
24	C	514	CLA	C4-C3-C5	3.17	120.25	115.41
26	d	404	BCR	C29-C30-C25	3.17	115.38	110.36
35	c	923	HTG	O5-C1-C2	3.18	114.50	110.19
37	D	407	LHG	O7-C7-C8	3.18	118.44	111.53
24	a	406	CLA	O2A-CGA-CBA	3.18	121.59	111.90
24	b	612	CLA	C3B-C4B-NB	3.19	113.33	109.21
24	A	407	CLA	CAC-C3C-C4C	3.19	129.47	124.83
37	d	407	LHG	O7-C7-C8	3.20	118.47	111.53
24	C	503	CLA	C3B-C4B-NB	3.21	113.35	109.21
24	c	905	CLA	CMC-C2C-C1C	3.21	129.98	125.02
24	b	608	CLA	C3B-C4B-NB	3.21	113.36	109.21
25	A	409	PHO	C4-C3-C5	3.21	120.31	115.41
24	C	506	CLA	C4-C3-C5	3.21	120.31	115.41
31	A	419	PL9	C15-C14-C16	3.21	120.32	115.41
24	B	610	CLA	CMC-C2C-C1C	3.21	129.99	125.02
24	A	407	CLA	C3B-C4B-NB	3.22	113.37	109.21
24	a	407	CLA	CAC-C3C-C4C	3.22	129.50	124.83
29	B	623	LMT	C4B-C3B-C2B	3.22	116.81	110.79
36	d	406	DGD	O5D-C1E-C2E	3.22	112.11	108.04
24	b	613	CLA	CAC-C3C-C4C	3.24	129.53	124.83
24	B	615	CLA	CMC-C2C-C1C	3.24	130.03	125.02
24	c	912	CLA	C3B-C4B-NB	3.24	113.40	109.21
27	a	402	SQD	O47-C7-C8	3.24	118.58	111.53
24	b	609	CLA	CMC-C2C-C1C	3.25	130.04	125.02
24	B	604	CLA	O2A-CGA-CBA	3.25	121.80	111.90
24	b	612	CLA	O2A-CGA-CBA	3.25	121.81	111.90
36	C	518	DGD	O2G-C1B-C2B	3.26	118.60	111.53
27	a	402	SQD	O48-C23-C24	3.26	121.82	111.90
24	A	410	CLA	C3B-C4B-NB	3.26	113.43	109.21
24	B	602	CLA	O2A-CGA-CBA	3.27	121.86	111.90
34	b	624	LMG	O8-C28-C29	3.27	121.86	111.90
24	b	620	CLA	CAC-C3C-C4C	3.27	129.58	124.83
24	B	614	CLA	C4-C3-C5	3.27	120.41	115.41
24	b	614	CLA	C3B-C4B-NB	3.28	113.44	109.21
24	B	612	CLA	C4-C3-C5	3.28	120.41	115.41
24	C	509	CLA	C4-C3-C5	3.28	120.41	115.41
37	E	101	LHG	O8-C23-C24	3.29	121.91	111.90
24	b	605	CLA	C4-C3-C5	3.29	120.43	115.41
24	c	910	CLA	CMC-C2C-C1C	3.29	130.12	125.02
31	D	404	PL9	C10-C9-C11	3.30	120.44	115.41
24	B	609	CLA	CMB-C2B-C3B	3.30	131.54	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	909	CLA	CAC-C3C-C4C	3.31	129.63	124.83
24	D	402	CLA	C3B-C4B-NB	3.31	113.48	109.21
24	B	602	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	b	606	CLA	CAC-C3C-C4C	3.31	129.63	124.83
27	A	412	SQD	O48-C23-C24	3.31	121.99	111.90
37	D	406	LHG	O8-C23-C24	3.32	122.03	111.90
38	V	201	HEM	C2D-C3D-C4D	3.33	107.14	101.50
31	a	417	PL9	C30-C29-C31	3.33	120.49	115.41
24	c	904	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	B	610	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	C	504	CLA	C4-C3-C5	3.33	120.50	115.41
24	C	511	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	C	512	CLA	C4-C3-C5	3.34	120.50	115.41
34	c	919	LMG	O8-C28-C29	3.35	122.11	111.90
24	B	617	CLA	CAC-C3C-C4C	3.36	129.71	124.83
34	C	520	LMG	O7-C10-C11	3.36	118.84	111.53
24	B	613	CLA	CAC-C3C-C4C	3.37	129.72	124.83
31	a	417	PL9	C10-C9-C11	3.37	120.55	115.41
27	F	101	SQD	O9-S-C6	3.37	109.78	106.94
24	a	406	CLA	CAC-C3C-C4C	3.38	129.73	124.83
26	B	619	BCR	C29-C30-C25	3.39	115.73	110.36
24	c	910	CLA	C3B-C4B-NB	3.40	113.61	109.21
24	B	605	CLA	C3B-C4B-NB	3.40	113.61	109.21
24	b	610	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	B	613	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	C	514	CLA	C3B-C4B-NB	3.41	113.62	109.21
27	f	102	SQD	C1-O5-C5	3.42	120.38	113.75
24	d	402	CLA	O2A-CGA-CBA	3.42	122.33	111.90
24	b	616	CLA	C4-C3-C5	3.42	120.64	115.41
24	A	410	CLA	C4-C3-C5	3.43	120.64	115.41
24	C	504	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	B	604	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	b	609	CLA	C4-C3-C5	3.45	120.68	115.41
24	c	909	CLA	C4-C3-C5	3.45	120.68	115.41
24	A	405	CLA	C3B-C4B-NB	3.46	113.68	109.21
34	C	520	LMG	O8-C28-C29	3.47	122.46	111.90
37	e	101	LHG	O7-C7-C8	3.47	119.07	111.53
24	C	509	CLA	C3B-C4B-NB	3.47	113.70	109.21
24	B	607	CLA	CMC-C2C-C1C	3.48	130.40	125.02
24	b	608	CLA	CMC-C2C-C1C	3.48	130.40	125.02
24	B	607	CLA	C4-C3-C5	3.48	120.72	115.41
24	a	409	CLA	C3B-C4B-NB	3.48	113.71	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	C3B-C4B-NB	3.49	113.72	109.21
34	c	920	LMG	C3-C4-C5	3.49	116.29	110.20
24	B	608	CLA	C3B-C4B-NB	3.50	113.73	109.21
34	c	919	LMG	O7-C10-C11	3.50	119.14	111.53
24	b	610	CLA	C4-C3-C5	3.50	120.76	115.41
24	b	617	CLA	C3B-C4B-NB	3.50	113.74	109.21
37	E	101	LHG	O7-C7-C8	3.52	119.17	111.53
24	D	402	CLA	C4-C3-C5	3.52	120.78	115.41
24	b	606	CLA	C3B-C4B-NB	3.52	113.77	109.21
24	b	608	CLA	CAC-C3C-C4C	3.53	129.95	124.83
24	b	607	CLA	C3B-C4B-NB	3.54	113.78	109.21
36	c	916	DGD	O2G-C1B-C2B	3.54	119.22	111.53
24	c	908	CLA	C3B-C4B-NB	3.54	113.78	109.21
24	d	402	CLA	C3B-C4B-NB	3.54	113.79	109.21
24	c	906	CLA	CAC-C3C-C4C	3.54	129.97	124.83
31	A	419	PL9	C20-C19-C21	3.54	120.82	115.41
24	d	402	CLA	CAC-C3C-C4C	3.55	129.98	124.83
24	c	905	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	C	510	CLA	CAC-C3C-C4C	3.55	129.98	124.83
29	b	601	LMT	O5'-C5'-C4'	3.55	117.25	109.75
24	C	510	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	c	911	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	B	609	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	b	618	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	A	410	CLA	CMC-C2C-C1C	3.59	130.58	125.02
25	a	420	PHO	CAC-C3C-C4C	3.59	129.35	125.16
34	z	101	LMG	O6-C5-C4	3.61	116.45	109.68
31	d	405	PL9	C10-C9-C11	3.62	120.93	115.41
24	B	615	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	B	617	CLA	C3B-C4B-NB	3.62	113.90	109.21
38	v	202	HEM	CMB-C2B-C3B	3.62	125.58	116.53
24	C	505	CLA	C3B-C4B-NB	3.63	113.90	109.21
24	b	607	CLA	O2A-CGA-CBA	3.63	122.96	111.90
36	c	918	DGD	O2G-C1B-C2B	3.64	119.44	111.53
24	C	502	CLA	CMC-C2C-C1C	3.64	130.65	125.02
34	z	101	LMG	O7-C10-C11	3.65	119.45	111.53
24	b	615	CLA	CAC-C3C-C4C	3.66	130.15	124.83
24	b	611	CLA	C3B-C4B-NB	3.66	113.95	109.21
27	A	416	SQD	O48-C23-C24	3.68	123.10	111.90
24	c	902	CLA	C3B-C4B-NB	3.69	113.98	109.21
27	A	416	SQD	O47-C7-C8	3.70	119.57	111.53
34	B	622	LMG	O8-C28-C29	3.72	123.22	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	C3B-C4B-NB	3.72	114.02	109.21
37	D	408	LHG	O7-C7-C8	3.72	119.62	111.53
24	b	615	CLA	C3B-C4B-NB	3.72	114.02	109.21
24	C	502	CLA	C3B-C4B-NB	3.73	114.03	109.21
25	a	420	PHO	C4-C3-C5	3.73	121.11	115.41
27	A	412	SQD	O9-S-C6	3.74	110.09	106.94
24	C	505	CLA	C4-C3-C5	3.75	121.14	115.41
24	b	620	CLA	C3B-C4B-NB	3.76	114.07	109.21
24	b	619	CLA	CAC-C3C-C4C	3.76	130.28	124.83
24	A	407	CLA	C4-C3-C5	3.76	121.15	115.41
24	B	607	CLA	C3B-C4B-NB	3.78	114.09	109.21
27	L	102	SQD	C3-C4-C5	3.78	116.80	110.20
36	D	405	DGD	C1D-C2D-C3D	3.79	117.44	109.97
24	a	406	CLA	O2D-CGD-CBD	3.79	116.50	111.30
24	C	507	CLA	C3B-C4B-NB	3.80	114.12	109.21
24	B	613	CLA	CMC-C2C-C1C	3.81	130.91	125.02
24	c	907	CLA	C3B-C4B-NB	3.81	114.14	109.21
24	b	619	CLA	C4-C3-C5	3.84	121.27	115.41
35	c	923	HTG	C1-O5-C5	3.84	120.07	112.74
35	D	411	HTG	C1'-S1-C1	3.85	105.61	100.30
24	a	406	CLA	C3B-C4B-NB	3.87	114.21	109.21
24	b	607	CLA	C4-C3-C5	3.88	121.34	115.41
38	V	201	HEM	CAD-C3D-C2D	3.89	124.41	113.22
38	e	102	HEM	CMB-C2B-C3B	3.90	126.26	116.53
24	d	403	CLA	C3B-C4B-NB	3.90	114.26	109.21
29	B	623	LMT	C3B-C4B-C5B	3.94	117.06	110.20
29	C	522	LMT	O1B-C4'-C3'	3.95	117.36	107.17
36	d	406	DGD	C3E-C4E-C5E	3.96	117.10	110.20
29	C	522	LMT	C1'-O5'-C5'	3.96	121.43	113.75
24	D	401	CLA	C3B-C4B-NB	3.97	114.34	109.21
36	C	517	DGD	O2G-C1B-C2B	3.98	120.17	111.53
37	d	409	LHG	O7-C7-C8	3.98	120.17	111.53
38	E	103	HEM	CAD-C3D-C4D	4.01	126.61	112.47
35	C	524	HTG	C1-O5-C5	4.02	120.40	112.74
24	A	406	CLA	C3B-C4B-NB	4.03	114.42	109.21
34	B	622	LMG	O7-C10-C11	4.05	120.32	111.53
24	c	909	CLA	C3B-C4B-NB	4.05	114.45	109.21
24	b	613	CLA	CMC-C2C-C1C	4.06	131.29	125.02
34	a	412	LMG	O7-C10-C11	4.06	120.36	111.53
24	B	604	CLA	C4-C3-C5	4.11	121.69	115.41
34	Z	101	LMG	O7-C10-C11	4.12	120.49	111.53
24	C	512	CLA	O2D-CGD-CBD	4.13	116.96	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	614	CLA	C3B-C4B-NB	4.13	114.55	109.21
24	c	906	CLA	C3B-C4B-NB	4.14	114.56	109.21
24	C	512	CLA	C3B-C4B-NB	4.14	114.56	109.21
38	e	102	HEM	CAD-C3D-C4D	4.15	127.11	112.47
38	v	202	HEM	CAD-C3D-C4D	4.16	127.15	112.47
37	l	101	LHG	O7-C7-C8	4.17	120.59	111.53
24	A	410	CLA	O2D-CGD-CBD	4.19	117.05	111.30
24	b	610	CLA	CMC-C2C-C1C	4.21	131.54	125.02
38	V	201	HEM	CMC-C2C-C3C	4.21	127.05	116.53
34	C	501	LMG	O7-C10-C11	4.25	120.76	111.53
36	c	917	DGD	O2G-C1B-C2B	4.26	120.79	111.53
34	C	521	LMG	O7-C10-C11	4.28	120.83	111.53
38	v	202	HEM	CMC-C2C-C3C	4.30	127.26	116.53
36	d	406	DGD	O2G-C1B-C2B	4.30	120.88	111.53
35	b	627	HTG	C1-O5-C5	4.34	121.02	112.74
29	B	623	LMT	O1B-C4'-C3'	4.36	118.44	107.17
24	b	619	CLA	C3B-C4B-NB	4.43	114.93	109.21
34	c	920	LMG	O7-C10-C11	4.43	121.15	111.53
27	f	102	SQD	O7-S-C6	4.44	110.69	106.94
38	E	103	HEM	CMB-C2B-C3B	4.47	127.69	116.53
24	A	406	CLA	C4-C3-C5	4.47	122.24	115.41
38	V	201	HEM	CMB-C2B-C3B	4.48	127.72	116.53
24	d	401	CLA	C3B-C4B-NB	4.49	115.01	109.21
38	E	103	HEM	CMC-C2C-C3C	4.50	127.77	116.53
35	B	625	HTG	C1'-S1-C1	4.51	106.52	100.30
38	V	201	HEM	CAD-C3D-C4D	4.52	128.42	112.47
36	D	405	DGD	O2G-C1B-C2B	4.56	121.44	111.53
27	L	102	SQD	O47-C7-C8	4.57	121.47	111.53
34	z	101	LMG	C3-C4-C5	4.58	118.17	110.20
38	v	202	HEM	CAD-C3D-C2D	4.60	126.43	113.22
38	e	102	HEM	CMC-C2C-C3C	4.67	128.20	116.53
31	a	417	PL9	C15-C14-C16	4.69	122.57	115.41
38	E	103	HEM	CAD-C3D-C2D	4.69	126.71	113.22
29	b	601	LMT	C1'-O5'-C5'	4.70	122.87	113.75
24	d	403	CLA	O2D-CGD-CBD	4.70	117.75	111.30
24	c	914	CLA	O2D-CGD-CBD	4.72	117.78	111.30
35	b	627	HTG	O5-C1-C2	4.74	116.62	110.19
38	e	102	HEM	CAD-C3D-C2D	4.74	126.85	113.22
27	B	621	SQD	O47-C7-C8	4.75	121.85	111.53
24	B	616	CLA	O2D-CGD-CBD	4.82	117.91	111.30
24	b	617	CLA	O2D-CGD-CBD	4.83	117.93	111.30
36	d	406	DGD	O6E-C5E-C4E	4.88	118.85	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	602	HTG	C1'-S1-C1	4.90	107.05	100.30
35	B	624	HTG	C1'-S1-C1	4.92	107.08	100.30
27	F	101	SQD	O47-C7-C8	4.99	122.37	111.53
24	c	912	CLA	O2D-CGD-CBD	5.04	118.22	111.30
27	A	412	SQD	O47-C7-C8	5.08	122.56	111.53
24	A	407	CLA	C2C-C1C-NC	5.08	114.02	110.24
25	A	409	PHO	CMD-C2D-C1D	5.08	133.33	125.06
25	a	420	PHO	C2D-C1D-ND	5.09	117.36	109.73
27	f	102	SQD	O47-C7-C8	5.13	122.67	111.53
25	A	409	PHO	C2D-C1D-ND	5.13	117.42	109.73
27	a	411	SQD	O47-C7-C8	5.29	123.03	111.53
24	c	904	CLA	O2D-CGD-CBD	5.30	118.57	111.30
25	A	409	PHO	O2D-CGD-CBD	5.30	118.58	111.30
25	A	408	PHO	C2D-C1D-ND	5.38	117.79	109.73
24	C	503	CLA	O2D-CGD-CBD	5.39	118.69	111.30
24	D	402	CLA	O2D-CGD-CBD	5.39	118.69	111.30
24	b	616	CLA	C2C-C1C-NC	5.39	114.26	110.24
35	V	202	HTG	C1'-S1-C1	5.42	107.76	100.30
24	b	612	CLA	O2D-CGD-CBD	5.43	118.74	111.30
24	B	610	CLA	O2D-CGD-CBD	5.45	118.77	111.30
24	a	407	CLA	C2C-C1C-NC	5.52	114.35	110.24
24	b	619	CLA	O2D-CGD-CBD	5.59	118.97	111.30
27	B	621	SQD	O7-S-C6	5.63	111.68	106.94
24	B	611	CLA	O2D-CGD-CBD	5.63	119.02	111.30
24	B	609	CLA	O2D-CGD-CBD	5.65	119.06	111.30
24	b	613	CLA	C2C-C1C-NC	5.67	114.46	110.24
24	C	513	CLA	C2C-C1C-NC	5.72	114.50	110.24
25	a	408	PHO	C2D-C1D-ND	5.73	118.32	109.73
27	F	101	SQD	O7-S-C6	5.76	111.80	106.94
24	B	608	CLA	O2D-CGD-CBD	5.76	119.20	111.30
24	b	605	CLA	C2C-C1C-NC	5.86	114.61	110.24
27	L	102	SQD	O6-C1-C2	5.86	115.44	108.04
24	b	613	CLA	O2D-CGD-CBD	5.88	119.36	111.30
24	c	911	CLA	O2D-CGD-CBD	5.92	119.42	111.30
24	B	605	CLA	O2D-CGD-CBD	5.92	119.43	111.30
24	c	912	CLA	C2C-C1C-NC	5.96	114.68	110.24
24	B	617	CLA	C2C-C1C-NC	5.97	114.69	110.24
24	C	504	CLA	O2D-CGD-CBD	5.97	119.49	111.30
24	B	612	CLA	O2D-CGD-CBD	5.97	119.49	111.30
24	A	406	CLA	O2D-CGD-CBD	5.98	119.50	111.30
24	A	410	CLA	C2C-C1C-NC	5.99	114.70	110.24
24	a	409	CLA	O2D-CGD-CBD	5.99	119.52	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	C2C-C1C-NC	5.99	114.70	110.24
24	d	401	CLA	O2D-CGD-CBD	5.99	119.52	111.30
24	A	407	CLA	O2D-CGD-CBD	6.00	119.53	111.30
25	a	408	PHO	O2D-CGD-CBD	6.01	119.55	111.30
24	c	913	CLA	C2C-C1C-NC	6.04	114.74	110.24
24	c	907	CLA	O2D-CGD-CBD	6.05	119.60	111.30
24	D	402	CLA	C2C-C1C-NC	6.06	114.76	110.24
24	C	507	CLA	O2D-CGD-CBD	6.07	119.62	111.30
24	b	614	CLA	O2D-CGD-CBD	6.11	119.68	111.30
35	B	633	HTG	C1'-S1-C1	6.12	108.73	100.30
24	c	914	CLA	C2C-C1C-NC	6.12	114.80	110.24
27	B	621	SQD	O6-C1-C2	6.16	115.82	108.04
24	B	604	CLA	C2C-C1C-NC	6.18	114.84	110.24
24	C	514	CLA	O2D-CGD-CBD	6.19	119.79	111.30
24	c	903	CLA	C2C-C1C-NC	6.19	114.85	110.24
24	b	610	CLA	C2C-C1C-NC	6.19	114.85	110.24
24	B	613	CLA	C2C-C1C-NC	6.21	114.87	110.24
24	B	616	CLA	C2C-C1C-NC	6.23	114.88	110.24
24	C	511	CLA	C2C-C1C-NC	6.23	114.88	110.24
24	b	606	CLA	C2C-C1C-NC	6.25	114.89	110.24
24	b	607	CLA	C2C-C1C-NC	6.26	114.91	110.24
24	d	402	CLA	O2D-CGD-CBD	6.29	119.93	111.30
24	c	911	CLA	C2C-C1C-NC	6.30	114.93	110.24
24	b	615	CLA	O2D-CGD-CBD	6.36	120.03	111.30
24	B	606	CLA	O2D-CGD-CBD	6.37	120.03	111.30
24	C	504	CLA	C2C-C1C-NC	6.38	114.99	110.24
24	C	514	CLA	C2C-C1C-NC	6.38	115.00	110.24
24	c	910	CLA	C2C-C1C-NC	6.40	115.00	110.24
24	D	401	CLA	O2D-CGD-CBD	6.40	120.08	111.30
24	B	602	CLA	C2C-C1C-NC	6.40	115.01	110.24
24	b	611	CLA	O2D-CGD-CBD	6.41	120.09	111.30
25	a	408	PHO	CMD-C2D-C1D	6.41	135.50	125.06
24	B	612	CLA	C2C-C1C-NC	6.42	115.02	110.24
35	d	412	HTG	C1'-S1-C1	6.42	109.15	100.30
24	c	909	CLA	O2D-CGD-CBD	6.42	120.11	111.30
25	a	420	PHO	CMD-C2D-C1D	6.45	135.55	125.06
24	b	609	CLA	C2C-C1C-NC	6.46	115.05	110.24
35	C	524	HTG	C1'-S1-C1	6.47	109.22	100.30
35	C	523	HTG	C1'-S1-C1	6.50	109.26	100.30
24	A	406	CLA	C2C-C1C-NC	6.51	115.09	110.24
24	B	603	CLA	C2C-C1C-NC	6.53	115.11	110.24
24	C	505	CLA	C2C-C1C-NC	6.55	115.12	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	620	CLA	C2C-C1C-NC	6.56	115.12	110.24
35	b	627	HTG	C1'-S1-C1	6.58	109.36	100.30
24	c	905	CLA	C2C-C1C-NC	6.60	115.16	110.24
24	C	513	CLA	O2D-CGD-CBD	6.61	120.37	111.30
24	b	618	CLA	C2C-C1C-NC	6.61	115.17	110.24
24	C	503	CLA	C2C-C1C-NC	6.67	115.21	110.24
24	C	510	CLA	O2D-CGD-CBD	6.68	120.46	111.30
24	B	603	CLA	O2D-CGD-CBD	6.68	120.46	111.30
24	b	612	CLA	C2C-C1C-NC	6.69	115.22	110.24
27	A	412	SQD	O6-C1-C2	6.69	116.49	108.04
24	a	407	CLA	O2D-CGD-CBD	6.70	120.49	111.30
24	c	913	CLA	O2D-CGD-CBD	6.71	120.51	111.30
24	a	409	CLA	C2C-C1C-NC	6.79	115.30	110.24
27	a	411	SQD	O6-C1-C2	6.80	116.62	108.04
24	b	620	CLA	O2D-CGD-CBD	6.82	120.66	111.30
24	B	605	CLA	C2C-C1C-NC	6.82	115.32	110.24
24	b	609	CLA	O2D-CGD-CBD	6.83	120.67	111.30
24	B	615	CLA	O2D-CGD-CBD	6.83	120.67	111.30
24	c	903	CLA	O2D-CGD-CBD	6.84	120.68	111.30
24	B	604	CLA	O2D-CGD-CBD	6.85	120.70	111.30
24	C	508	CLA	C2C-C1C-NC	6.86	115.35	110.24
24	B	615	CLA	C2C-C1C-NC	6.89	115.37	110.24
24	b	605	CLA	O2D-CGD-CBD	6.89	120.76	111.30
24	c	909	CLA	C2C-C1C-NC	6.90	115.38	110.24
24	B	607	CLA	O2D-CGD-CBD	6.91	120.77	111.30
35	c	922	HTG	C1'-S1-C1	6.92	109.84	100.30
24	B	614	CLA	C2C-C1C-NC	6.93	115.41	110.24
24	B	611	CLA	C2C-C1C-NC	6.95	115.42	110.24
24	C	506	CLA	C2C-C1C-NC	6.98	115.44	110.24
24	b	606	CLA	O2D-CGD-CBD	6.99	120.89	111.30
24	C	502	CLA	C2C-C1C-NC	7.00	115.45	110.24
25	A	408	PHO	CMD-C2D-C1D	7.03	136.50	125.06
24	c	904	CLA	C2C-C1C-NC	7.03	115.48	110.24
24	c	902	CLA	C2C-C1C-NC	7.07	115.50	110.24
24	C	510	CLA	C2C-C1C-NC	7.07	115.50	110.24
35	b	626	HTG	C1'-S1-C1	7.08	110.06	100.30
24	b	616	CLA	O2D-CGD-CBD	7.09	121.03	111.30
24	C	508	CLA	O2D-CGD-CBD	7.09	121.03	111.30
24	c	902	CLA	O2D-CGD-CBD	7.10	121.03	111.30
24	b	615	CLA	C2C-C1C-NC	7.11	115.54	110.24
24	c	910	CLA	O2D-CGD-CBD	7.14	121.09	111.30
24	b	611	CLA	C2C-C1C-NC	7.18	115.59	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C2C-C1C-NC	7.18	115.59	110.24
24	C	512	CLA	C2C-C1C-NC	7.19	115.59	110.24
25	a	420	PHO	O2D-CGD-CBD	7.19	121.16	111.30
24	C	502	CLA	O2D-CGD-CBD	7.25	121.24	111.30
24	B	602	CLA	O2D-CGD-CBD	7.25	121.24	111.30
24	b	608	CLA	C2C-C1C-NC	7.25	115.64	110.24
24	c	907	CLA	C2C-C1C-NC	7.33	115.70	110.24
24	C	506	CLA	O2D-CGD-CBD	7.40	121.45	111.30
24	b	619	CLA	C2C-C1C-NC	7.41	115.76	110.24
24	c	906	CLA	O2D-CGD-CBD	7.41	121.46	111.30
24	d	402	CLA	C2C-C1C-NC	7.41	115.76	110.24
24	c	905	CLA	O2D-CGD-CBD	7.42	121.48	111.30
24	c	908	CLA	C2C-C1C-NC	7.44	115.78	110.24
24	B	608	CLA	C2C-C1C-NC	7.47	115.80	110.24
24	C	509	CLA	C2C-C1C-NC	7.48	115.81	110.24
24	A	405	CLA	C2C-C1C-NC	7.50	115.83	110.24
24	C	507	CLA	C2C-C1C-NC	7.51	115.83	110.24
24	C	505	CLA	O2D-CGD-CBD	7.52	121.62	111.30
24	C	511	CLA	O2D-CGD-CBD	7.53	121.63	111.30
35	b	603	HTG	C1'-S1-C1	7.55	110.71	100.30
24	b	607	CLA	O2D-CGD-CBD	7.57	121.68	111.30
24	d	403	CLA	C2C-C1C-NC	7.58	115.88	110.24
24	d	401	CLA	C2C-C1C-NC	7.58	115.89	110.24
35	c	923	HTG	C1'-S1-C1	7.64	110.83	100.30
24	B	613	CLA	O2D-CGD-CBD	7.65	121.79	111.30
24	B	609	CLA	C2C-C1C-NC	7.65	115.94	110.24
24	b	617	CLA	C2C-C1C-NC	7.65	115.94	110.24
24	b	618	CLA	O2D-CGD-CBD	7.69	121.85	111.30
24	c	906	CLA	C2C-C1C-NC	7.71	115.98	110.24
24	a	406	CLA	C2C-C1C-NC	7.73	116.00	110.24
24	b	608	CLA	O2D-CGD-CBD	7.75	121.94	111.30
25	A	408	PHO	O2D-CGD-CBD	7.76	121.95	111.30
24	D	401	CLA	C2C-C1C-NC	7.77	116.03	110.24
27	L	102	SQD	O7-S-C6	7.87	113.57	106.94
24	C	509	CLA	O2D-CGD-CBD	7.88	122.11	111.30
24	B	607	CLA	C2C-C1C-NC	7.89	116.12	110.24
24	b	610	CLA	O2D-CGD-CBD	7.95	122.21	111.30
35	B	634	HTG	C1'-S1-C1	8.00	111.33	100.30
24	B	617	CLA	O2D-CGD-CBD	8.14	122.46	111.30
24	B	606	CLA	C2C-C1C-NC	8.23	116.37	110.24
27	F	101	SQD	O6-C1-C2	8.43	118.69	108.04
35	B	626	HTG	C1'-S1-C1	8.77	112.39	100.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	908	CLA	O2D-CGD-CBD	8.92	123.54	111.30

All (182) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	c	904	CLA	NC
24	c	904	CLA	ND
24	c	904	CLA	NA
24	C	506	CLA	ND
24	C	503	CLA	NC
24	C	503	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	D	401	CLA	ND
24	D	401	CLA	NA
24	a	407	CLA	NC
24	a	407	CLA	NA
24	A	410	CLA	NC
24	A	410	CLA	NA
24	b	618	CLA	NC
24	b	618	CLA	ND
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	C	505	CLA	NC
24	C	505	CLA	ND
24	C	505	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	612	CLA	NC
24	B	612	CLA	ND
24	B	612	CLA	NA
24	b	619	CLA	NA

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Mol	Chain	Res	Type	Atom
24	b	619	CLA	NC
24	b	619	CLA	ND
24	d	402	CLA	ND
24	c	914	CLA	NC
24	c	914	CLA	ND
24	c	914	CLA	NA
24	c	911	CLA	NC
24	c	911	CLA	ND
24	c	911	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	a	409	CLA	NC
24	a	409	CLA	ND
24	a	409	CLA	NA
24	d	403	CLA	NC
24	d	403	CLA	NA
24	c	912	CLA	NC
24	c	912	CLA	ND
24	c	912	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	c	905	CLA	NC
24	c	905	CLA	ND
24	c	905	CLA	NA
24	C	514	CLA	NC
24	C	514	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	c	913	CLA	NC

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Mol	Chain	Res	Type	Atom
24	c	913	CLA	ND
24	c	913	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	609	CLA	NC
24	B	609	CLA	NA
24	d	401	CLA	ND
24	d	401	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	D	402	CLA	NC
24	D	402	CLA	ND
24	D	402	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	c	903	CLA	NC
24	c	903	CLA	ND
24	c	903	CLA	NA
24	c	908	CLA	NC
24	c	908	CLA	ND
24	c	908	CLA	NA
24	b	620	CLA	NA
24	b	620	CLA	NC
24	b	620	CLA	ND
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	614	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	b	611	CLA	NC
24	b	611	CLA	ND

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Mol	Chain	Res	Type	Atom
24	a	406	CLA	NC
24	a	406	CLA	ND
24	a	406	CLA	NA
24	A	405	CLA	NC
24	A	405	CLA	ND
24	c	909	CLA	NC
24	c	909	CLA	ND
24	c	909	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	c	910	CLA	NC
24	c	910	CLA	ND
24	c	910	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	NA
24	c	906	CLA	ND
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	b	608	CLA	NC
24	b	608	CLA	ND
24	b	608	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA

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Mol	Chain	Res	Type	Atom
24	B	617	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	A	407	CLA	NC
24	A	407	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	ND
24	A	406	CLA	NA
24	c	902	CLA	NC
24	c	902	CLA	ND
24	c	902	CLA	NA
24	c	907	CLA	NC
24	c	907	CLA	ND
24	c	907	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	NA

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C45-O47-C7-C8
36	d	406	DGD	C2G-O2G-C1B-C2B
27	F	101	SQD	C45-O47-C7-O49
34	Z	101	LMG	C8-O7-C10-O9
27	f	102	SQD	C45-O47-C7-O49
27	F	101	SQD	C45-O47-C7-C8
34	Z	101	LMG	C8-O7-C10-C11
27	f	102	SQD	C45-O47-C7-C8

There are no ring outliers.

85 monomers are involved in 212 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	405	CLA	2	0
24	A	406	CLA	8	0
24	A	407	CLA	2	0
25	A	409	PHO	3	0
24	A	410	CLA	3	0
26	A	411	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	412	SQD	5	0
28	A	414	GOL	2	0
27	A	416	SQD	2	0
31	A	419	PL9	5	0
24	B	602	CLA	4	0
24	B	603	CLA	2	0
24	B	604	CLA	1	0
24	B	605	CLA	6	0
24	B	606	CLA	4	0
24	B	607	CLA	3	0
24	B	608	CLA	4	0
24	B	609	CLA	6	0
24	B	610	CLA	3	0
24	B	612	CLA	3	0
24	B	613	CLA	4	0
24	B	614	CLA	5	0
24	B	615	CLA	1	0
24	B	616	CLA	5	0
24	B	617	CLA	7	0
26	B	618	BCR	1	0
26	B	619	BCR	3	0
26	B	620	BCR	2	0
27	B	621	SQD	3	0
34	B	622	LMG	1	0
29	B	623	LMT	1	0
35	B	625	HTG	1	0
28	B	631	GOL	2	0
28	B	632	GOL	2	0
35	B	633	HTG	2	0
35	B	634	HTG	1	0
29	B	636	LMT	1	0
28	B	637	GOL	1	0
34	C	501	LMG	2	0
24	C	502	CLA	3	0
24	C	503	CLA	4	0
24	C	504	CLA	1	0
24	C	505	CLA	1	0
24	C	506	CLA	4	0
24	C	507	CLA	7	0
24	C	508	CLA	5	0
24	C	509	CLA	2	0
24	C	510	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	511	CLA	5	0
24	C	512	CLA	2	0
24	C	513	CLA	3	0
24	C	514	CLA	5	0
26	C	515	BCR	1	0
36	C	517	DGD	4	0
36	C	518	DGD	2	0
36	C	519	DGD	2	0
34	C	520	LMG	2	0
34	C	521	LMG	3	0
29	C	522	LMT	2	0
35	C	524	HTG	1	0
28	C	525	GOL	2	0
24	D	401	CLA	4	0
24	D	402	CLA	6	0
26	D	403	BCR	2	0
31	D	404	PL9	1	0
36	D	405	DGD	5	0
37	D	406	LHG	2	0
37	D	408	LHG	8	0
35	D	411	HTG	2	0
37	E	101	LHG	2	0
29	E	102	LMT	1	0
27	F	101	SQD	3	0
26	H	101	BCR	4	0
36	H	102	DGD	1	0
34	J	101	LMG	7	0
26	K	102	BCR	2	0
26	K	103	BCR	3	0
37	L	101	LHG	2	0
27	L	102	SQD	2	0
29	M	101	LMT	3	0
35	O	303	HTG	1	0
28	T	101	GOL	1	0
26	T	102	BCR	3	0
28	V	203	GOL	1	0
34	Z	101	LMG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	0.48	22 (6%) 22 31	13, 21, 38, 73	0
1	a	334/344 (97%)	0.63	37 (11%) 7 11	15, 23, 47, 90	0
2	B	504/505 (99%)	0.21	27 (5%) 29 41	15, 25, 48, 78	0
2	b	504/505 (99%)	0.31	37 (7%) 18 28	16, 27, 59, 92	0
3	C	451/455 (99%)	0.19	18 (3%) 42 53	18, 30, 46, 73	0
3	c	455/455 (100%)	0.33	31 (6%) 20 30	21, 33, 49, 92	0
4	D	342/342 (100%)	0.63	38 (11%) 7 11	14, 22, 37, 97	0
4	d	341/342 (99%)	0.41	17 (4%) 32 44	16, 25, 39, 90	0
5	E	81/84 (96%)	0.90	9 (11%) 7 11	26, 37, 66, 92	0
5	e	81/84 (96%)	1.18	14 (17%) 2 3	30, 42, 71, 92	0
6	F	34/44 (77%)	0.37	4 (11%) 6 10	23, 30, 50, 61	0
6	f	32/44 (72%)	0.36	3 (9%) 11 17	30, 34, 79, 84	0
7	H	65/65 (100%)	0.27	2 (3%) 52 62	23, 31, 46, 110	0
7	h	65/65 (100%)	0.78	8 (12%) 5 9	27, 35, 52, 105	0
8	I	37/38 (97%)	0.65	5 (13%) 4 7	26, 33, 88, 108	0
8	i	37/38 (97%)	0.60	3 (8%) 15 23	27, 33, 73, 102	0
9	J	38/39 (97%)	0.63	6 (15%) 3 4	24, 35, 84, 98	0
9	j	39/39 (100%)	0.39	1 (2%) 59 69	29, 38, 84, 96	0
10	K	37/37 (100%)	0.30	1 (2%) 58 68	27, 35, 54, 65	0
10	k	37/37 (100%)	1.00	8 (21%) 1 1	30, 38, 55, 68	0
11	L	37/37 (100%)	0.67	5 (13%) 4 7	15, 19, 56, 82	0
11	l	37/37 (100%)	0.84	5 (13%) 4 7	16, 20, 58, 83	0
12	M	33/36 (91%)	0.76	3 (9%) 11 18	15, 21, 45, 89	0
12	m	33/36 (91%)	0.70	3 (9%) 11 18	16, 21, 41, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.35	17 (6%) 19 29	16, 32, 66, 110	0
13	o	243/244 (99%)	0.76	47 (19%) 2 2	19, 33, 71, 125	0
14	T	29/32 (90%)	0.88	3 (10%) 9 14	16, 20, 43, 89	0
14	t	29/32 (90%)	0.51	2 (6%) 20 30	16, 20, 46, 89	0
15	U	97/104 (93%)	0.40	5 (5%) 31 42	21, 31, 54, 84	0
15	u	97/104 (93%)	-0.01	0 100 100	23, 33, 51, 84	0
16	V	137/137 (100%)	-0.03	0 100 100	20, 31, 51, 69	0
16	v	137/137 (100%)	0.56	11 (8%) 15 24	24, 36, 57, 70	0
17	Y	29/30 (96%)	1.70	7 (24%) 1 1	35, 47, 82, 101	0
17	y	29/30 (96%)	1.54	8 (27%) 1 0	38, 50, 83, 100	0
18	X	39/40 (97%)	0.66	6 (15%) 3 4	31, 38, 75, 102	0
18	x	39/40 (97%)	1.58	11 (28%) 1 0	33, 41, 83, 102	0
19	Z	62/62 (100%)	1.40	18 (29%) 1 0	36, 47, 83, 96	0
19	z	62/62 (100%)	2.96	35 (56%) 0 0	42, 49, 82, 96	0
20	R	34/34 (100%)	7.22	34 (100%) 0 0	55, 75, 98, 106	0
All	All	5294/5384 (98%)	0.54	511 (9%) 10 16	13, 29, 61, 125	0

All (511) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	17.9
17	Y	18	VAL	12.0
7	H	65	LEU	11.3
20	R	18	TRP	11.1
19	z	3	ILE	10.7
20	R	24	LEU	10.0
5	e	5	THR	9.9
20	R	3	TRP	9.9
20	R	23	ILE	9.9
20	R	6	LEU	9.3
20	R	14	LEU	9.1
17	Y	19	ILE	9.1
20	R	31	VAL	9.0
20	R	19	ALA	9.0
20	R	7	VAL	8.9
20	R	20	VAL	8.8
20	R	32	GLN	8.7

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Mol	Chain	Res	Type	RSRZ
20	R	25	PRO	8.2
20	R	10	LEU	8.1
20	R	26	TYR	8.0
1	a	11	ALA	8.0
19	Z	3	ILE	7.6
7	h	65	LEU	7.5
20	R	28	VAL	7.5
17	y	18	VAL	7.4
18	X	40	SER	7.3
19	z	42	LEU	7.2
19	z	5	PHE	7.2
20	R	27	ALA	7.2
19	z	4	LEU	7.2
20	R	9	LEU	7.0
18	x	2	THR	7.0
20	R	34	LEU	7.0
17	y	19	ILE	7.0
2	b	495	PHE	6.9
13	o	59	LYS	6.9
8	I	37	LEU	6.9
18	x	40	SER	6.9
13	O	56	PRO	6.8
19	z	61	VAL	6.8
20	R	5	VAL	6.8
20	R	15	ALA	6.7
9	j	1	MET	6.7
20	R	33	LYS	6.5
20	R	13	LEU	6.5
20	R	30	GLN	6.4
20	R	29	LYS	6.4
8	i	37	LEU	6.4
17	Y	22	LEU	6.4
19	Z	7	LEU	6.3
20	R	21	ARG	6.2
5	E	84	LYS	6.2
20	R	35	LEU	6.1
1	A	11	ALA	6.0
18	x	37	VAL	5.9
19	Z	62	VAL	5.8
19	z	60	PHE	5.8
20	R	16	ALA	5.8
2	b	486	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
2	b	85	GLY	5.7
9	J	2	SER	5.7
18	x	38	GLN	5.6
2	b	505	ARG	5.6
3	C	23	ALA	5.6
13	O	62	GLU	5.6
19	Z	1	MET	5.6
19	z	2	THR	5.5
9	J	3	GLU	5.5
13	o	61	GLN	5.4
20	R	8	VAL	5.4
2	B	486	LEU	5.3
2	B	86	ILE	5.3
7	h	66	GLY	5.2
14	T	30	THR	5.2
10	k	18	PHE	5.2
20	R	2	ASP	5.1
5	e	25	ILE	5.1
2	b	293	ALA	5.1
13	o	63	ALA	5.1
11	l	1	MET	5.1
19	Z	4	LEU	5.0
19	z	7	LEU	5.0
20	R	22	ASN	4.9
1	A	13	LEU	4.9
13	o	26	ALA	4.9
13	o	246	ALA	4.8
20	R	17	GLY	4.8
13	o	36	GLN	4.7
19	z	18	VAL	4.7
16	v	17	LYS	4.7
13	o	35	SER	4.7
4	D	12	ARG	4.6
18	X	2	THR	4.5
19	z	57	LEU	4.5
5	e	4	THR	4.4
16	v	16	GLY	4.4
8	i	36	ASP	4.4
10	k	13	GLU	4.4
2	b	487	SER	4.4
7	h	64	ALA	4.3
19	Z	31	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
13	o	135	SER	4.3
13	O	61	GLN	4.3
7	H	64	ALA	4.3
13	o	56	PRO	4.3
3	c	143	TYR	4.3
19	z	1	MET	4.2
8	I	38	GLU	4.2
6	f	14	PRO	4.2
2	b	504	THR	4.2
13	o	24	ASP	4.2
2	b	493	TRP	4.2
10	k	14	ALA	4.1
2	B	494	GLY	4.1
13	O	4	THR	4.1
8	I	36	ASP	4.1
19	z	9	LEU	4.1
6	f	16	PHE	4.1
20	R	12	VAL	4.1
19	Z	33	TRP	4.1
2	b	494	GLY	4.0
13	o	25	THR	4.0
20	R	4	ARG	4.0
17	Y	20	ALA	4.0
14	t	30	THR	4.0
2	b	484	PRO	4.0
2	b	489	GLU	4.0
3	C	143	TYR	3.9
13	o	34	SER	3.9
2	b	84	THR	3.9
2	b	496	TYR	3.9
14	t	29	ILE	3.9
2	B	298	LEU	3.9
1	A	12	ASN	3.8
13	o	32	ILE	3.8
5	E	17	VAL	3.8
19	z	41	PHE	3.8
2	b	294	SER	3.8
2	b	497	GLN	3.7
13	o	134	THR	3.7
17	y	22	LEU	3.7
19	z	59	PHE	3.7
3	c	134	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
5	e	32	ILE	3.6
2	b	290	ALA	3.6
7	h	6	TRP	3.6
12	m	34	LYS	3.6
19	z	43	GLY	3.6
5	e	21	VAL	3.6
12	M	33	GLN	3.6
19	Z	35	ARG	3.6
6	F	16	PHE	3.6
17	y	20	ALA	3.6
6	F	15	ILE	3.6
11	l	3	PRO	3.5
2	b	502	VAL	3.5
16	v	14	SER	3.5
4	D	11	GLU	3.5
18	x	30	ALA	3.5
19	z	33	TRP	3.5
13	o	23	ASP	3.5
19	z	46	LEU	3.5
1	A	202	VAL	3.5
1	a	192	ILE	3.5
2	b	86[A]	ILE	3.5
18	x	39	ARG	3.5
19	Z	32	ASP	3.4
13	O	27	ARG	3.4
3	c	155	ASN	3.4
13	o	199	LEU	3.4
4	D	279	LEU	3.4
3	C	254	THR	3.4
1	a	197	PHE	3.3
2	b	488	PRO	3.3
13	O	26	ALA	3.3
2	B	85	GLY	3.3
1	a	13	LEU	3.3
2	b	295	GLY	3.3
1	A	200	LEU	3.3
19	Z	34	ASP	3.3
13	O	25	THR	3.3
13	o	243	ILE	3.3
10	k	12	PRO	3.2
15	U	58	VAL	3.2
18	x	34	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	b	490	GLN	3.2
3	c	432	VAL	3.2
17	Y	21	GLN	3.2
4	d	325	ILE	3.2
19	z	40	ILE	3.2
1	a	200	LEU	3.2
4	D	153	PHE	3.2
2	b	491	VAL	3.2
13	o	62	GLU	3.2
10	k	17	ILE	3.2
19	Z	60	PHE	3.2
4	D	278	GLY	3.1
19	z	39	LEU	3.1
2	B	495	PHE	3.1
20	R	11	PRO	3.1
16	v	10	VAL	3.1
13	O	138	THR	3.1
13	o	4	THR	3.1
18	X	31	ILE	3.1
1	A	205	VAL	3.1
4	D	201	VAL	3.1
4	D	149	PRO	3.1
4	D	289	LEU	3.1
2	B	485	GLU	3.1
6	F	14	PRO	3.1
1	A	197	PHE	3.1
13	o	58	ASN	3.1
1	A	193	LEU	3.0
15	U	79	LEU	3.0
3	C	432	VAL	3.0
19	z	27	TYR	3.0
15	U	73	GLN	3.0
19	z	28	ALA	3.0
13	o	132	ASN	3.0
1	A	206	PHE	3.0
4	d	152	VAL	3.0
5	E	21	VAL	3.0
13	o	37	THR	3.0
19	Z	30	PRO	3.0
5	E	6	GLY	3.0
3	c	140	LEU	3.0
3	C	257	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	152	VAL	3.0
13	o	133	VAL	3.0
2	B	127	ARG	3.0
13	O	137	THR	2.9
4	D	156	VAL	2.9
2	B	505	ARG	2.9
1	A	14	TRP	2.9
2	b	298	LEU	2.9
8	I	34	ARG	2.9
4	D	280	TRP	2.9
4	D	150	ILE	2.9
12	M	34	LYS	2.9
16	v	26	TYR	2.9
2	b	297	THR	2.9
3	c	159	THR	2.9
18	x	35	ASP	2.9
19	z	20	VAL	2.9
16	v	15	GLU	2.9
1	a	288	LEU	2.9
2	b	291	SER	2.9
19	z	29	SER	2.9
13	o	95	PHE	2.9
5	e	26	THR	2.9
6	f	15	ILE	2.9
16	v	19	ILE	2.9
2	b	296	ALA	2.9
4	D	191	TRP	2.9
5	E	79	PHE	2.8
13	o	65	PHE	2.8
2	b	485	GLU	2.8
18	x	3	ILE	2.8
11	L	1	MET	2.8
16	v	12	LEU	2.8
17	Y	25	ILE	2.8
13	o	131	PRO	2.8
9	J	4	GLY	2.8
4	d	74	LEU	2.8
4	D	148	ALA	2.8
3	c	146	PHE	2.8
1	A	278	TRP	2.8
1	a	193	LEU	2.8
2	B	461	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
13	o	22	LEU	2.8
19	z	6	GLN	2.8
17	y	41	VAL	2.8
3	c	147	PHE	2.8
1	A	288	LEU	2.7
13	O	130	GLN	2.7
1	a	300	PHE	2.7
10	k	21	LEU	2.7
4	D	178	ILE	2.7
1	a	157	VAL	2.7
1	a	280	VAL	2.7
4	D	202	ALA	2.7
5	e	37	PHE	2.7
5	e	42	LEU	2.7
4	d	328	TRP	2.7
1	a	290	ILE	2.7
4	D	17	ILE	2.7
13	o	33	ASP	2.7
19	z	56	VAL	2.7
2	B	295	GLY	2.7
3	C	260	ALA	2.7
13	O	60	ARG	2.7
3	c	145	SER	2.7
1	A	192	ILE	2.7
13	o	66	VAL	2.7
7	h	3	ARG	2.7
19	z	35	ARG	2.7
11	L	31	PHE	2.7
3	C	433	LEU	2.7
4	D	182	LEU	2.7
11	l	27	LEU	2.7
3	C	436	PHE	2.6
13	o	27	ARG	2.6
16	v	106	ASN	2.6
3	C	145[A]	SER	2.6
1	a	285	PHE	2.6
10	K	30	VAL	2.6
15	U	70	ARG	2.6
2	b	126	PRO	2.6
2	b	302	TRP	2.6
4	D	193	LEU	2.6
19	Z	57	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
13	O	24	ASP	2.6
19	z	58	ASN	2.6
1	a	202	VAL	2.6
13	o	204	VAL	2.6
17	y	25	ILE	2.6
5	e	61	ARG	2.6
8	i	38	GLU	2.6
9	J	6	ARG	2.6
3	C	155	ASN	2.6
4	d	205	LEU	2.6
12	m	16	LEU	2.6
14	T	9	ILE	2.6
12	m	33	GLN	2.6
3	c	259	TRP	2.5
1	a	299	GLY	2.5
1	A	186	PHE	2.5
3	c	204	LEU	2.5
4	d	185	PHE	2.5
2	B	457	VAL	2.5
2	b	127	ARG	2.5
4	d	24	ARG	2.5
13	o	60	ARG	2.5
4	d	182	LEU	2.5
5	e	10	PHE	2.5
13	o	57	LYS	2.5
3	c	19	ASN	2.5
1	a	205	VAL	2.5
4	D	175	VAL	2.5
4	D	286	VAL	2.5
4	d	12	ARG	2.5
2	B	165	GLY	2.5
1	A	287	ALA	2.5
4	D	196	PHE	2.5
18	x	36	LYS	2.5
19	Z	6	GLN	2.5
19	z	30	PRO	2.5
3	c	411	ALA	2.5
5	E	81	GLU	2.5
11	L	23	LEU	2.5
4	d	184	PHE	2.5
4	d	196	PHE	2.5
19	z	38	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	297	LEU	2.5
1	a	196	PRO	2.5
3	c	255	THR	2.5
3	c	435	PHE	2.4
2	b	499	VAL	2.4
13	o	136	ILE	2.4
4	D	146	PHE	2.4
5	E	22	ILE	2.4
13	o	202	ALA	2.4
17	Y	43	ARG	2.4
19	z	14	ILE	2.4
4	D	275	PRO	2.4
13	O	131	PRO	2.4
13	o	31	PRO	2.4
13	o	38	TYR	2.4
13	O	5	LEU	2.4
7	h	22	ALA	2.4
2	b	129	GLY	2.4
13	o	201	VAL	2.4
4	D	238	THR	2.4
19	Z	36	SER	2.4
2	b	120	LEU	2.4
4	D	291	LEU	2.4
1	A	196	PRO	2.4
1	a	156	ALA	2.4
4	D	192	THR	2.4
14	T	13	ILE	2.3
1	a	284	TRP	2.3
19	z	31	GLN	2.3
1	a	341	LEU	2.3
4	D	290	ALA	2.3
4	D	185	PHE	2.3
1	a	160	ILE	2.3
3	c	131	TYR	2.3
12	M	16[A]	LEU	2.3
19	z	52	LEU	2.3
2	B	84	THR	2.3
3	c	429	SER	2.3
3	C	259	TRP	2.3
2	B	454	ALA	2.3
1	A	201	GLY	2.3
1	a	283	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	146	PHE	2.3
13	O	136	ILE	2.3
1	a	235	TYR	2.3
6	F	17	THR	2.3
10	k	15	TYR	2.3
19	Z	49	ALA	2.3
1	a	293	MET	2.3
10	k	11	LEU	2.3
17	y	21	GLN	2.3
4	D	154	VAL	2.3
2	b	501	ASP	2.3
7	h	63	LYS	2.3
18	X	3	ILE	2.3
19	Z	2	THR	2.3
1	a	287	ALA	2.3
2	B	459	ALA	2.3
1	a	194	MET	2.3
1	a	326	LEU	2.2
3	C	425	TRP	2.2
4	d	156	VAL	2.2
3	C	142	GLU	2.2
3	c	427	ALA	2.2
5	e	14	ILE	2.2
11	l	2	GLU	2.2
13	o	30	TYR	2.2
3	c	20	SER	2.2
3	c	433	LEU	2.2
13	o	43	LEU	2.2
18	x	8	LYS	2.2
2	B	293	ALA	2.2
1	a	184	ILE	2.2
5	E	25	ILE	2.2
2	B	488	PRO	2.2
4	D	160	TYR	2.2
2	B	292	LEU	2.2
5	e	80	LEU	2.2
2	B	297	THR	2.2
3	C	255	THR	2.2
16	v	110	LYS	2.2
2	b	301	ALA	2.2
1	a	180	PHE	2.2
4	D	295[A]	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	a	163	ILE	2.2
15	U	74	ILE	2.2
1	A	282	GLY	2.2
4	d	324	GLY	2.2
18	X	38	GLN	2.2
2	B	408	GLY	2.2
4	d	179	PHE	2.2
13	o	206	GLY	2.2
2	B	305	ILE	2.2
2	B	489	GLU	2.2
3	c	142	GLU	2.2
9	J	7	ILE	2.2
1	a	297	LEU	2.2
3	c	253	LEU	2.2
2	B	502	VAL	2.2
13	o	87	VAL	2.2
4	d	283	ALA	2.1
13	o	142	PHE	2.1
7	h	20	LYS	2.1
2	B	504	THR	2.1
11	L	29	LEU	2.1
11	l	25	LEU	2.1
1	A	294	ALA	2.1
1	a	188	ALA	2.1
1	a	203	ALA	2.1
1	a	330	VAL	2.1
2	B	301	ALA	2.1
19	Z	53	VAL	2.1
3	c	151	TRP	2.1
4	D	181	PHE	2.1
3	c	428	THR	2.1
19	z	34	ASP	2.1
1	a	161	TYR	2.1
16	v	21	LEU	2.1
1	a	279	PRO	2.1
3	c	410	VAL	2.1
4	D	276	VAL	2.1
19	z	53	VAL	2.1
2	b	223	GLN	2.1
13	o	208	THR	2.1
3	C	147	PHE	2.1
4	D	179	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	282	GLY	2.1
3	C	253	LEU	2.1
4	d	321	LEU	2.1
13	O	59	LYS	2.1
3	c	183	GLY	2.1
9	J	5	GLY	2.1
1	A	285	PHE	2.1
1	a	182	PHE	2.1
4	D	114	ILE	2.1
3	c	271	TYR	2.1
4	d	187	GLY	2.1
11	L	2	GLU	2.0
3	C	262	ARG	2.0
3	c	127	PHE	2.0
3	c	284	PHE	2.0
5	E	57	ALA	2.0
13	o	29	ALA	2.0
13	o	211	ILE	2.0
17	y	43	ARG	2.0
18	X	34	ILE	2.0
13	O	87	VAL	2.0
5	e	23	HIS	2.0
8	I	33	LYS	2.0
3	c	144	SER	2.0
4	D	157	PHE	2.0
1	A	210	LEU	2.0
2	b	498	LYS	2.0
4	D	174	GLY	2.0
5	e	74	GLN	2.0
2	B	304	ALA	2.0
13	o	209	GLY	2.0
3	c	160	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.98	0.12	-	21,31,39,42	0
12	FME	M	1	10/11	0.97	0.13	-	23,36,70,74	0
12	FME	m	1	10/11	0.93	0.16	-	13,32,67,68	0
14	FME	T	1	10/11	0.96	0.16	-	18,26,40,49	0
8	FME	I	1	10/11	0.95	0.13	-	22,34,38,38	0
14	FME	t	1	10/11	0.96	0.12	-	12,22,31,68	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	GOL	c	925	6/6	0.89	0.23	14.47	34,52,63,66	0
28	GOL	b	633	6/6	0.94	0.36	11.62	34,60,65,65	0
28	GOL	V	203	6/6	0.75	0.43	9.52	50,64,71,72	0
29	LMT	E	102	35/35	0.55	0.35	7.75	43,80,109,115	0
29	LMT	f	103	35/35	0.60	0.37	7.72	43,86,107,111	0
36	DGD	d	406	62/66	0.61	0.44	7.38	38,89,122,130	0
28	GOL	B	631	6/6	0.86	0.22	7.25	30,48,62,65	0
35	HTG	d	412	16/19	0.70	0.31	7.12	38,78,97,98	0
28	GOL	V	206	6/6	0.84	0.27	6.95	47,63,66,66	0
32	UNL	J	102	10/-	0.76	0.34	6.71	39,51,64,67	0
32	UNL	j	102	10/-	0.74	0.30	6.67	47,57,63,63	0
27	SQD	a	402	54/54	0.80	0.20	6.39	29,55,76,90	0
35	HTG	C	524	19/19	0.75	0.30	6.37	41,69,99,100	0
31	PL9	a	417	55/55	0.72	0.26	6.29	41,73,92,99	0
29	LMT	B	636	25/35	0.86	0.22	6.07	24,61,106,122	0
28	GOL	B	627	6/6	0.92	0.16	5.83	23,36,45,72	0
28	GOL	C	525	6/6	0.92	0.20	5.64	32,41,61,69	0
28	GOL	B	629	6/6	0.84	0.21	5.33	28,42,50,56	0
32	UNL	d	410	17/-	0.87	0.18	5.18	34,48,82,82	0
28	GOL	a	415	6/6	0.75	0.23	5.09	48,62,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	GOL	T	101	6/6	0.88	0.29	5.06	54,60,61,69	0
29	LMT	c	921	35/35	0.83	0.40	4.99	46,76,97,104	0
31	PL9	A	419	55/55	0.81	0.23	4.78	28,56,91,98	0
29	LMT	b	601	25/35	0.83	0.27	4.71	18,55,104,111	0
29	LMT	a	401	35/35	0.83	0.19	4.52	21,53,74,80	0
35	HTG	c	923	19/19	0.78	0.30	4.17	45,80,94,97	0
35	HTG	V	202	19/19	0.89	0.18	4.10	40,59,77,163	0
35	HTG	D	411	16/19	0.78	0.26	3.98	38,102,111,112	0
27	SQD	A	416	54/54	0.82	0.20	3.97	26,51,78,85	0
34	LMG	Z	101	37/55	0.74	0.28	3.90	30,75,96,112	0
26	BCR	d	404	40/40	0.89	0.15	3.72	27,36,54,60	0
28	GOL	A	415	6/6	0.80	0.20	3.52	36,49,64,64	0
35	HTG	B	625	19/19	0.91	0.20	3.49	28,43,74,86	0
32	UNL	D	410	40/-	0.82	0.20	3.43	24,54,93,101	0
34	LMG	j	101	51/55	0.92	0.17	3.38	25,35,71,81	0
34	LMG	C	501	51/55	0.80	0.20	3.34	34,56,76,85	0
32	UNL	d	411	36/-	0.80	0.23	3.34	32,56,104,111	0
29	LMT	m	102	35/35	0.68	0.24	3.31	33,61,79,95	0
36	DGD	D	405	62/66	0.54	0.39	3.31	48,79,113,122	0
28	GOL	F	103	6/6	0.90	0.19	3.30	60,65,71,71	0
29	LMT	A	417	35/35	0.85	0.19	3.29	22,57,79,97	0
28	GOL	b	632	6/6	0.84	0.19	3.26	38,52,59,59	0
28	GOL	B	628	6/6	0.86	0.29	3.26	33,42,54,72	0
29	LMT	m	104	35/35	0.77	0.24	3.20	29,59,85,86	0
26	BCR	b	622	40/40	0.92	0.18	3.07	14,24,43,51	0
34	LMG	J	101	51/55	0.90	0.19	2.99	18,32,75,81	0
32	UNL	i	101	40/-	0.77	0.25	2.95	28,62,105,117	0
29	LMT	C	522	35/35	0.74	0.38	2.89	52,81,102,104	0
32	UNL	d	413	18/-	0.77	0.19	2.85	30,52,81,84	0
24	CLA	B	602	65/65	0.92	0.16	2.80	22,40,80,101	0
34	LMG	z	101	39/55	0.74	0.33	2.78	45,82,99,107	0
28	GOL	t	102	6/6	0.89	0.25	2.77	22,59,67,67	0
28	GOL	f	101	6/6	0.81	0.25	2.73	44,50,62,64	0
34	LMG	b	624	51/55	0.89	0.23	2.68	21,36,57,81	0
23	BCT	A	404	4/4	0.94	0.15	2.51	21,24,36,47	0
32	UNL	K	101	34/-	0.69	0.30	2.51	37,61,83,88	0
28	GOL	v	203	6/6	0.75	0.31	2.50	39,74,86,87	0
28	GOL	C	526	6/6	0.95	0.19	2.46	17,21,26,26	0
28	GOL	b	631	6/6	0.91	0.16	2.41	28,41,48,51	0
24	CLA	b	605	65/65	0.92	0.18	2.37	29,48,89,102	0
28	GOL	b	628	6/6	0.91	0.13	2.33	30,35,42,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
27	SQD	L	102	54/54	0.77	0.22	2.29	24,52,86,91	0
35	HTG	b	626	19/19	0.90	0.20	2.29	30,50,86,86	0
23	BCT	a	419	4/4	0.93	0.15	2.25	21,32,41,50	0
27	SQD	B	621	54/54	0.77	0.21	2.21	26,55,94,104	0
28	GOL	A	413	6/6	0.93	0.11	2.16	23,30,33,36	0
32	UNL	I	101	40/-	0.78	0.23	2.14	27,62,110,120	0
25	PHO	a	420	64/64	0.93	0.20	2.12	17,24,30,33	0
34	LMG	a	412	51/55	0.78	0.21	2.08	33,62,84,90	0
28	GOL	A	414	6/6	0.87	0.17	2.08	30,40,43,49	0
37	LHG	l	101	49/49	0.90	0.18	2.02	15,27,39,56	0
27	SQD	a	411	54/54	0.91	0.22	2.01	32,52,73,81	0
26	BCR	B	619	40/40	0.93	0.14	1.89	15,23,46,49	0
37	LHG	d	407	49/49	0.92	0.20	1.78	15,31,44,53	0
26	BCR	D	403	40/40	0.92	0.14	1.73	19,30,58,70	0
34	LMG	C	521	51/55	0.78	0.25	1.71	32,69,88,108	0
37	LHG	L	101	49/49	0.94	0.21	1.71	12,26,38,46	0
35	HTG	b	602	19/19	0.88	0.15	1.70	29,45,65,68	0
29	LMT	b	625	25/35	0.71	0.29	1.67	44,67,109,119	0
37	LHG	E	101	42/49	0.82	0.22	1.66	22,63,78,93	0
37	LHG	D	406	49/49	0.92	0.22	1.65	14,26,38,52	0
34	LMG	B	622	51/55	0.86	0.23	1.63	19,32,49,71	0
28	GOL	a	413	6/6	0.91	0.11	1.62	30,32,37,42	0
32	UNL	D	409	17/-	0.87	0.16	1.58	30,40,63,66	0
24	CLA	d	402	65/65	0.95	0.23	1.55	16,20,36,46	0
31	PL9	d	405	55/55	0.92	0.18	1.53	13,19,33,44	0
28	GOL	c	924	6/6	0.97	0.20	1.47	24,24,25,29	0
39	MG	j	103	1/1	0.97	0.14	1.44	33,33,33,33	0
24	CLA	d	403	65/65	0.93	0.12	1.40	26,31,79,93	0
37	LHG	D	408	49/49	0.94	0.18	1.37	17,29,88,100	0
24	CLA	A	407	65/65	0.94	0.25	1.36	13,20,71,73	0
24	CLA	c	914	65/65	0.88	0.25	1.36	35,48,81,87	0
24	CLA	a	407	65/65	0.94	0.23	1.34	18,23,72,84	0
32	UNL	X	101	18/-	0.87	0.15	1.30	29,44,62,79	0
24	CLA	b	615	65/65	0.93	0.15	1.28	17,22,38,46	0
24	CLA	B	617	65/65	0.95	0.15	1.26	16,28,79,88	0
31	PL9	D	404	55/55	0.91	0.20	1.25	11,18,31,41	0
28	GOL	a	414	6/6	0.94	0.13	1.23	25,34,43,53	0
26	BCR	b	621	40/40	0.93	0.16	1.21	14,24,33,38	0
35	HTG	B	633	19/19	0.88	0.16	1.21	28,54,70,76	0
24	CLA	b	609	65/65	0.95	0.11	1.21	16,24,37,44	0
24	CLA	c	909	65/65	0.93	0.15	1.19	23,28,67,91	0
24	CLA	A	405	65/65	0.95	0.23	1.15	13,17,27,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
27	SQD	A	412	54/54	0.90	0.20	1.15	15,45,72,85	0
36	DGD	C	519	62/66	0.94	0.20	1.15	18,29,48,55	0
35	HTG	b	627	19/19	0.72	0.27	1.13	49,86,110,116	0
36	DGD	c	918	62/66	0.91	0.20	1.13	25,31,52,70	0
37	LHG	e	101	42/49	0.67	0.29	1.11	52,89,118,129	0
28	GOL	o	302	6/6	0.90	0.14	1.09	44,50,53,58	0
26	BCR	B	618	40/40	0.93	0.14	1.06	11,23,32,35	0
24	CLA	b	617	65/65	0.95	0.15	1.05	14,22,44,52	0
24	CLA	b	618	65/65	0.93	0.14	1.02	14,24,78,80	0
24	CLA	A	406	65/65	0.96	0.20	1.02	12,16,30,35	0
37	LHG	D	407	49/49	0.95	0.15	1.01	13,22,44,57	0
35	HTG	B	624	19/19	0.95	0.11	1.01	20,32,43,46	0
24	CLA	c	911	65/65	0.94	0.16	1.00	24,31,43,53	0
24	CLA	D	401	65/65	0.95	0.24	0.99	12,16,32,36	0
28	GOL	b	629	6/6	0.93	0.15	0.98	27,36,50,54	0
28	GOL	V	205	6/6	0.93	0.16	0.97	34,41,45,52	0
24	CLA	B	611	65/65	0.95	0.10	0.94	17,25,33,50	0
36	DGD	c	916	62/66	0.92	0.17	0.92	22,31,64,82	0
24	CLA	B	607	65/65	0.94	0.12	0.91	16,25,70,76	0
24	CLA	d	401	65/65	0.95	0.19	0.90	14,18,27,47	0
37	LHG	d	408	49/49	0.94	0.14	0.89	15,23,41,54	0
27	SQD	f	102	43/54	0.86	0.25	0.87	41,75,103,108	0
24	CLA	b	608	65/65	0.95	0.14	0.87	15,23,51,62	0
25	PHO	A	409	64/64	0.95	0.21	0.86	13,20,29,35	0
24	CLA	b	610	65/65	0.93	0.11	0.86	18,31,78,87	0
24	CLA	b	611	65/65	0.95	0.16	0.84	13,20,31,34	0
37	LHG	d	409	49/49	0.95	0.17	0.83	21,32,85,88	0
34	LMG	C	520	51/55	0.83	0.23	0.83	22,52,72,90	0
34	LMG	c	919	51/55	0.83	0.20	0.83	29,57,78,81	0
28	GOL	V	204	6/6	0.93	0.14	0.82	19,26,30,37	0
29	LMT	B	623	35/35	0.81	0.22	0.81	26,74,96,101	0
36	DGD	C	518	62/66	0.92	0.20	0.80	19,29,78,90	0
26	BCR	A	411	40/40	0.94	0.11	0.78	15,22,29,31	0
28	GOL	b	630	6/6	0.93	0.13	0.77	35,39,50,53	0
26	BCR	t	101	40/40	0.92	0.12	0.77	12,26,45,48	0
24	CLA	a	409	65/65	0.95	0.12	0.76	18,26,79,83	0
24	CLA	B	614	65/65	0.94	0.16	0.75	12,20,43,55	0
28	GOL	B	632	6/6	0.92	0.15	0.75	24,40,53,57	0
36	DGD	h	102	62/66	0.90	0.14	0.75	19,31,48,60	0
25	PHO	A	408	64/64	0.95	0.17	0.74	12,16,23,24	0
35	HTG	O	303	19/19	0.95	0.11	0.72	23,32,46,55	0
24	CLA	A	410	65/65	0.96	0.11	0.71	17,26,80,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	CLA	a	406	65/65	0.95	0.21	0.69	15,17,32,38	0
29	LMT	M	101	35/35	0.73	0.21	0.68	23,52,69,77	0
24	CLA	B	612	65/65	0.95	0.15	0.66	12,18,30,37	0
24	CLA	c	903	65/65	0.94	0.15	0.66	24,30,41,51	0
24	CLA	C	509	65/65	0.94	0.14	0.64	18,25,67,82	0
36	DGD	H	102	62/66	0.90	0.17	0.64	16,28,46,59	0
24	CLA	B	610	65/65	0.92	0.12	0.61	17,24,36,45	0
26	BCR	K	103	40/40	0.93	0.11	0.61	24,30,40,43	0
24	CLA	c	902	65/65	0.92	0.12	0.59	26,32,45,52	0
24	CLA	C	505	65/65	0.93	0.18	0.57	18,27,47,61	0
24	CLA	B	615	65/65	0.94	0.12	0.57	12,21,66,79	0
24	CLA	D	402	65/65	0.94	0.12	0.54	18,27,68,84	0
26	BCR	y	101	40/40	0.91	0.14	0.51	29,37,57,63	0
24	CLA	B	613	65/65	0.95	0.11	0.44	13,20,27,33	0
36	DGD	c	917	62/66	0.91	0.18	0.43	26,35,61,87	0
24	CLA	B	616	65/65	0.95	0.11	0.43	16,23,42,45	0
26	BCR	T	102	40/40	0.93	0.14	0.42	13,26,37,42	0
24	CLA	C	506	65/65	0.95	0.10	0.40	18,27,47,54	0
24	CLA	c	906	65/65	0.91	0.13	0.36	21,28,44,56	0
24	CLA	B	608	65/65	0.92	0.16	0.35	11,19,28,40	0
38	HEM	e	102	43/43	0.95	0.17	0.35	37,46,76,95	0
26	BCR	K	102	40/40	0.94	0.12	0.35	22,30,39,47	0
24	CLA	b	616	65/65	0.94	0.10	0.34	16,23,32,44	0
26	BCR	a	410	40/40	0.93	0.10	0.32	15,23,28,32	0
24	CLA	c	904	65/65	0.91	0.12	0.31	26,33,44,47	0
34	LMG	c	920	51/55	0.81	0.25	0.31	33,74,88,93	0
24	CLA	c	913	65/65	0.91	0.16	0.31	31,40,59,65	0
24	CLA	B	609	65/65	0.95	0.14	0.30	15,24,30,36	0
36	DGD	C	517	62/66	0.94	0.12	0.29	19,28,60,72	0
24	CLA	B	606	65/65	0.94	0.10	0.27	13,20,31,41	0
27	SQD	F	101	43/54	0.90	0.24	0.27	34,59,81,90	0
24	CLA	B	605	65/65	0.94	0.14	0.26	13,19,44,57	0
26	BCR	k	101	40/40	0.92	0.17	0.26	34,45,63,75	0
24	CLA	b	606	65/65	0.93	0.12	0.24	22,28,38,48	0
29	LMT	m	103	35/35	0.83	0.17	0.20	19,48,62,74	0
24	CLA	C	502	65/65	0.94	0.11	0.17	22,30,42,54	0
25	PHO	a	408	64/64	0.94	0.15	0.17	15,18,27,30	0
24	CLA	c	905	65/65	0.91	0.16	0.16	25,32,49,68	0
26	BCR	H	101	40/40	0.90	0.13	0.13	19,32,45,59	0
24	CLA	C	514	65/65	0.92	0.14	0.11	30,42,67,73	0
24	CLA	B	604	65/65	0.93	0.11	0.10	16,25,32,38	0
24	CLA	C	511	65/65	0.93	0.15	0.07	21,29,38,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	CLA	b	607	65/65	0.96	0.10	0.06	21,28,38,50	0
24	CLA	C	513	65/65	0.91	0.13	0.06	27,40,59,71	0
28	GOL	v	205	6/6	0.95	0.17	0.05	23,35,46,50	0
24	CLA	c	908	65/65	0.91	0.12	0.00	26,33,49,60	0
26	BCR	c	915	40/40	0.91	0.12	-0.00	25,34,42,45	0
38	HEM	v	202	43/43	0.97	0.11	-0.02	28,31,40,46	0
26	BCR	k	102	40/40	0.90	0.14	-0.03	30,37,50,61	0
24	CLA	c	910	65/65	0.94	0.12	-0.04	27,34,47,53	0
24	CLA	b	613	65/65	0.92	0.11	-0.05	23,29,42,48	0
24	CLA	B	603	65/65	0.92	0.12	-0.05	17,24,36,47	0
24	CLA	C	510	65/65	0.94	0.11	-0.07	23,30,45,62	0
24	CLA	C	504	65/65	0.94	0.11	-0.08	22,28,40,45	0
28	GOL	v	204	6/6	0.87	0.17	-0.09	54,66,71,80	0
24	CLA	b	620	65/65	0.94	0.13	-0.11	19,33,77,78	0
26	BCR	b	623	40/40	0.94	0.09	-0.11	18,31,42,48	0
24	CLA	b	614	65/65	0.94	0.10	-0.11	20,29,39,42	0
24	CLA	c	912	65/65	0.93	0.12	-0.16	27,36,50,54	0
24	CLA	C	507	65/65	0.92	0.13	-0.16	25,40,75,77	0
24	CLA	b	619	65/65	0.93	0.11	-0.17	20,30,49,51	0
24	CLA	C	508	65/65	0.94	0.12	-0.22	23,35,47,54	0
24	CLA	C	512	65/65	0.93	0.11	-0.22	22,30,39,45	0
26	BCR	h	101	40/40	0.90	0.12	-0.23	25,35,48,52	0
24	CLA	C	503	65/65	0.94	0.12	-0.26	20,25,39,63	0
24	CLA	c	907	65/65	0.94	0.12	-0.29	28,37,64,72	0
26	BCR	B	620	40/40	0.93	0.09	-0.35	16,26,39,49	0
26	BCR	C	515	40/40	0.93	0.10	-0.37	29,38,49,53	0
28	GOL	B	630	6/6	0.93	0.09	-0.46	26,32,40,42	0
24	CLA	b	612	65/65	0.95	0.10	-0.49	21,28,40,43	0
38	HEM	V	201	43/43	0.97	0.09	-0.56	22,25,32,39	0
38	HEM	E	103	43/43	0.97	0.12	-0.65	23,35,45,56	0
33	CA	O	301	1/1	0.97	0.14	-0.76	53,53,53,53	0
26	BCR	C	516	40/40	0.95	0.09	-0.80	23,32,42,43	0
39	MG	J	103	1/1	0.98	0.06	-1.50	27,27,27,27	0
21	FE2	A	401	1/1	0.99	0.07	-1.78	24,24,24,24	0
30	OEX	a	416	10/10	0.98	0.10	-1.94	18,21,24,34	0
22	CL	a	405	1/1	0.99	0.09	-2.03	26,26,26,26	0
30	OEX	A	418	10/10	0.99	0.09	-2.26	15,20,24,28	0
22	CL	A	403	1/1	0.99	0.06	-2.33	19,19,19,19	0
21	FE2	a	403	1/1	0.99	0.08	-2.87	28,28,28,28	0
22	CL	a	404	1/1	0.98	0.07	-2.95	20,20,20,20	0
33	CA	c	901	1/1	0.97	0.04	-3.34	44,44,44,44	0
22	CL	A	402	1/1	0.99	0.07	-4.96	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	CA	o	301	1/1	0.98	0.04	-5.19	54,54,54,54	0
22	CL	v	201	1/1	0.94	0.08	-	62,62,62,62	0
28	GOL	T	103	6/6	0.81	0.24	-	52,68,70,79	0
33	CA	B	601	1/1	0.78	0.09	-	83,83,83,83	0
35	HTG	c	922	19/19	0.80	0.21	-	43,67,84,95	0
35	HTG	C	523	19/19	0.92	0.19	-	54,62,86,88	0
35	HTG	b	603	19/19	0.65	0.26	-	46,84,110,111	0
33	CA	b	604	1/1	0.47	0.25	-	117,117,117,117	0
22	CL	U	201	1/1	0.96	0.07	-	50,50,50,50	0
32	UNL	m	101	10/-	0.81	0.22	-	35,50,55,61	0
28	GOL	O	302	6/6	0.78	0.23	-	49,55,57,61	0
32	UNL	M	102	10/-	0.81	0.21	-	28,38,57,58	0
33	CA	F	102	1/1	0.97	0.09	-	69,69,69,69	0
32	UNL	a	418	30/-	0.72	0.31	-	42,66,98,106	0
33	CA	f	104	1/1	0.91	0.07	-	77,77,77,77	0
35	HTG	B	634	19/19	0.62	0.31	-	32,76,109,127	0
32	UNL	c	926	32/-	0.70	0.37	-	39,79,98,105	0
32	UNL	B	635	33/-	0.73	0.25	-	33,58,102,102	0
32	UNL	A	420	28/-	0.64	0.28	-	50,71,78,86	0
35	HTG	B	626	19/19	0.60	0.37	-	48,81,94,95	0
32	UNL	b	634	33/-	0.68	0.29	-	29,62,111,117	0
28	GOL	B	637	6/6	0.62	0.26	-	51,72,83,86	0

6.5 Other polymers (i)

There are no such residues in this entry.