Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:05 PM GMT

PDB ID	:	4UB8
Title	:	Native structure of photosystem II (dataset-2) 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:

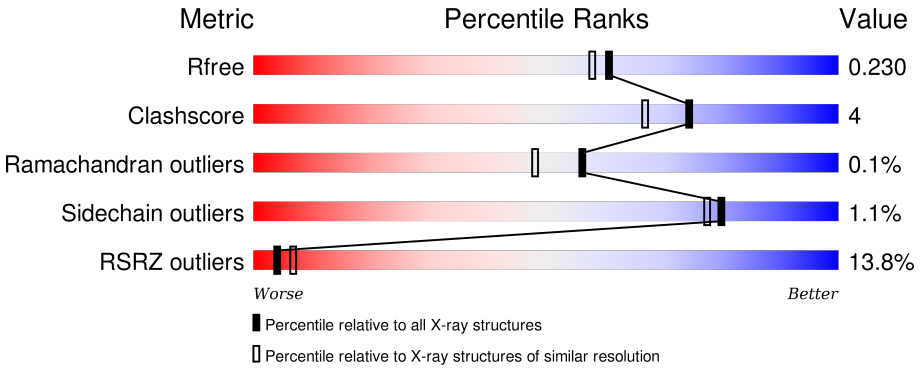
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	14% 90% 6%
1	a	344	20% 97%
2	B	505	9% 90% 10%
2	b	505	10% 99%
3	C	455	6% 90% 9%

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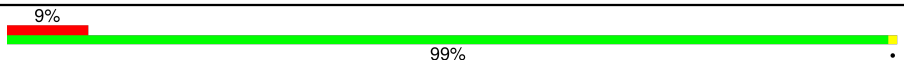
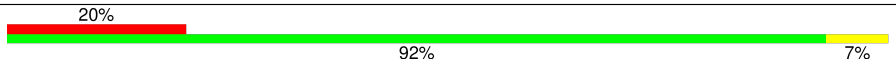
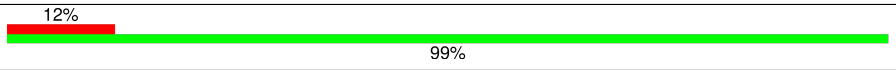
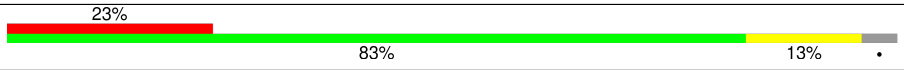
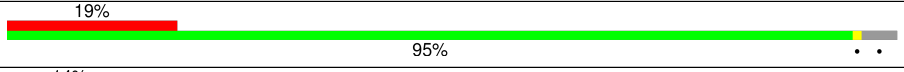
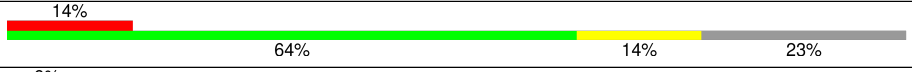
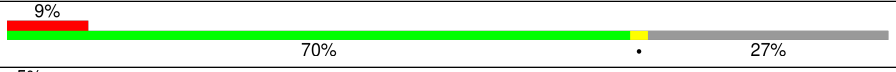
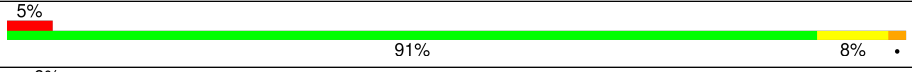
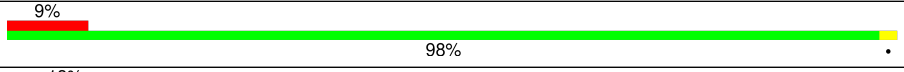
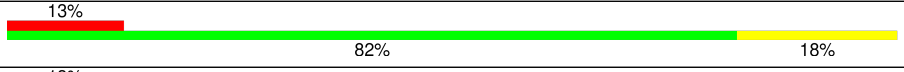
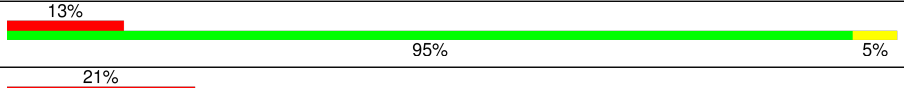
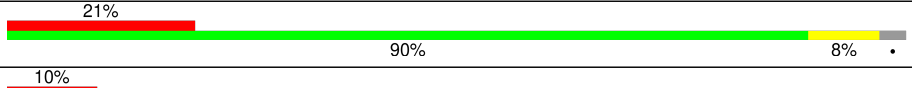
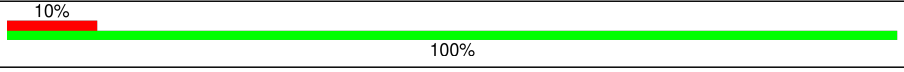
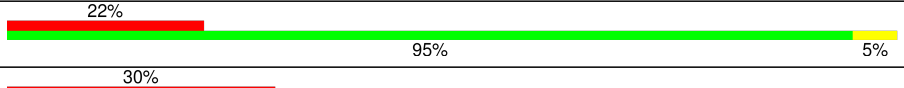
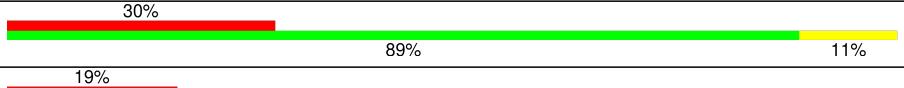
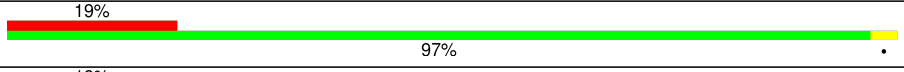
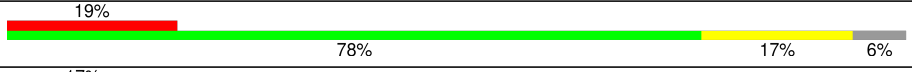
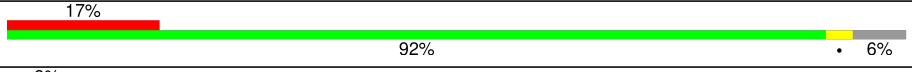
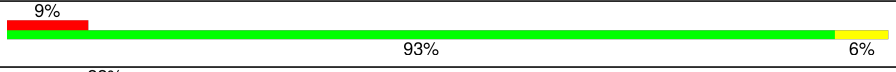
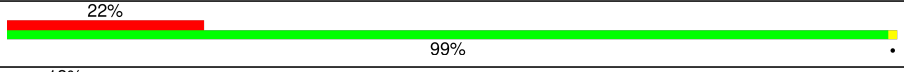
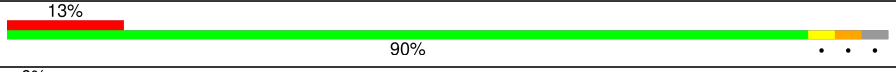
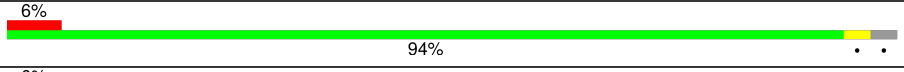
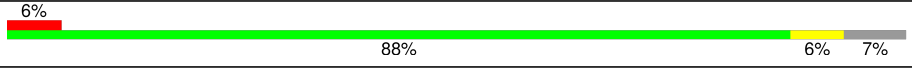
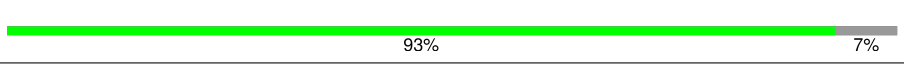
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	104	
15	u	104	

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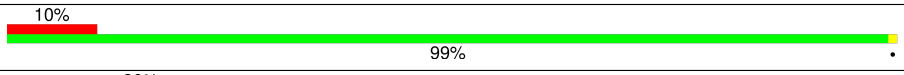
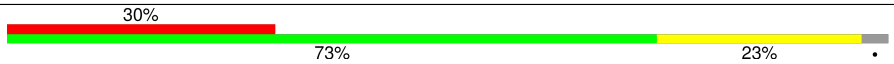
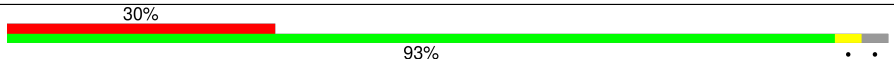
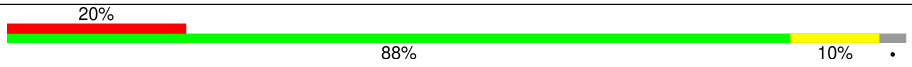
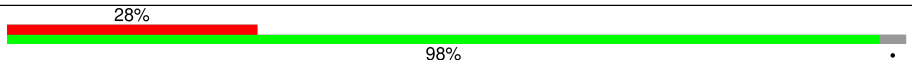
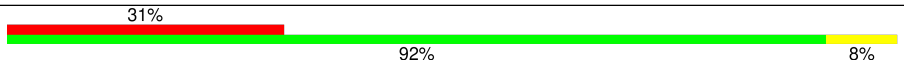
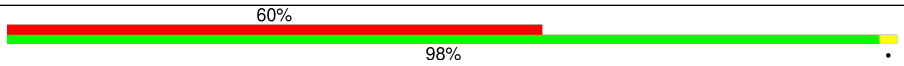
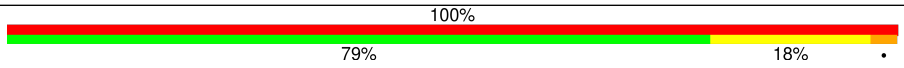
Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
23	BCT	a	418	-	-	-	X
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	409	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	-	-	-
24	CLA	B	617	X	-	-	X
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	606	X	-	-	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	b	621	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	404	X	-	-	-
26	BCR	B	619	-	-	-	X
26	BCR	b	623	-	-	-	X
26	BCR	d	405	-	-	-	X
27	SQD	A	416	-	-	-	X
27	SQD	a	402	-	-	-	X
27	SQD	l	101	-	-	-	X
28	GOL	A	413	-	-	-	X
28	GOL	A	414	-	-	-	X
28	GOL	B	625	-	-	-	X
28	GOL	B	626	-	-	-	X
28	GOL	B	627	-	-	-	X
28	GOL	B	628	-	-	-	X
28	GOL	B	629	-	-	-	X
28	GOL	C	524	-	-	-	X
28	GOL	F	103	-	-	-	X
28	GOL	V	205	-	-	-	X
28	GOL	V	206	-	-	-	X
28	GOL	V	207	-	-	-	X
28	GOL	V	208	-	-	-	X
28	GOL	a	412	-	-	-	X
28	GOL	a	413	-	-	-	X
28	GOL	b	632	-	-	-	X
28	GOL	b	633	-	-	-	X
28	GOL	c	525	-	-	-	X
28	GOL	c	527	-	-	-	X
28	GOL	f	104	-	-	-	X
28	GOL	t	102	-	-	-	X
28	GOL	v	203	-	-	-	X
29	UNL	C	526	-	-	-	X
29	UNL	D	413	-	-	-	X
29	UNL	I	101	-	-	-	X
29	UNL	J	103	-	-	-	X
29	UNL	X	101	-	-	-	X
29	UNL	d	412	-	-	-	X
29	UNL	d	413	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	UNL	i	101	-	-	-	X
29	UNL	j	103	-	-	-	X
29	UNL	k	101	-	-	-	X
29	UNL	k	102	-	-	-	X
30	LMT	A	417	-	-	-	X
30	LMT	B	634	-	-	-	X
30	LMT	E	102	-	-	-	X
30	LMT	I	102	-	-	-	X
30	LMT	M	101	-	-	-	X
30	LMT	a	401	-	-	-	X
30	LMT	a	417	-	-	-	X
30	LMT	b	602	-	-	-	X
30	LMT	f	102	-	-	-	X
30	LMT	m	103	-	-	-	X
32	PL9	A	419	-	-	-	X
32	PL9	a	416	-	-	-	X
34	LMG	C	501	-	-	-	X
34	LMG	J	101	-	-	-	X
34	LMG	Z	101	-	-	-	X
34	LMG	b	625	-	-	-	X
34	LMG	j	101	-	-	-	X
34	LMG	z	101	-	-	-	X
35	HTG	B	631	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	411	-	-	-	X
35	HTG	V	204	-	-	-	X
35	HTG	b	627	-	-	-	X
35	HTG	c	523	-	-	-	X
36	DGD	D	407	-	-	-	X
36	DGD	d	407	-	-	-	X
39	MG	j	102	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 53958 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
			2631	1725	431	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2634	1727	431	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	10	0
			4023	2642	667	701	13			
2	b	504	Total	C	N	O	S	0	11	0
			4028	2645	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	5	0
			3506	2296	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	0	0
			2726	1805	445	464	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 662	C 432	N 107	O 123	0	0	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 282	C 188	N 43	O 49	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 293	C 204	N 43	O 46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 309	C 207	N 48	O 53	S 1	0	1	0
11	l	37	Total 309	C 207	N 48	O 53	S 1	0	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total 1883	C 1178	N 315	O 385	S 5	0	4	0
13	o	243	Total 1879	C 1175	N 315	O 384	S 5	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total 264	C 185	N 36	O 41	S 2	0	1	0
14	t	30	Total 264	C 185	N 36	O 41	S 2	0	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total 774	C 491	N 129	O 154	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	0	0	0

- 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	1	0
			292	196	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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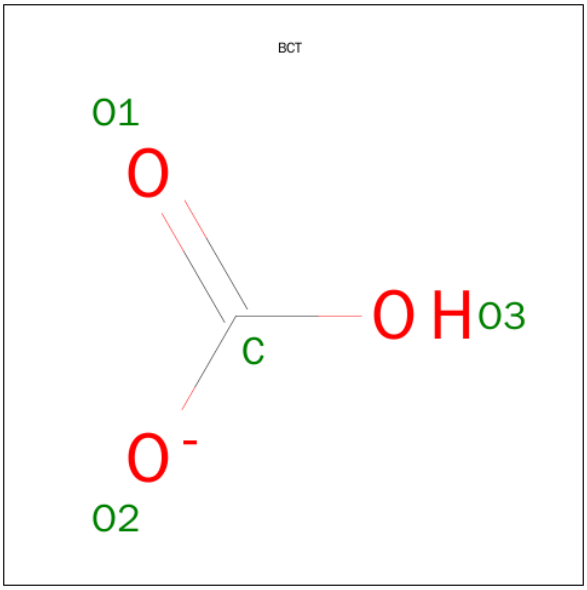
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

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

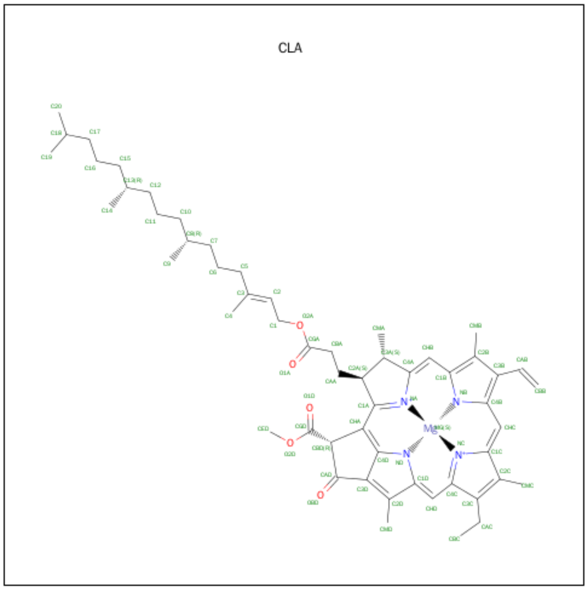
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 2 2	0	0
22	A	2	Total Cl 2 2	0	0
22	V	1	Total Cl 1 1	0	0
22	u	1	Total Cl 1 1	0	0

- 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	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

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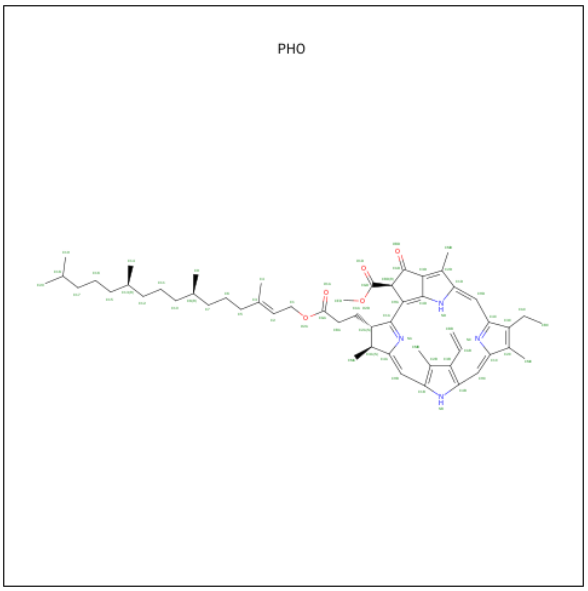
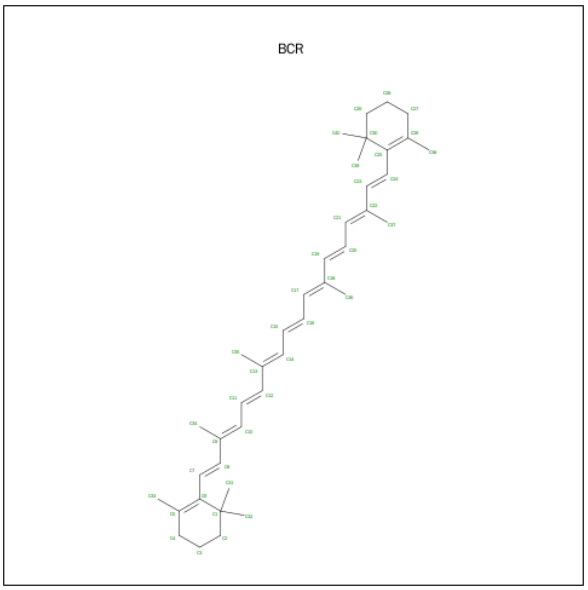
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

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



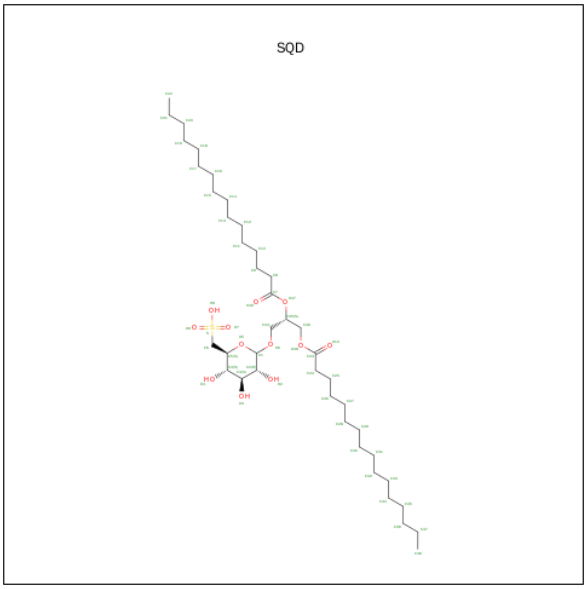
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



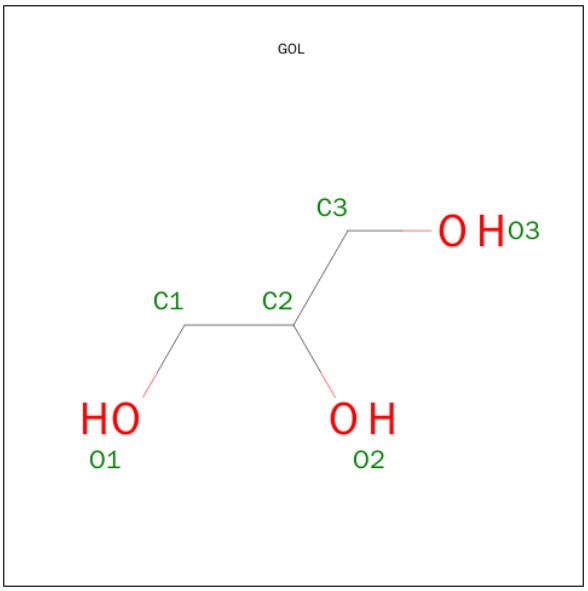
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total 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	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	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	F	1	Total	C	O	S	0	0
			43	30	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	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		

- 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	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	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	c	1	Total	C	O	0	0
			6	3	3		
28	f	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		

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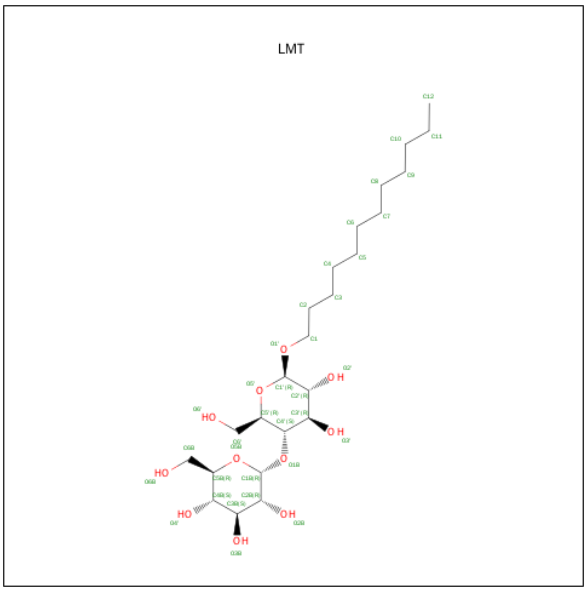
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	v	1	Total C O 6 3 3	0	0
28	v	1	Total C O 6 3 3	0	0

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

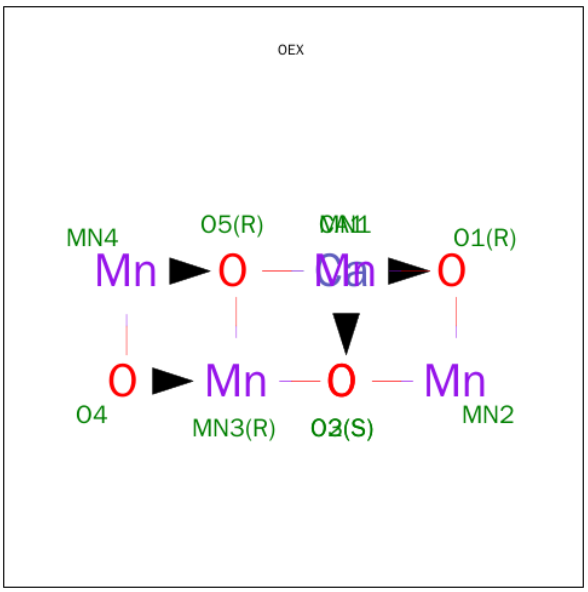
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	J	1	Total C 10 10	0	0
29	i	1	Total C O 40 35 5	0	0
29	D	2	Total C O 57 51 6	0	0
29	k	2	Total C O 42 37 5	0	0
29	B	1	Total C O 33 28 5	0	0
29	I	1	Total C O 40 35 5	0	0
29	C	1	Total C O 34 29 5	0	0
29	a	1	Total C O 30 25 5	0	0
29	x	1	Total C 10 10	0	0
29	A	1	Total C O 28 23 5	0	0
29	j	1	Total C 10 10	0	0
29	X	1	Total C 10 10	0	0
29	d	2	Total C O 53 47 6	0	0
29	m	1	Total C 10 10	0	0
29	b	1	Total C O 33 28 5	0	0
29	M	1	Total C 10 10	0	0

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



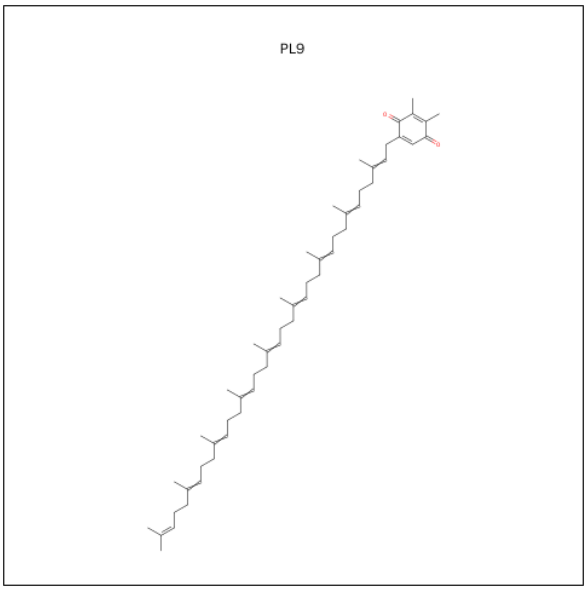
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			33	22	11		
30	B	1	Total	C	O	0	0
			25	19	6		
30	D	1	Total	C	O	0	0
			35	24	11		
30	E	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	b	1	Total	C	O	0	0
			25	19	6		
30	f	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 32 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: $C_{53}H_{80}O_2$).

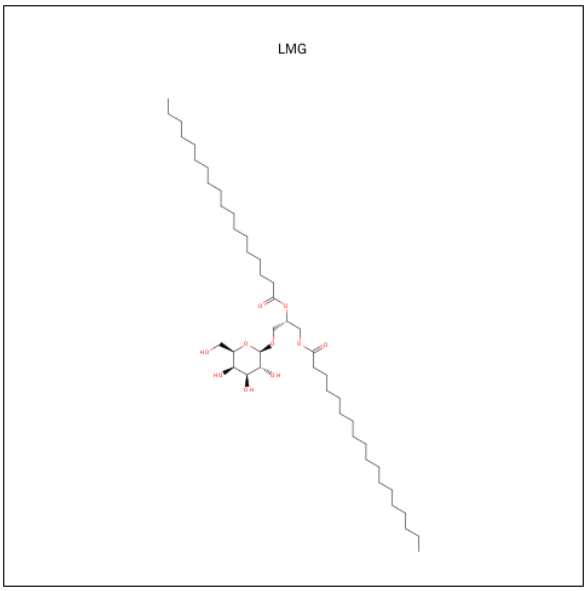


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 55 53 2	0	0
32	D	1	Total C O 55 53 2	0	0
32	a	1	Total C O 55 53 2	0	0
32	d	1	Total C O 55 53 2	0	0

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

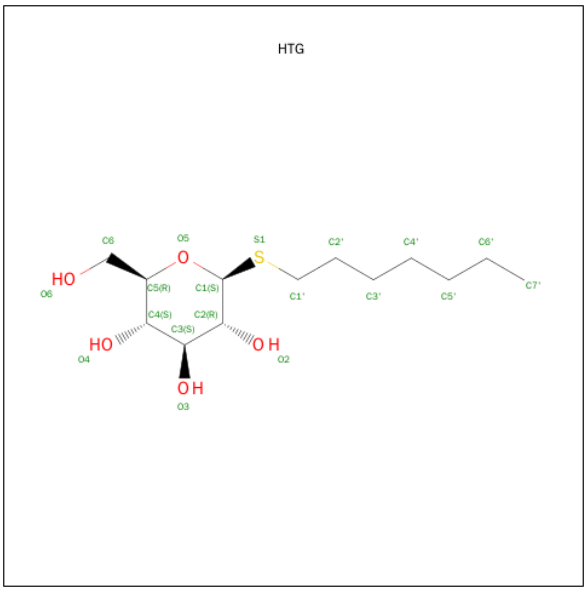
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0

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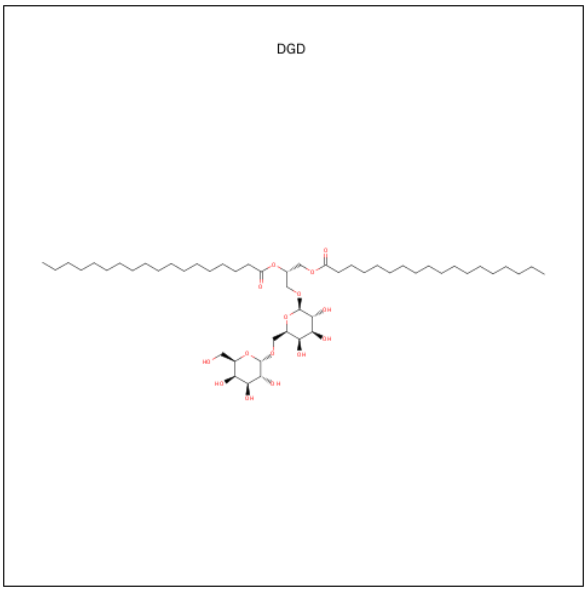
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0

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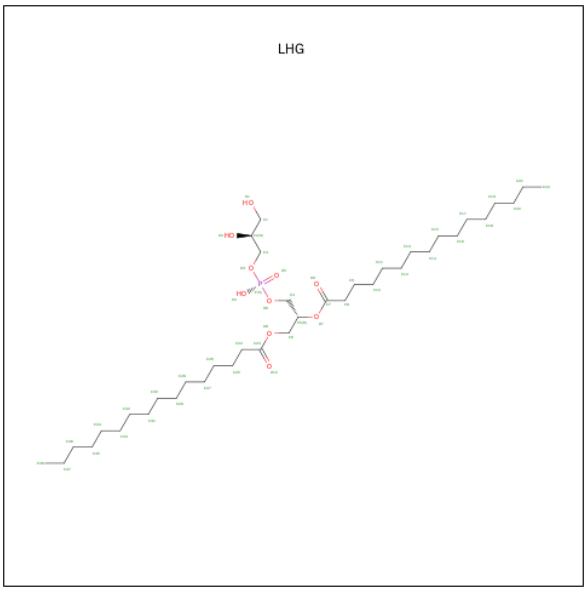
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

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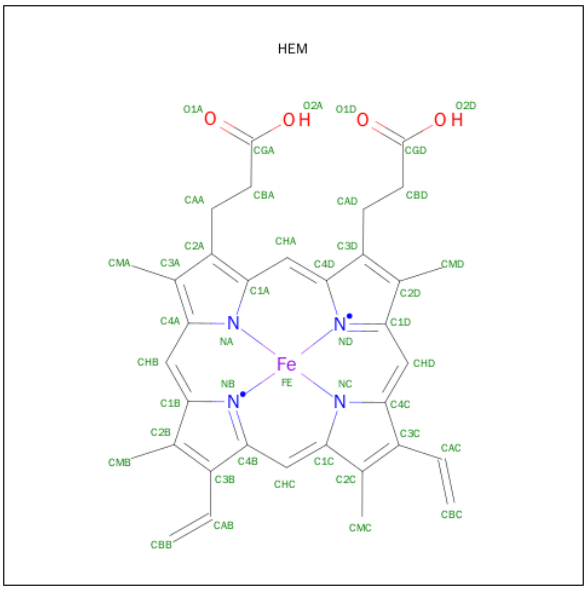
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- 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	146	Total O 149 149	0	3
40	B	277	Total O 280 280	0	3
40	C	206	Total O 209 209	0	3
40	D	157	Total O 161 161	0	4
40	E	28	Total O 28 28	0	0
40	F	7	Total O 7 7	0	0
40	H	39	Total O 40 40	0	1
40	I	8	Total O 8 8	0	0
40	J	12	Total O 12 12	0	0
40	K	6	Total O 6 6	0	0
40	L	12	Total O 12 12	0	0
40	M	15	Total O 15 15	0	0
40	O	164	Total O 165 165	0	1
40	T	12	Total O 13 13	0	1
40	U	75	Total O 76 76	0	1
40	V	111	Total O 111 111	0	0
40	Y	1	Total O 1 1	0	0
40	X	8	Total O 8 8	0	0
40	a	151	Total O 151 151	0	0
40	b	247	Total O 249 249	0	2
40	c	187	Total O 189 189	0	2
40	d	136	Total O 139 139	0	3

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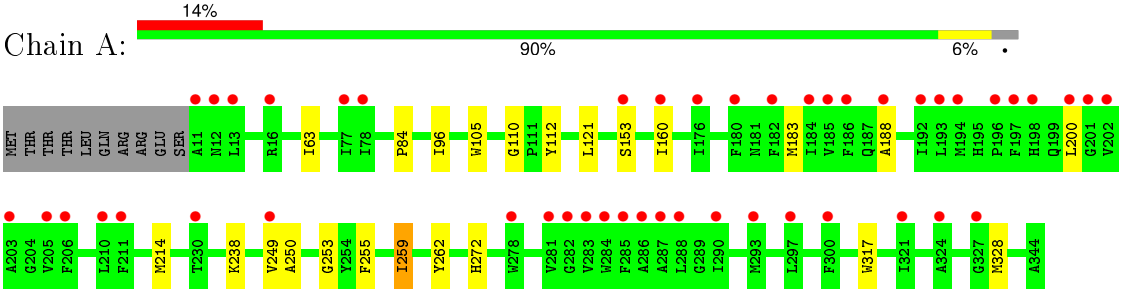
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	e	15	Total O 15 15	0	0
40	f	7	Total O 7 7	0	0
40	h	36	Total O 36 36	0	0
40	i	5	Total O 5 5	0	0
40	j	7	Total O 7 7	0	0
40	k	3	Total O 3 3	0	0
40	l	10	Total O 10 10	0	0
40	m	12	Total O 12 12	0	0
40	o	137	Total O 137 137	0	0
40	t	10	Total O 10 10	0	0
40	u	89	Total O 89 89	0	0
40	v	80	Total O 80 80	0	0
40	y	4	Total O 4 4	0	0
40	x	5	Total O 5 5	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.

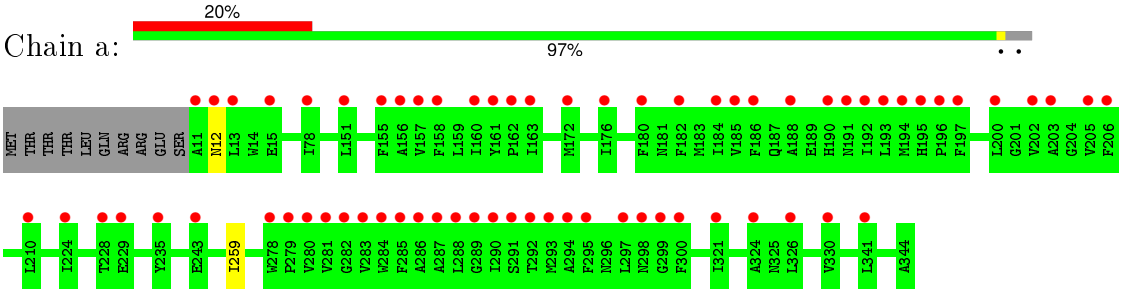
- Molecule 1: Photosystem Q(B) protein

Chain A:



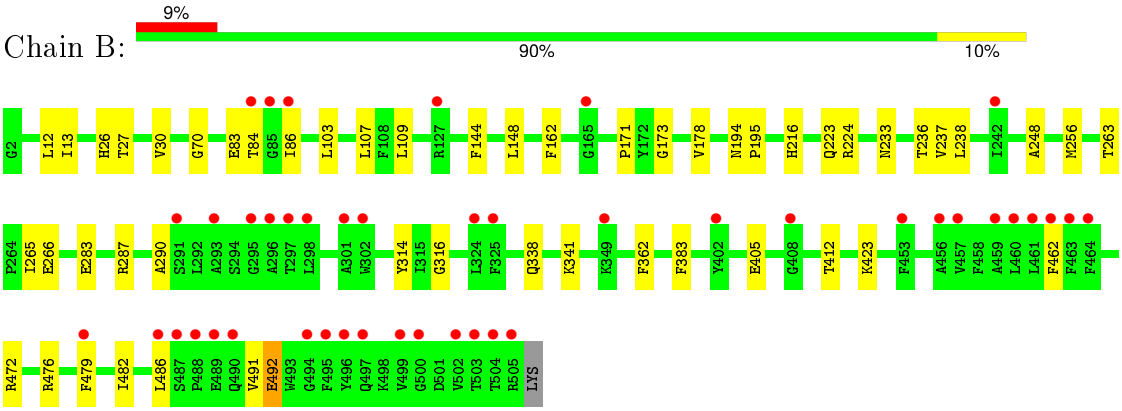
- Molecule 1: Photosystem Q(B) protein

Chain a:



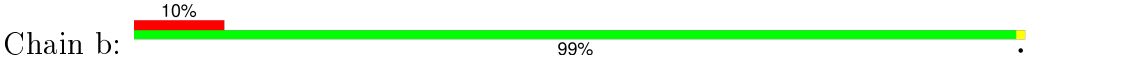
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

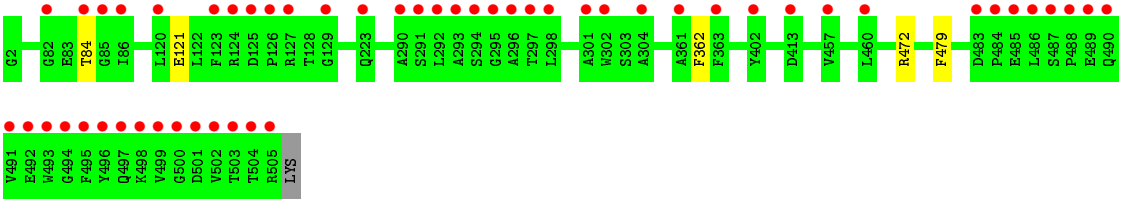
Chain B:



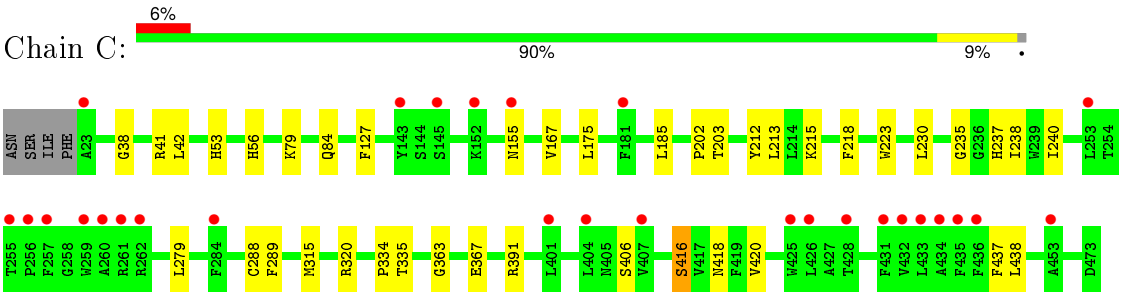
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

Chain b:

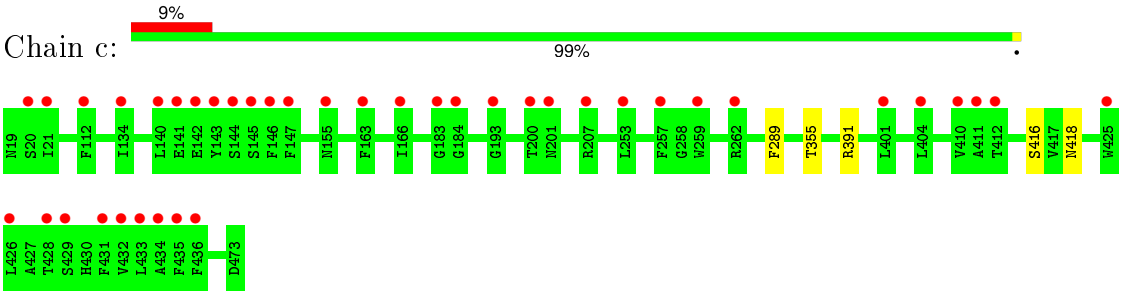




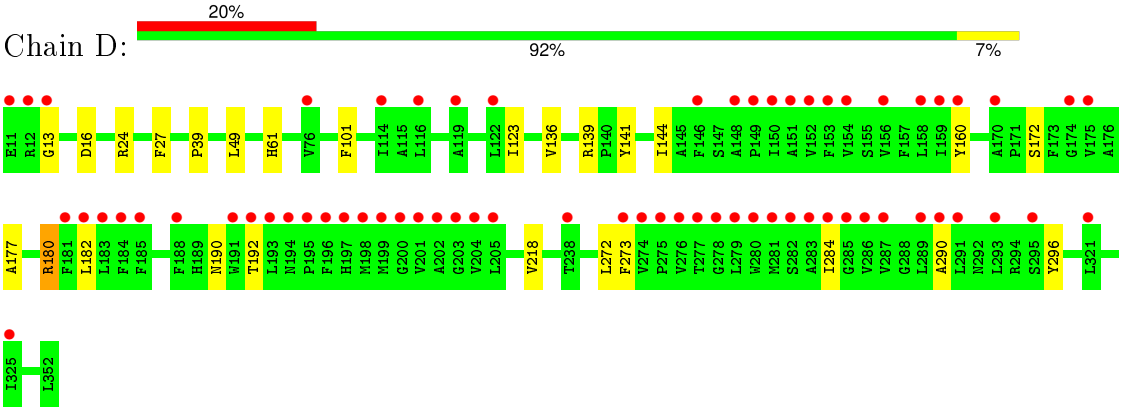
• Molecule 3: Photosystem II 44 kDa reaction center protein



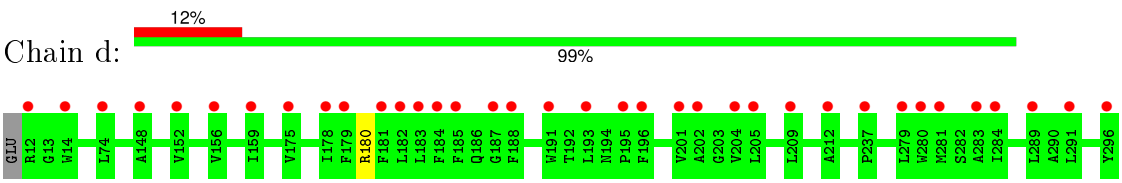
• Molecule 3: Photosystem II 44 kDa reaction center protein

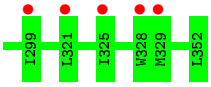


• Molecule 4: Photosystem II D2 protein



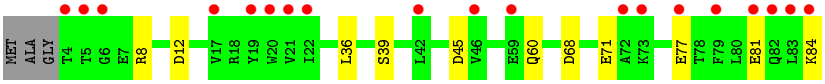
• Molecule 4: Photosystem II D2 protein





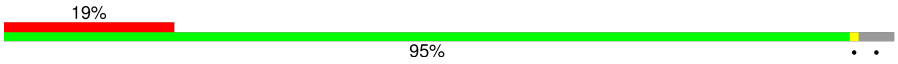
• Molecule 5: Cytochrome b559 subunit alpha

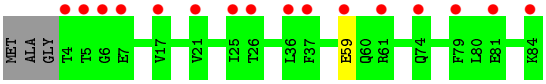
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

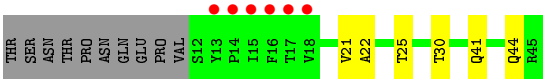
Chain e:





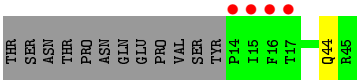
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



• Molecule 6: Cytochrome b559 subunit beta

Chain f:

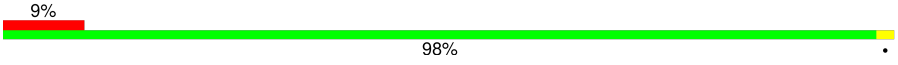


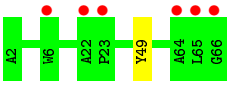
• Molecule 7: Photosystem II reaction center protein H

Chain H:

• Molecule 7: Photosystem II reaction center protein H

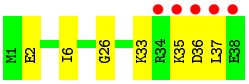
Chain h:





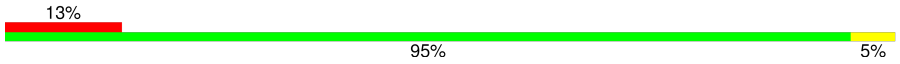
• Molecule 8: Photosystem II reaction center protein I

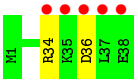
Chain I:



• Molecule 8: Photosystem II reaction center protein I

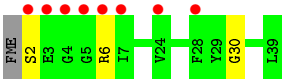
Chain i:





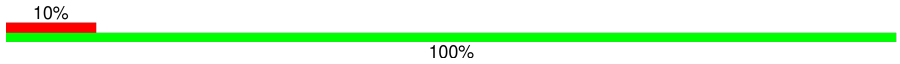
• Molecule 9: Photosystem II reaction center protein J

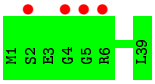
Chain J:



• Molecule 9: Photosystem II reaction center protein J

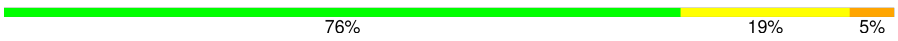
Chain j:

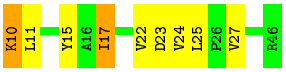




• Molecule 10: Photosystem II reaction center protein K

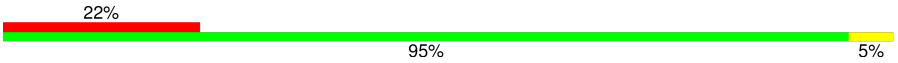
Chain K:

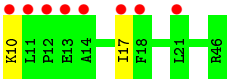




• Molecule 10: Photosystem II reaction center protein K

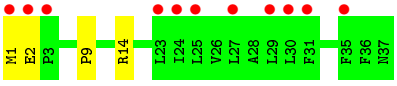
Chain k:





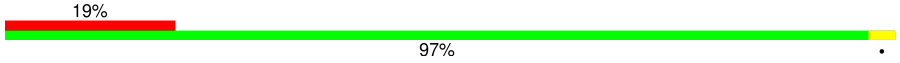
• Molecule 11: Photosystem II reaction center protein L

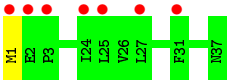
Chain L:



• Molecule 11: Photosystem II reaction center protein L

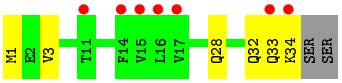
Chain l:





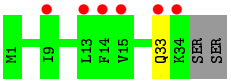
• Molecule 12: Photosystem II reaction center protein M

Chain M:



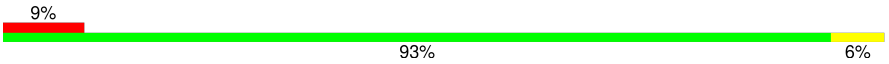
• Molecule 12: Photosystem II reaction center protein M

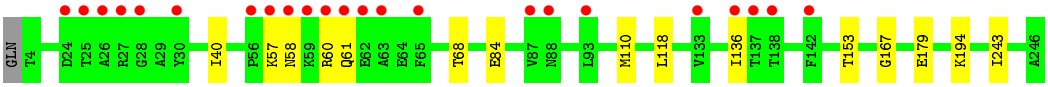
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

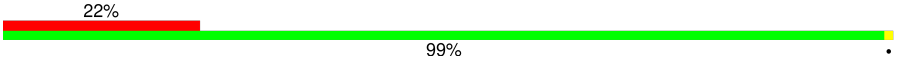
Chain O:

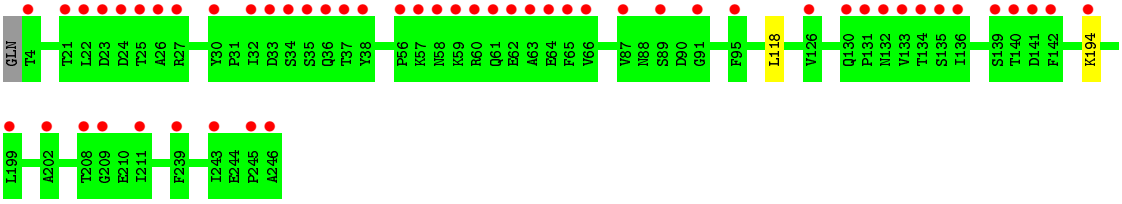




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

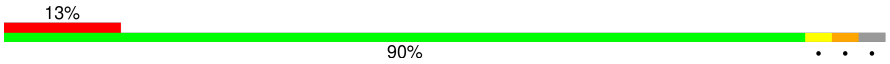
Chain o:

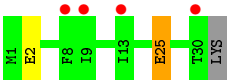




• Molecule 14: Photosystem II reaction center protein T

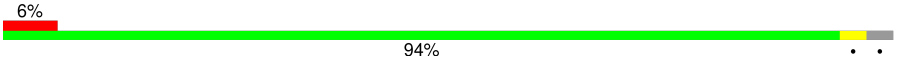
Chain T:

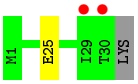




• Molecule 14: Photosystem II reaction center protein T

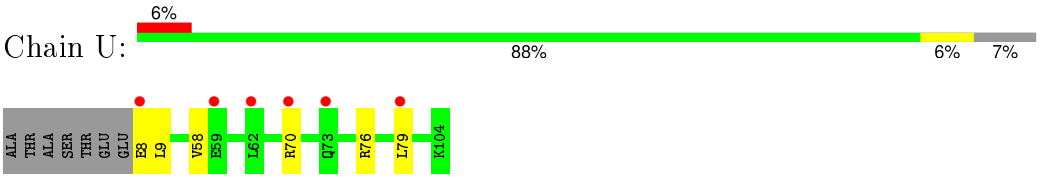
Chain t:





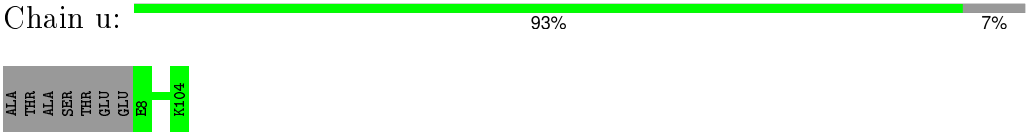
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



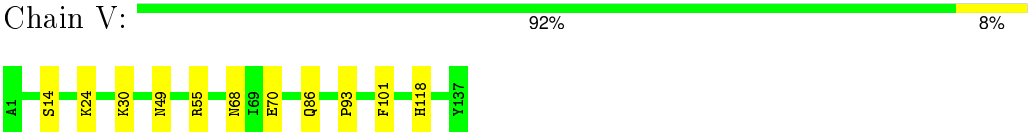
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



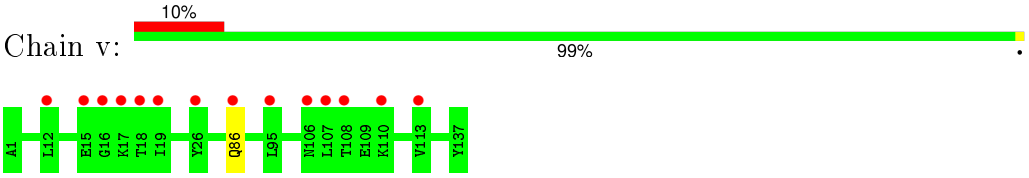
• Molecule 16: Cytochrome c-550

Chain V:



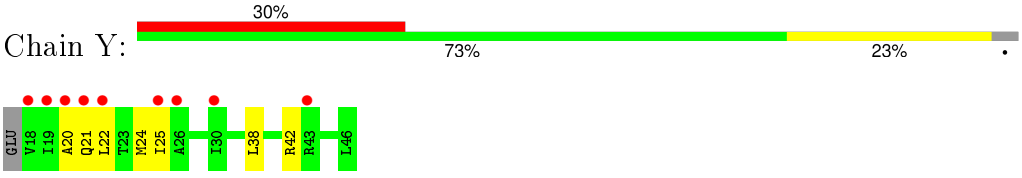
• Molecule 16: Cytochrome c-550

Chain v:



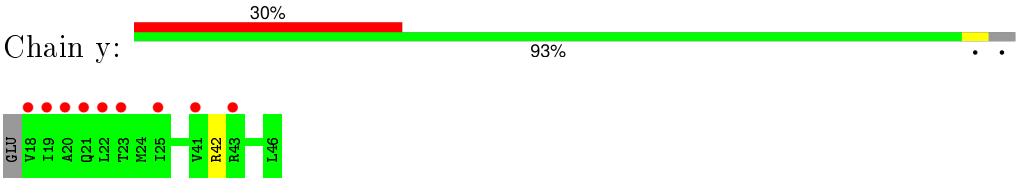
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



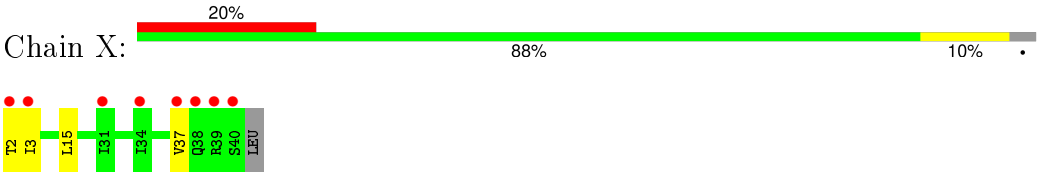
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



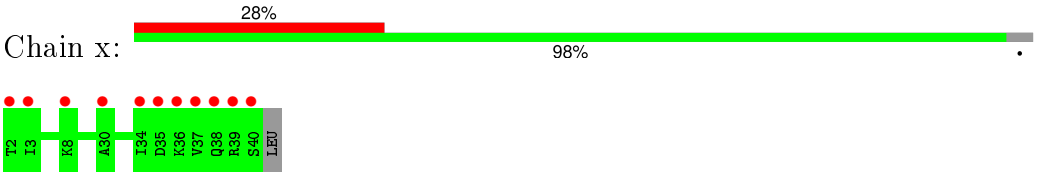
• Molecule 18: Photosystem II reaction center protein X

Chain X:



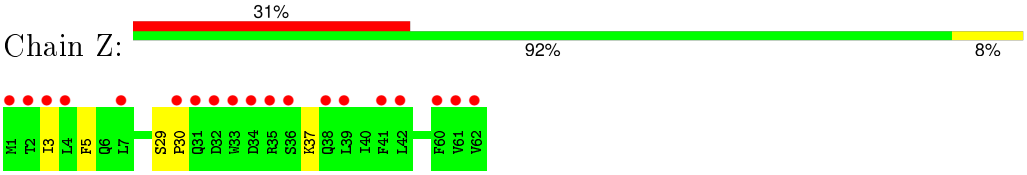
• Molecule 18: Photosystem II reaction center protein X

Chain x:



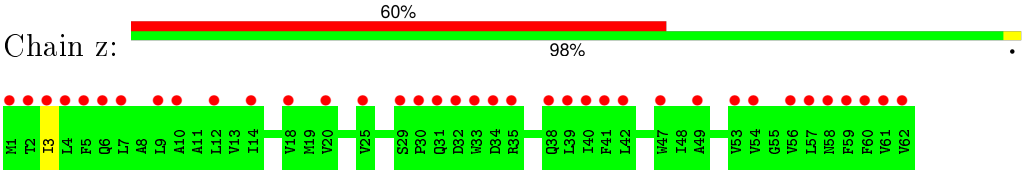
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



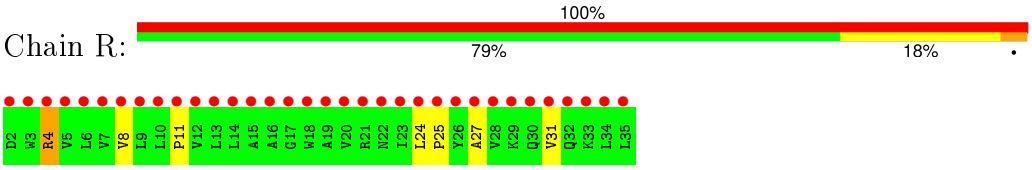
• Molecule 19: Photosystem II reaction center protein Z

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	123.81Å 230.00Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 – 1.95 61.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.90-1.95) 85.6 (61.90-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.225 0.195 , 0.230	Depositor DCC
R_{free} test set	29289 reflections (6.01%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 585991 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53958	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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	0.53	0/2725	0.59	0/3716
1	a	0.55	0/2731	0.58	0/3724
2	B	0.49	0/4193	0.56	0/5712
2	b	0.47	0/4201	0.55	0/5723
3	C	0.46	0/3634	0.54	0/4947
3	c	0.46	0/3676	0.54	0/5004
4	D	0.53	0/2821	0.56	0/3844
4	d	0.52	0/2818	0.55	0/3840
5	E	0.36	0/693	0.52	0/944
5	e	0.33	0/681	0.52	0/928
6	F	0.39	0/284	0.48	0/387
6	f	0.37	0/265	0.51	0/360
7	H	0.40	0/535	0.53	0/728
7	h	0.35	0/524	0.50	0/713
8	I	0.38	0/311	0.51	0/419
8	i	0.40	0/311	0.50	0/419
9	J	0.37	0/278	0.46	0/376
9	j	0.38	0/278	0.48	0/376
10	K	0.36	0/303	0.48	0/416
10	k	0.36	0/303	0.51	0/416
11	L	0.48	0/319	0.49	0/433
11	l	0.49	0/319	0.50	0/433
12	M	0.43	0/270	0.58	0/368
12	m	0.47	0/262	0.58	0/357
13	O	0.41	0/1926	0.56	0/2611
13	o	0.40	0/1919	0.57	0/2601
14	T	0.54	0/266	0.56	0/362
14	t	0.54	0/266	0.56	0/362
15	U	0.44	0/785	0.55	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.45	0/1096	0.54	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.41	0/1085	0.53	0/1473
17	Y	0.29	0/216	0.46	0/289
17	y	0.28	0/216	0.46	0/289
18	X	0.34	0/298	0.44	0/403
18	x	0.34	0/290	0.48	0/392
19	Z	0.31	0/490	0.43	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.24	0/279	0.38	0/383
All	All	0.46	0/43142	0.55	0/58701

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	2631	0	2538	24	0
1	a	2634	0	2543	0	0
2	B	4023	0	3904	52	0
2	b	4028	0	3910	0	0
3	C	3506	0	3439	33	0
3	c	3544	0	3480	0	0
4	D	2726	0	2627	27	0
4	d	2720	0	2626	0	0
5	E	668	0	658	8	0
5	e	662	0	648	0	0
6	F	275	0	282	4	0
6	f	257	0	269	0	0
7	H	519	0	545	8	0
7	h	511	0	532	0	0
8	I	314	0	328	5	0
8	i	314	0	328	0	0
9	J	272	0	279	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	282	0	290	0	0
10	K	293	0	305	8	0
10	k	293	0	305	0	0
11	L	309	0	327	3	0
11	l	309	0	327	0	0
12	M	274	0	299	8	0
12	m	269	0	288	0	0
13	O	1883	0	1865	10	0
13	o	1879	0	1858	0	0
14	T	264	0	267	3	0
14	t	264	0	267	0	0
15	U	774	0	773	3	0
15	u	774	0	773	0	0
16	V	1072	0	1086	9	0
16	v	1064	0	1073	0	0
17	Y	215	0	246	5	0
17	y	215	0	246	0	0
18	X	292	0	328	3	0
18	x	287	0	317	0	0
19	Z	479	0	516	4	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	V	1	0	0	1	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	195	0	216	13	0
24	B	1040	0	1152	50	0
24	C	845	0	936	53	0
24	D	195	0	216	11	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	2	0
25	a	64	0	74	0	0
25	d	64	0	74	0	0
26	A	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	120	0	168	6	0
26	C	80	0	112	7	0
26	D	40	0	56	4	0
26	H	40	0	56	6	0
26	K	40	0	56	2	0
26	T	40	0	56	5	0
26	Y	40	0	56	2	0
26	a	40	0	56	0	0
26	b	120	0	168	0	0
26	c	80	0	112	0	0
26	d	40	0	56	0	0
26	h	40	0	56	0	0
26	k	40	0	56	0	0
26	t	40	0	56	0	0
26	y	40	0	56	0	0
27	A	108	0	156	8	0
27	F	43	0	53	5	0
27	a	108	0	155	0	0
27	b	54	0	78	0	0
27	f	43	0	53	0	0
27	l	54	0	78	0	0
28	A	18	0	24	4	0
28	B	42	0	56	4	0
28	C	12	0	16	3	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	1	0
28	V	30	0	40	4	0
28	a	12	0	16	0	0
28	b	30	0	40	0	0
28	c	18	0	24	0	0
28	f	6	0	7	0	0
28	t	6	0	8	0	0
28	v	24	0	32	0	0
29	A	28	0	0	0	0
29	B	33	0	0	0	0
29	C	34	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	M	10	0	0	0	0
29	X	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	30	0	0	0	0
29	b	33	0	0	0	0
29	d	53	0	0	0	0
29	i	40	0	0	0	0
29	j	10	0	0	0	0
29	k	42	0	0	0	0
29	m	10	0	0	0	0
29	x	10	0	0	0	0
30	A	33	0	39	0	0
30	B	25	0	35	1	0
30	D	35	0	46	1	0
30	E	35	0	46	0	0
30	I	35	0	46	2	0
30	M	70	0	92	3	0
30	a	70	0	92	0	0
30	b	50	0	70	0	0
30	f	35	0	46	0	0
30	m	70	0	92	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	55	0	80	4	0
32	D	55	0	80	0	0
32	a	55	0	80	0	0
32	d	55	0	80	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	2	0
34	C	153	0	216	11	0
34	J	51	0	72	3	0
34	Z	37	0	44	6	0
34	b	51	0	72	0	0
34	c	153	0	216	0	0
34	j	51	0	72	0	0
34	z	39	0	48	0	0
35	B	95	0	130	1	0
35	C	38	0	52	3	0
35	D	16	0	17	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	O	19	0	26	0	0
35	V	19	0	26	1	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	10	0
36	D	62	0	82	6	0
36	H	62	0	82	2	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	12	0
37	E	42	0	57	6	0
37	L	49	0	74	1	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	149	0	0	2	0
40	B	280	0	0	6	0
40	C	209	0	0	4	0
40	D	161	0	0	2	0
40	E	28	0	0	1	0
40	F	7	0	0	0	0
40	H	40	0	0	0	0
40	I	8	0	0	0	0
40	J	12	0	0	1	0
40	K	6	0	0	1	0
40	L	12	0	0	1	0
40	M	15	0	0	0	0
40	O	165	0	0	2	0
40	T	13	0	0	0	0
40	U	76	0	0	2	0
40	V	111	0	0	1	0
40	X	8	0	0	0	0
40	Y	1	0	0	0	0
40	a	151	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	b	249	0	0	0	0
40	c	189	0	0	0	0
40	d	139	0	0	0	0
40	e	15	0	0	0	0
40	f	7	0	0	0	0
40	h	36	0	0	0	0
40	i	5	0	0	0	0
40	j	7	0	0	0	0
40	k	3	0	0	0	0
40	l	10	0	0	0	0
40	m	12	0	0	0	0
40	o	137	0	0	0	0
40	t	10	0	0	0	0
40	u	89	0	0	0	0
40	v	80	0	0	0	0
40	x	5	0	0	0	0
40	y	4	0	0	0	0
All	All	53958	0	52755	346	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 4.

All (346) 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	32:A:419:PL9:H102	1.51	0.93
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.30	0.92
24:B:616:CLA:H71	24:B:617:CLA:H192	1.64	0.78
24:C:503:CLA:H193	35:C:522:HTG:H3'1	1.67	0.74
24:C:504:CLA:H61	24:C:514:CLA:H42	27.00	0.74
24:C:507:CLA:HMC2	24:C:508:CLA:H102	1.68	0.73
8:I:26:GLY:HA3	30:I:102:LMT:H6'1	1.70	0.73
1:A:253:GLY:HA3	2:B:491:VAL:HG12	3.53	0.73
24:C:503:CLA:H202	24:C:509:CLA:HBB1	29.02	0.72
26:B:620:BCR:HC8	26:B:620:BCR:H331	1.73	0.71
32:A:419:PL9:H471	27:F:101:SQD:H302	1.71	0.71
36:D:407:DGD:HD4	5:E:45:ASP:HB3	1.73	0.70
24:C:508:CLA:HMC2	24:C:509:CLA:H102	29.18	0.68
24:C:510:CLA:HBB1	24:C:510:CLA:HMB1	1.77	0.66
13:O:58:ASN:HD21	13:O:61:GLN:HB2	1.60	0.66
4:D:101:PHE:HB3	36:D:407:DGD:HG2	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:411:SQD:H251	37:D:410:LHG:H131	1.78	0.66
24:A:406:CLA:HBB1	24:A:406:CLA:HMB1	1.92	0.65
18:X:2:THR:HG22	18:X:3:ILE:HG12	4.88	0.65
24:B:615:CLA:H18	34:B:621:LMG:H421	1.78	0.64
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.80	0.62
3:C:213[B]:LEU:HD11	26:C:516:BCR:H373	4.79	0.62
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.82	0.62
2:B:248:ALA:HA	24:B:604:CLA:H42	1.81	0.62
1:A:238:LYS:NZ	40:A:628:HOH:O	65.39	0.61
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.82	0.61
2:B:266:GLU:HB3	28:B:628:GOL:H11	1.82	0.61
1:A:183:MET:HA	24:A:405:CLA:HMD2	1.83	0.61
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.81	0.61
24:B:606:CLA:HBB1	24:B:606:CLA:HHC	1.81	0.60
24:C:511:CLA:HBB1	24:C:511:CLA:HMB1	1.94	0.60
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.82	0.60
3:C:213[A]:LEU:HG	24:C:508:CLA:H202	14.70	0.60
32:A:419:PL9:H502	4:D:39:PRO:HG3	1.83	0.60
27:A:416:SQD:H271	2:B:109:LEU:HD13	60.04	0.59
3:C:167:VAL:HG13	24:C:514:CLA:H71	13.26	0.59
24:D:401:CLA:HMB1	24:D:401:CLA:HBB1	1.87	0.59
2:B:12:LEU:HB2	24:B:617:CLA:HMC2	13.30	0.58
36:D:407:DGD:HAW1	27:F:101:SQD:H383	4.37	0.58
2:B:266:GLU:HB3	28:B:633:GOL:H11	25.83	0.57
40:B:953:HOH:O	7:H:12[A]:ARG:NH2	2.38	0.57
5:E:45:ASP:OD2	20:R:4:ARG:NH2	2.38	0.57
24:C:505:CLA:HBB1	24:C:505:CLA:HHC	4.33	0.57
1:A:183:MET:HA	24:A:406:CLA:HMD2	12.21	0.57
24:B:602:CLA:H91	26:H:101:BCR:H21C	1.86	0.56
24:C:513:CLA:HMB1	24:C:513:CLA:HBB1	2.34	0.56
24:C:513:CLA:H101	24:C:514:CLA:H141	1.87	0.56
24:C:503:CLA:C4D	24:C:505:CLA:H2	17.62	0.56
1:A:262:TYR:HB3	37:E:101:LHG:HC62	4.53	0.56
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	1.87	0.55
3:C:438:LEU:HD11	24:C:507:CLA:HBB1	17.25	0.55
2:B:462:PHE:CE1	24:B:614:CLA:HMB3	2.41	0.55
6:F:30:THR:HG21	34:J:101:LMG:H412	1.88	0.55
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.19	0.55
28:A:413:GOL:H11	12:M:1:FME:HG2	1.88	0.55
34:B:621:LMG:H242	4:D:284:ILE:HD13	1.86	0.55
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:D:411:HTG:H1	7:H:25:TRP:CG	2.75	0.55
24:C:514:CLA:HAB	26:C:515:BCR:H24C	1.88	0.55
37:D:410:LHG:H112	37:D:410:LHG:H382	1.88	0.55
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.41	0.55
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.64	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.88	0.55
24:A:405:CLA:HBB1	24:A:405:CLA:HMB1	1.89	0.54
28:A:412:GOL:H11	12:M:1:FME:HG2	19.33	0.54
4:D:24:ARG:HD3	18:X:37:VAL:HG22	2.00	0.54
24:A:406:CLA:H91	34:J:101:LMG:H221	1.88	0.54
30:B:634:LMT:H2'	28:B:635:GOL:H2	1.88	0.54
4:D:13:GLY:HA3	35:D:411:HTG:H62	1.89	0.54
2:B:216:HIS:HE1	24:B:614:CLA:C1A	26.58	0.54
2:B:103:LEU:HD21	24:B:610:CLA:HMC3	26.26	0.54
24:C:507:CLA:HMB1	24:C:507:CLA:HBB1	1.88	0.54
2:B:482:ILE:HD12	2:B:486:LEU:HD13	2.11	0.54
3:C:215:LYS:HG3	3:C:223:TRP:HA	4.36	0.54
26:D:405:BCR:H313	36:D:407:DGD:HA91	2.48	0.53
24:D:404:CLA:H162	7:H:33:VAL:HG13	11.14	0.53
34:C:501:LMG:H242	24:C:507:CLA:H92	14.83	0.53
6:F:21:VAL:O	6:F:25:THR:HG23	2.08	0.53
10:K:17:ILE:H	10:K:17:ILE:HD13	1.73	0.53
12:M:28:GLN:O	12:M:32:GLN:HG3	2.10	0.53
11:L:2:GLU:O	40:L:207:HOH:O	3.23	0.53
16:V:70:GLU:HB2	28:V:205:GOL:H12	1.90	0.52
32:A:419:PL9:H13	32:A:419:PL9:H101	1.90	0.52
36:D:407:DGD:O1B	36:D:407:DGD:O2D	2.32	0.52
37:D:410:LHG:H132	37:D:410:LHG:H372	1.91	0.52
26:B:620:BCR:C8	26:B:620:BCR:H331	2.35	0.52
24:B:617:CLA:HMB1	24:B:617:CLA:HBB1	1.92	0.52
3:C:437:PHE:CE1	24:C:511:CLA:HMB3	2.45	0.52
12:M:33:GLN:HB2	12:M:33:GLN:HB2	0.00	0.52
2:B:86[B]:ILE:HD12	2:B:86[B]:ILE:H	1.74	0.52
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.91	0.51
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.91	0.51
4:D:61:HIS:HD2	40:D:599:HOH:O	1.92	0.51
4:D:192:THR:HG23	24:D:403:CLA:HBC2	1.91	0.51
3:C:41:ARG:NH1	24:C:513:CLA:HMD1	19.82	0.51
8:I:36:ASP:OD1	8:I:36:ASP:N	2.43	0.51
3:C:391:ARG:NH2	40:C:776:HOH:O	2.44	0.51
24:C:508:CLA:H71	26:C:516:BCR:H10C	12.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121[A]:LEU:HD21	24:A:409:CLA:HMB3	5.50	0.50
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.15	0.50
28:C:525:GOL:H2	40:C:708:HOH:O	12.32	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.50
24:C:503:CLA:H42	24:C:504:CLA:HMD1	7.41	0.50
3:C:155:ASN:OD1	40:C:757:HOH:O	2.19	0.50
40:U:230[A]:HOH:O	22:V:202:CL:CL	2.56	0.50
26:H:101:BCR:H331	26:H:101:BCR:C8	2.42	0.50
3:C:212:TYR:O	3:C:215:LYS:HG2	4.56	0.50
24:C:512:CLA:HMB1	24:C:512:CLA:HBB1	2.29	0.49
2:B:412:THR:O	40:B:758:HOH:O	76.24	0.49
5:E:77:GLU:O	5:E:81:GLU:HG2	2.77	0.49
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.92	0.49
19:Z:37:LYS:NZ	34:Z:101:LMG:HC5	3.64	0.49
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	1.93	0.49
2:B:103:LEU:HB2	24:B:611:CLA:H62	13.82	0.49
27:A:411:SQD:H302	24:C:510:CLA:H71	25.60	0.49
34:C:501:LMG:H152	36:C:517:DGD:HA82	1.94	0.49
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.92	0.49
10:K:15:TYR:CZ	19:Z:5:PHE:HZ	2.51	0.49
1:A:153:SER:HB2	24:A:406:CLA:H43	18.78	0.49
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.18	0.49
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.48	0.49
4:D:24:ARG:NH2	27:F:101:SQD:O4	2.46	0.49
3:C:38:GLY:HA3	24:C:513:CLA:HMD3	17.43	0.48
10:K:24:VAL:HG13	17:Y:25:ILE:HD13	2.08	0.48
3:C:320:ARG:HB2	28:C:525:GOL:H32	17.15	0.48
24:B:610:CLA:HHC	24:B:610:CLA:HBB1	2.18	0.48
27:A:411:SQD:H142	37:D:410:LHG:H152	4.52	0.48
8:I:2:GLU:O	8:I:6:ILE:HG12	2.14	0.48
24:B:611:CLA:HBB1	24:B:611:CLA:HHC	1.96	0.48
24:A:405:CLA:CBD	24:D:401:CLA:HAC2	2.43	0.48
3:C:79:LYS:HB3	3:C:84:GLN:NE2	2.46	0.48
26:H:101:BCR:H331	26:H:101:BCR:HC8	1.95	0.48
24:D:404:CLA:H142	7:H:36:GLY:HA3	7.21	0.48
26:T:102:BCR:H311	26:T:102:BCR:HC8	1.95	0.48
3:C:363:GLY:O	3:C:367:GLU:HG2	2.42	0.48
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.48
24:B:608:CLA:HBB1	24:B:608:CLA:HMB1	2.59	0.47
24:C:514:CLA:HBC1	34:Z:101:LMG:H171	1.96	0.47
26:T:102:BCR:H331	26:T:102:BCR:HC7	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:E:101:LHG:H241	37:E:101:LHG:HC61	1.70	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.14	0.47
24:C:508:CLA:C3D	24:C:509:CLA:H193	28.27	0.47
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.96	0.47
16:V:30:LYS:HD3	16:V:118:HIS:NE2	3.39	0.47
34:C:501:LMG:H211	36:C:517:DGD:HA61	1.96	0.47
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.50	0.47
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.96	0.47
28:B:635:GOL:H31	30:M:101:LMT:H6D	1.96	0.47
16:V:14:SER:HA	28:V:208:GOL:H12	1.97	0.47
9:J:2:SER:N	40:J:208:HOH:O	2.48	0.47
13:O:84:GLU:OE2	40:O:543:HOH:O	2.20	0.47
24:B:606:CLA:H91	26:H:101:BCR:H21C	22.23	0.47
2:B:248:ALA:HA	24:B:608:CLA:H42	25.01	0.46
27:A:411:SQD:H251	37:D:410:LHG:H121	3.64	0.46
34:J:101:LMG:H221	34:J:101:LMG:H192	4.75	0.46
24:B:609:CLA:H43	24:B:610:CLA:H2	8.05	0.46
16:V:24:LYS:HD3	28:V:207:GOL:H2	1.98	0.46
10:K:10:LYS:N	10:K:10:LYS:HD2	2.34	0.46
1:A:84:PRO:HA	1:A:112:TYR:CG	2.50	0.46
4:D:49:LEU:HD13	26:D:405:BCR:C15	2.45	0.46
1:A:160:ILE:HD11	36:C:517:DGD:HBT2	1.98	0.46
24:C:502:CLA:H192	24:C:507:CLA:C1B	2.45	0.46
2:B:476:ARG:NH1	40:B:951:HOH:O	2.46	0.46
24:B:612:CLA:H161	24:B:612:CLA:H192	1.81	0.46
3:C:437:PHE:CE1	24:C:512:CLA:HMB3	14.46	0.46
35:D:411:HTG:H1	7:H:25:TRP:CD1	2.53	0.46
24:C:509:CLA:H122	24:C:509:CLA:H162	1.75	0.46
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.90	0.46
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.46	0.46
36:C:518:DGD:HA81	36:C:518:DGD:HAE2	1.68	0.46
4:D:141:TYR:OH	37:D:408:LHG:O4	2.29	0.45
37:D:410:LHG:H331	37:D:410:LHG:H302	1.57	0.45
2:B:162:PHE:O	24:B:611:CLA:HHD	30.81	0.45
4:D:123:ILE:HD11	36:H:102:DGD:HAE1	1.97	0.45
3:C:38:GLY:HA3	24:C:512:CLA:HMD3	1.98	0.45
24:B:609:CLA:HMD2	24:B:617:CLA:H203	29.77	0.45
37:D:410:LHG:H141	37:D:410:LHG:H322	1.99	0.45
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.73	0.45
25:A:408:PHO:NC	25:A:408:PHO:ND	2.67	0.45
2:B:83:GLU:C	2:B:86[B]:ILE:HD11	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:ILE:HD11	36:H:102:DGD:HAH2	1.97	0.45
36:C:519:DGD:HBF1	37:D:410:LHG:H211	1.98	0.45
24:D:404:CLA:H171	18:X:15[A]:LEU:HD13	1.99	0.45
24:D:404:CLA:HBA1	24:D:404:CLA:H3A	2.00	0.45
2:B:223:GLN:NE2	40:B:937:HOH:O	2.30	0.45
4:D:141:TYR:HA	4:D:144:ILE:HD12	1.99	0.45
20:R:8:VAL:O	20:R:11:PRO:HD2	2.17	0.45
3:C:218:PHE:HE2	34:C:501:LMG:H111	1.80	0.45
34:Z:101:LMG:H142	34:Z:101:LMG:H111	2.52	0.45
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.07	0.44
2:B:256:MET:HA	2:B:263:THR:HG21	2.26	0.44
24:C:504:CLA:HAB	34:C:521:LMG:H241	1.99	0.44
3:C:288:CYS:SG	36:C:517:DGD:HB32	2.58	0.44
28:A:412:GOL:C1	12:M:1:FME:HG2	18.81	0.44
2:B:338:GLN:HA	13:O:57:LYS:HE3	40.65	0.44
4:D:16:ASP:OD2	30:D:402:LMT:O6'	2.34	0.44
1:A:200:LEU:HG	36:C:519:DGD:HAT2	1.98	0.44
26:T:102:BCR:H321	26:T:102:BCR:HC8	1.99	0.44
26:A:410:BCR:H371	26:A:410:BCR:H24C	1.76	0.44
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.71	0.44
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.53	0.44
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.76	0.44
24:C:514:CLA:HMD1	34:Z:101:LMG:HC8	1.99	0.44
36:C:519:DGD:HAE2	36:C:519:DGD:HA81	2.01	0.44
40:A:615[B]:HOH:O	16:V:30:LYS:HE2	2.17	0.44
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.44
2:B:233:ASN:O	2:B:236:THR:HG22	2.18	0.44
26:B:619:BCR:H371	26:B:619:BCR:H24C	1.81	0.44
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.64	0.44
11:L:9:PRO:HA	30:M:102:LMT:H6D	16.81	0.44
28:A:413:GOL:C1	12:M:1:FME:HG2	2.48	0.44
8:I:35:LYS:O	8:I:37:LEU:N	2.61	0.44
5:E:60:GLN:NE2	40:E:228:HOH:O	2.51	0.44
34:C:520:LMG:H182	34:C:520:LMG:H301	5.59	0.44
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.00	0.44
1:A:96:ILE:HD12	24:A:409:CLA:HMD1	2.00	0.44
16:V:55[B]:ARG:NH1	40:V:388:HOH:O	2.51	0.44
5:E:68:ASP:OD1	5:E:71:GLU:N	2.42	0.44
27:F:101:SQD:H342	27:F:101:SQD:H311	1.65	0.43
26:Y:101:BCR:H351	26:Y:101:BCR:H15C	1.89	0.43
24:C:502:CLA:HMD2	24:C:503:CLA:H101	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ALA:O	40:B:730:HOH:O	40.60	0.43
35:V:204:HTG:H4'1	35:V:204:HTG:H1'1	1.78	0.43
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.79	0.43
13:O:136:ILE:HD12	13:O:243:ILE:HD13	4.75	0.43
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.99	0.43
4:D:273:PHE:CE2	37:L:101:LHG:H112	2.52	0.43
4:D:272:LEU:C	4:D:272:LEU:HD23	2.40	0.43
24:B:607:CLA:H102	24:B:607:CLA:H61	1.72	0.43
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.57	0.43
17:Y:20:ALA:O	17:Y:24:MET:HG2	2.18	0.43
2:B:13:ILE:HG12	24:B:613:CLA:HAC2	2.01	0.43
24:B:615:CLA:H71	24:B:615:CLA:H112	1.62	0.43
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.53	0.43
24:B:614:CLA:H43	37:D:408:LHG:H372	2.01	0.43
27:A:411:SQD:H361	27:A:411:SQD:H332	4.73	0.43
3:C:279:LEU:HD22	24:C:510:CLA:HED2	2.00	0.43
5:E:8:ARG:HH21	5:E:12:ASP:HB3	2.97	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	2.01	0.43
2:B:30:VAL:HG12	24:B:610:CLA:HHD	31.15	0.43
24:B:615:CLA:H62	24:B:615:CLA:H41	1.88	0.43
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.86	0.43
27:A:411:SQD:H131	37:D:410:LHG:H142	1.99	0.43
24:A:406:CLA:HMD3	4:D:182:LEU:HD11	2.00	0.43
24:D:401:CLA:H203	24:D:401:CLA:H162	1.80	0.43
26:T:102:BCR:H371	26:T:102:BCR:H24C	1.84	0.43
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.53	0.43
24:C:511:CLA:H191	24:C:514:CLA:HAC1	20.96	0.43
24:C:505:CLA:HBB1	34:C:521:LMG:H231	17.70	0.43
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.34	0.43
12:M:34:LYS:HG2	30:M:102:LMT:O3B	2.18	0.43
3:C:406:SER:HA	3:C:420:VAL:HG23	2.16	0.43
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.48	0.43
24:C:510:CLA:H203	36:C:518:DGD:HA92	33.55	0.43
34:C:520:LMG:H242	34:C:520:LMG:H211	1.81	0.43
9:J:6:ARG:H	9:J:6:ARG:HG2	1.69	0.43
4:D:139:ARG:NH2	40:D:635:HOH:O	51.45	0.43
2:B:26:HIS:HB2	24:B:613:CLA:HMB2	2.00	0.42
15:U:76:ARG:NH2	40:U:201:HOH:O	2.51	0.42
24:C:507:CLA:HAA1	24:C:507:CLA:HBD	2.30	0.42
2:B:283:GLU:OE2	2:B:287[B]:ARG:NE	2.51	0.42
24:B:606:CLA:H143	24:B:606:CLA:C1B	16.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:514:CLA:HAB	26:C:515:BCR:H371	2.00	0.42
37:E:101:LHG:H152	6:F:22:ALA:HB1	2.71	0.42
3:C:202:PRO:HD2	35:C:523:HTG:H62	2.01	0.42
2:B:238:LEU:N	24:B:617:CLA:HMD3	22.30	0.42
24:B:611:CLA:H111	24:B:611:CLA:H152	4.37	0.42
26:B:618:BCR:H371	26:B:618:BCR:H24C	1.77	0.42
34:C:520:LMG:H192	10:K:27:VAL:HG11	2.02	0.42
5:E:84:LYS:HA	5:E:84:LYS:HD3	1.91	0.42
2:B:492:GLU:HG3	40:B:915:HOH:O	2.19	0.42
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.85	0.42
36:C:518:DGD:HB61	36:C:518:DGD:HB32	3.36	0.42
24:B:607:CLA:H142	24:B:607:CLA:H111	1.83	0.42
3:C:127:PHE:CE1	34:Z:101:LMG:H152	5.34	0.42
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.01	0.42
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.92	0.42
26:C:516:BCR:H371	26:C:516:BCR:H24C	1.73	0.42
24:B:615:CLA:HBD	24:B:615:CLA:HAA1	2.00	0.42
25:A:408:PHO:H161	24:D:401:CLA:HMB3	32.73	0.42
1:A:259:ILE:HA	37:E:101:LHG:H202	5.02	0.42
13:O:179:GLU:HG2	40:O:499:HOH:O	2.19	0.42
3:C:218:PHE:CE2	34:C:501:LMG:H111	2.54	0.42
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.02	0.42
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.86	0.42
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.20	0.42
19:Z:37:LYS:HZ3	34:Z:101:LMG:HC5	4.07	0.41
24:A:405:CLA:HBD	24:D:401:CLA:HAC2	2.00	0.41
24:A:409:CLA:H102	24:A:409:CLA:H61	1.76	0.41
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.08	0.41
24:B:617:CLA:H62	24:B:617:CLA:H41	1.52	0.41
24:C:512:CLA:HMB2	26:K:101:BCR:H382	2.02	0.41
16:V:68:ASN:OD1	28:V:205:GOL:H2	2.19	0.41
15:U:8:GLU:HG2	15:U:9:LEU:H	1.84	0.41
1:A:253:GLY:HA3	2:B:491:VAL:HB	2.02	0.41
13:O:58:ASN:C	13:O:60:ARG:H	2.49	0.41
35:B:623:HTG:H1	35:B:623:HTG:H2'2	1.86	0.41
2:B:491:VAL:HG13	4:D:136:VAL:HG13	3.29	0.41
5:E:36:LEU:HA	5:E:39:SER:OG	2.20	0.41
24:C:503:CLA:C3D	24:C:505:CLA:H2	18.64	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.84	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.41
26:B:620:BCR:H24C	26:B:620:BCR:H371	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:102:BCR:H11C	26:T:102:BCR:H341	1.97	0.41
20:R:24:LEU:N	20:R:25:PRO:HD2	2.36	0.41
27:F:101:SQD:H45	27:F:101:SQD:H81	4.74	0.41
24:C:502:CLA:H42	24:C:503:CLA:HMD1	2.02	0.41
24:C:507:CLA:H52	30:I:102:LMT:H71	2.02	0.41
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.90	0.41
28:C:524:GOL:O1	16:V:49:ASN:ND2	2.48	0.41
24:B:617:CLA:H93	24:B:617:CLA:H61	1.95	0.41
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	2.03	0.41
3:C:42:LEU:HD21	24:C:513:CLA:H2A	18.64	0.41
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.03	0.41
26:D:405:BCR:HC22	36:D:407:DGD:HA72	2.89	0.41
2:B:216:HIS:CE1	24:B:614:CLA:NA	25.95	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.41
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.66	0.41
24:B:606:CLA:H72	24:B:606:CLA:H2	4.80	0.41
2:B:237:VAL:HG12	24:B:617:CLA:HMD1	21.39	0.41
24:C:514:CLA:O1A	40:C:782:HOH:O	49.22	0.41
24:D:401:CLA:H43	24:D:401:CLA:O1A	2.20	0.41
24:B:605:CLA:HMB1	24:B:605:CLA:HBB1	2.03	0.41
10:K:25:LEU:HB2	40:K:201:HOH:O	2.21	0.41
20:R:27:ALA:O	20:R:31:VAL:HG23	2.21	0.41
27:A:416:SQD:H301	27:A:416:SQD:H272	1.85	0.40
26:D:405:BCR:H351	26:D:405:BCR:H15C	1.97	0.40
2:B:237:VAL:HG12	24:B:613:CLA:HMD1	2.03	0.40
2:B:238:LEU:N	24:B:613:CLA:HMD3	2.36	0.40
24:C:508:CLA:H92	24:C:508:CLA:H61	1.75	0.40
3:C:56:HIS:HB2	24:C:511:CLA:HMB2	8.48	0.40
26:A:410:BCR:H11C	26:A:410:BCR:H341	1.95	0.40
3:C:53:HIS:CB	24:C:513:CLA:HMD1	2.52	0.40
8:I:33:LYS:HA	8:I:33:LYS:HD3	1.89	0.40
37:D:410:LHG:H242	37:D:410:LHG:H272	1.95	0.40
24:B:604:CLA:HAB	24:B:606:CLA:H171	2.03	0.40
24:B:610:CLA:H62	24:B:610:CLA:H41	4.32	0.40
24:B:613:CLA:HAB	4:D:123:ILE:HG12	28.02	0.40
24:B:617:CLA:H152	24:B:617:CLA:H111	1.93	0.40
26:H:101:BCR:HC32	26:H:101:BCR:H312	2.05	0.40
1:A:153:SER:CB	24:A:406:CLA:H43	18.49	0.40
4:D:27:PHE:CD1	37:E:101:LHG:HC12	2.57	0.40
37:E:101:LHG:H282	37:E:101:LHG:H251	3.79	0.40
26:A:410:BCR:H15C	26:A:410:BCR:H351	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:506:CLA:HMD2	34:C:520:LMG:H291	39.46	0.40
3:C:238:ILE:HD13	35:C:523:HTG:H2'1	2.03	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%)	330 (98%)	4 (1%)	1 (0%)	46 35
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	46 35
2	B	512/505 (101%)	507 (99%)	5 (1%)	0	100 100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100 100
3	C	454/455 (100%)	445 (98%)	7 (2%)	2 (0%)	39 27
3	c	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	39 27
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100 100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100 100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100 100
5	e	79/84 (94%)	77 (98%)	2 (2%)	0	100 100
6	F	32/44 (73%)	32 (100%)	0	0	100 100
6	f	30/44 (68%)	30 (100%)	0	0	100 100
7	H	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%)	35 (97%)	1 (3%)	0	100 100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	245/244 (100%)	242 (99%)	3 (1%)	0	100	100
13	o	244/244 (100%)	238 (98%)	6 (2%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	29/31 (94%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	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%)	27 (100%)	0	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5279/5382 (98%)	5168 (98%)	104 (2%)	7 (0%)	56	48

All (7) 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
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	273/279 (98%)	272 (100%)	1 (0%)	93 93
2	B	412/403 (102%)	407 (99%)	5 (1%)	78 75
2	b	413/403 (102%)	408 (99%)	5 (1%)	78 75
3	C	357/356 (100%)	352 (99%)	5 (1%)	74 70
3	c	362/356 (102%)	358 (99%)	4 (1%)	80 77
4	D	277/277 (100%)	276 (100%)	1 (0%)	93 93
4	d	277/277 (100%)	276 (100%)	1 (0%)	93 93
5	E	74/73 (101%)	74 (100%)	0	100 100
5	e	72/73 (99%)	71 (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	26/26 (100%)	26 (100%)	0	100 100
9	j	26/26 (100%)	26 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20 7
10	k	30/30 (100%)	28 (93%)	2 (7%)	20 7
11	L	36/35 (103%)	35 (97%)	1 (3%)	51 39
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%)	29 (97%)	1 (3%)	45 32
13	O	210/207 (101%)	208 (99%)	2 (1%)	82 80
13	o	209/207 (101%)	207 (99%)	2 (1%)	82 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	T	27/27 (100%)	25 (93%)	2 (7%)	17 5
14	t	27/27 (100%)	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%)	116 (99%)	1 (1%)	84 83
17	Y	22/23 (96%)	22 (100%)	0	100 100
17	y	22/23 (96%)	21 (96%)	1 (4%)	34 18
18	X	33/33 (100%)	33 (100%)	0	100 100
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65 58
19	z	52/52 (100%)	51 (98%)	1 (2%)	65 58
20	R	29/29 (100%)	28 (97%)	1 (3%)	44 30
All	All	4383/4399 (100%)	4331 (99%)	52 (1%)	80 75

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	84	THR
2	B	362	PHE
2	B	472	ARG
2	B	479	PHE
2	B	492	GLU
3	C	289	PHE
3	C	315	MET
3	C	416[A]	SER
3	C	416[B]	SER
3	C	418	ASN
4	D	180	ARG
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	10	LYS
10	K	17	ILE
11	L	1	MET
13	O	118	LEU

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Mol	Chain	Res	Type
13	O	194	LYS
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	70	ARG
16	V	86	GLN
19	Z	3	ILE
20	R	4	ARG
1	a	12	ASN
2	b	84	THR
2	b	121	GLU
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	418	ASN
4	d	180	ARG
5	e	59	GLU
6	f	44	GLN
7	h	49	TYR
8	i	34	ARG
10	k	10	LYS
10	k	17	ILE
11	l	1	MET
12	m	33	GLN
13	o	118	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
16	v	86	GLN
17	y	42	ARG
19	z	3	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
4	D	142	ASN
19	Z	31	GLN
2	b	497	GLN
13	o	109	GLN

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Mol	Chain	Res	Type
15	u	81	HIS
19	z	6	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 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	0.56	0	6,9,11	1.64	3 (50%)
12	FME	M	1	12	8,9,10	0.56	0	6,9,11	1.67	2 (33%)
14	FME	T	1	14	8,9,10	0.61	0	6,9,11	1.84	3 (50%)
8	FME	i	1	8	8,9,10	0.56	0	6,9,11	1.43	1 (16%)
9	FME	j	1	9	8,9,10	0.57	0	6,9,11	1.54	2 (33%)
12	FME	m	1	12	8,9,10	0.62	0	6,9,11	1.29	1 (16%)
14	FME	t	1	14	8,9,10	0.79	0	6,9,11	2.35	3 (50%)

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
9	FME	j	1	9	-	0/6/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-3.56	119.63	124.76
14	t	1	FME	O-C-CA	-3.22	116.92	125.44
14	T	1	FME	O-C-CA	-3.01	117.48	125.44
9	j	1	FME	O1-CN-N	-2.84	120.67	124.76
12	M	1	FME	O1-CN-N	-2.64	120.95	124.76
8	I	1	FME	O1-CN-N	-2.38	121.33	124.76
8	I	1	FME	O-C-CA	-2.35	119.23	125.44
14	T	1	FME	O1-CN-N	-2.33	121.40	124.76
8	i	1	FME	O-C-CA	-2.30	119.36	125.44
14	T	1	FME	CA-N-CN	-2.29	119.31	122.82
12	m	1	FME	O-C-CA	-2.28	119.43	125.44
14	t	1	FME	CE-SD-CG	-2.21	92.84	100.37
9	j	1	FME	O-C-CA	-2.17	119.71	125.44
12	M	1	FME	O-C-CA	-2.14	119.80	125.44
8	I	1	FME	CA-N-CN	-2.11	119.58	122.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 252 ligands modelled in this entry, 19 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	1.98	12 (21%)	61,113,113	2.16	20 (32%)
24	CLA	A	406	40	55,73,73	1.95	11 (20%)	61,113,113	2.12	22 (36%)
25	PHO	A	407	-	67,69,69	2.12	16 (23%)	84,99,99	1.88	20 (23%)
25	PHO	A	408	-	67,69,69	2.04	14 (20%)	84,99,99	1.97	23 (27%)
24	CLA	A	409	-	55,73,73	1.96	12 (21%)	61,113,113	2.06	20 (32%)
26	BCR	A	410	-	41,41,41	0.98	1 (2%)	56,56,56	1.33	5 (8%)
27	SQD	A	411	-	53,54,54	1.35	3 (5%)	61,65,65	1.66	10 (16%)
28	GOL	A	412	-	5,5,5	0.21	0	5,5,5	0.62	0
28	GOL	A	413	-	5,5,5	0.42	0	5,5,5	0.58	0
28	GOL	A	414	-	5,5,5	0.38	0	5,5,5	0.19	0
27	SQD	A	416	-	53,54,54	1.41	3 (5%)	61,65,65	1.20	7 (11%)
30	LMT	A	417	-	34,34,36	0.38	0	45,45,47	1.05	3 (6%)
31	OEX	A	418	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
32	PL9	A	419	-	55,55,55	0.63	1 (1%)	68,69,69	2.01	26 (38%)
24	CLA	B	602	40	55,73,73	1.95	12 (21%)	61,113,113	2.10	18 (29%)
24	CLA	B	603	-	55,73,73	1.94	12 (21%)	61,113,113	2.20	22 (36%)
24	CLA	B	604	-	55,73,73	1.98	12 (21%)	61,113,113	2.25	23 (37%)
24	CLA	B	605	-	55,73,73	1.80	12 (21%)	61,113,113	2.24	19 (31%)
24	CLA	B	606	-	55,73,73	1.87	12 (21%)	61,113,113	2.25	19 (31%)
24	CLA	B	607	-	55,73,73	1.90	12 (21%)	61,113,113	2.27	21 (34%)
24	CLA	B	608	40	55,73,73	1.94	12 (21%)	61,113,113	2.14	22 (36%)
24	CLA	B	609	-	55,73,73	1.98	12 (21%)	61,113,113	2.09	17 (27%)
24	CLA	B	610	-	55,73,73	1.88	11 (20%)	61,113,113	2.09	19 (31%)
24	CLA	B	611	40	55,73,73	1.92	12 (21%)	61,113,113	2.15	21 (34%)
24	CLA	B	612	-	55,73,73	1.94	12 (21%)	61,113,113	2.11	19 (31%)
24	CLA	B	613	-	55,73,73	1.93	12 (21%)	61,113,113	2.09	16 (26%)
24	CLA	B	614	-	55,73,73	1.94	12 (21%)	61,113,113	2.05	18 (29%)
24	CLA	B	615	-	55,73,73	1.86	11 (20%)	61,113,113	2.26	21 (34%)
24	CLA	B	616	-	55,73,73	1.87	12 (21%)	61,113,113	2.05	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	617	-	55,73,73	1.96	12 (21%)	61,113,113	2.24	19 (31%)
26	BCR	B	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.26	5 (8%)
26	BCR	B	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.01	3 (5%)
26	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.48	11 (19%)
34	LMG	B	621	-	51,51,55	0.88	2 (3%)	59,59,63	1.03	4 (6%)
35	HTG	B	622	-	19,19,19	1.12	1 (5%)	22,24,24	1.63	3 (13%)
35	HTG	B	623	-	19,19,19	0.82	1 (5%)	22,24,24	1.43	1 (4%)
35	HTG	B	624	-	19,19,19	0.99	1 (5%)	22,24,24	2.17	3 (13%)
28	GOL	B	625	-	5,5,5	0.29	0	5,5,5	0.59	0
28	GOL	B	626	-	5,5,5	0.28	0	5,5,5	0.47	0
28	GOL	B	627	-	5,5,5	0.30	0	5,5,5	0.65	0
28	GOL	B	628	-	5,5,5	0.39	0	5,5,5	0.23	0
28	GOL	B	629	-	5,5,5	0.29	0	5,5,5	0.36	0
35	HTG	B	630	-	19,19,19	0.91	1 (5%)	22,24,24	1.61	1 (4%)
35	HTG	B	631	-	19,19,19	0.96	2 (10%)	22,24,24	1.75	2 (9%)
28	GOL	B	633	-	5,5,5	0.26	0	5,5,5	0.63	0
30	LMT	B	634	-	25,25,36	0.47	0	30,30,47	0.74	0
28	GOL	B	635	-	5,5,5	0.36	0	5,5,5	0.29	0
34	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.12	3 (5%)
24	CLA	C	502	-	55,73,73	1.91	12 (21%)	61,113,113	2.13	18 (29%)
24	CLA	C	503	-	55,73,73	1.94	12 (21%)	61,113,113	2.15	20 (32%)
24	CLA	C	504	-	55,73,73	1.96	12 (21%)	61,113,113	2.02	19 (31%)
24	CLA	C	505	40	55,73,73	1.93	12 (21%)	61,113,113	2.18	16 (26%)
24	CLA	C	506	-	55,73,73	1.95	12 (21%)	61,113,113	2.14	17 (27%)
24	CLA	C	507	-	55,73,73	1.91	12 (21%)	61,113,113	2.18	17 (27%)
24	CLA	C	508	40	55,73,73	1.93	12 (21%)	61,113,113	2.12	19 (31%)
24	CLA	C	509	-	55,73,73	1.97	12 (21%)	61,113,113	2.20	19 (31%)
24	CLA	C	510	-	55,73,73	1.98	12 (21%)	61,113,113	2.22	19 (31%)
24	CLA	C	511	-	55,73,73	1.97	12 (21%)	61,113,113	2.12	16 (26%)
24	CLA	C	512	3	55,73,73	1.89	12 (21%)	61,113,113	1.98	13 (21%)
24	CLA	C	513	-	55,73,73	1.92	12 (21%)	61,113,113	2.19	21 (34%)
24	CLA	C	514	-	55,73,73	1.92	12 (21%)	61,113,113	2.10	19 (31%)
26	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.40	5 (8%)
26	BCR	C	516	-	41,41,41	0.98	1 (2%)	56,56,56	1.41	9 (16%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.06	5 (6%)
36	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DGD	C	519	-	63,63,67	0.79	2 (3%)	77,77,81	0.91	4 (5%)
34	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.10	4 (6%)
34	LMG	C	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.15	4 (6%)
35	HTG	C	522	-	19,19,19	0.94	2 (10%)	22,24,24	1.57	2 (9%)
35	HTG	C	523	-	19,19,19	0.95	1 (5%)	22,24,24	1.96	4 (18%)
28	GOL	C	524	-	5,5,5	0.30	0	5,5,5	0.89	0
28	GOL	C	525	-	5,5,5	0.27	0	5,5,5	0.68	0
24	CLA	D	401	40	55,73,73	1.97	12 (21%)	61,113,113	2.21	22 (36%)
30	LMT	D	402	-	36,36,36	0.46	0	47,47,47	1.03	3 (6%)
24	CLA	D	403	-	55,73,73	1.93	12 (21%)	61,113,113	2.15	20 (32%)
24	CLA	D	404	-	55,73,73	1.92	12 (21%)	61,113,113	2.12	18 (29%)
26	BCR	D	405	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	12 (21%)
32	PL9	D	406	-	55,55,55	0.79	2 (3%)	68,69,69	1.64	19 (27%)
36	DGD	D	407	-	63,63,67	0.93	3 (4%)	77,77,81	1.31	9 (11%)
37	LHG	D	408	-	48,48,48	0.83	2 (4%)	49,54,54	1.11	5 (10%)
37	LHG	D	409	-	48,48,48	0.83	2 (4%)	49,54,54	1.08	5 (10%)
37	LHG	D	410	-	48,48,48	0.90	2 (4%)	49,54,54	0.97	3 (6%)
35	HTG	D	411	-	16,16,19	1.08	2 (12%)	19,21,24	1.14	2 (10%)
37	LHG	E	101	-	41,41,48	0.98	2 (4%)	42,47,54	1.10	3 (7%)
30	LMT	E	102	-	36,36,36	0.45	0	47,47,47	0.78	0
38	HEM	E	103	5,6	30,50,50	2.27	7 (23%)	24,82,82	2.49	12 (50%)
27	SQD	F	101	-	42,43,54	1.41	3 (7%)	50,54,65	1.75	9 (18%)
28	GOL	F	103	33	5,5,5	0.35	0	5,5,5	0.32	0
26	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.28	5 (8%)
36	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.91	4 (5%)
30	LMT	I	102	-	36,36,36	0.44	0	47,47,47	1.21	5 (10%)
34	LMG	J	101	39	51,51,55	0.81	2 (3%)	59,59,63	1.01	4 (6%)
26	BCR	K	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.47	12 (21%)
37	LHG	L	101	-	48,48,48	0.86	2 (4%)	49,54,54	1.17	4 (8%)
30	LMT	M	101	-	36,36,36	0.56	1 (2%)	47,47,47	0.87	0
30	LMT	M	102	-	36,36,36	0.39	0	47,47,47	0.89	0
28	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.33	0
35	HTG	O	303	-	19,19,19	1.00	1 (5%)	22,24,24	1.09	1 (4%)
28	GOL	T	101	-	5,5,5	0.44	0	5,5,5	0.29	0
26	BCR	T	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.41	10 (17%)
28	GOL	T	103	-	5,5,5	0.38	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	V	201	-	5,5,5	0.33	0	5,5,5	0.45	0
38	HEM	V	203	16	30,50,50	2.20	7 (23%)	24,82,82	2.46	10 (41%)
35	HTG	V	204	-	19,19,19	0.93	2 (10%)	22,24,24	1.47	3 (13%)
28	GOL	V	205	-	5,5,5	0.33	0	5,5,5	0.30	0
28	GOL	V	206	-	5,5,5	0.33	0	5,5,5	0.43	0
28	GOL	V	207	-	5,5,5	0.34	0	5,5,5	0.48	0
28	GOL	V	208	-	5,5,5	0.34	0	5,5,5	0.24	0
26	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.52	8 (14%)
34	LMG	Z	101	-	37,37,55	0.93	2 (5%)	45,45,63	1.44	6 (13%)
30	LMT	a	401	-	36,36,36	0.44	0	47,47,47	0.99	2 (4%)
27	SQD	a	402	-	53,54,54	1.39	3 (5%)	61,65,65	1.22	6 (9%)
24	CLA	a	406	-	55,73,73	1.92	12 (21%)	61,113,113	2.14	19 (31%)
24	CLA	a	407	40	55,73,73	1.91	12 (21%)	61,113,113	2.10	20 (32%)
25	PHO	a	408	-	67,69,69	2.11	15 (22%)	84,99,99	1.93	18 (21%)
24	CLA	a	409	-	55,73,73	1.90	13 (23%)	61,113,113	2.20	19 (31%)
26	BCR	a	410	-	41,41,41	1.11	1 (2%)	56,56,56	1.35	9 (16%)
27	SQD	a	411	-	53,54,54	1.30	3 (5%)	61,65,65	1.68	11 (18%)
28	GOL	a	412	-	5,5,5	0.32	0	5,5,5	0.50	0
28	GOL	a	413	-	5,5,5	0.40	0	5,5,5	0.30	0
31	OEX	a	415	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
32	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.97	20 (29%)
30	LMT	a	417	-	36,36,36	0.43	0	47,47,47	0.86	1 (2%)
23	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
27	SQD	b	601	-	53,54,54	1.32	3 (5%)	61,65,65	1.81	10 (16%)
30	LMT	b	602	-	25,25,36	0.45	0	30,30,47	1.27	3 (10%)
35	HTG	b	603	-	19,19,19	1.00	1 (5%)	22,24,24	1.58	1 (4%)
35	HTG	b	604	-	19,19,19	0.95	2 (10%)	22,24,24	1.31	2 (9%)
24	CLA	b	606	40	55,73,73	1.96	11 (20%)	61,113,113	2.10	17 (27%)
24	CLA	b	607	-	55,73,73	1.98	12 (21%)	61,113,113	2.22	20 (32%)
24	CLA	b	608	-	55,73,73	1.95	12 (21%)	61,113,113	2.35	21 (34%)
24	CLA	b	609	-	55,73,73	1.94	12 (21%)	61,113,113	2.23	17 (27%)
24	CLA	b	610	-	55,73,73	1.85	12 (21%)	61,113,113	2.20	20 (32%)
24	CLA	b	611	-	55,73,73	1.91	12 (21%)	61,113,113	2.15	21 (34%)
24	CLA	b	612	40	55,73,73	1.87	11 (20%)	61,113,113	2.25	22 (36%)
24	CLA	b	613	-	55,73,73	1.94	12 (21%)	61,113,113	2.14	24 (39%)
24	CLA	b	614	-	55,73,73	1.94	12 (21%)	61,113,113	2.15	21 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	615	40	55,73,73	1.98	12 (21%)	61,113,113	2.06	18 (29%)
24	CLA	b	616	-	55,73,73	1.91	12 (21%)	61,113,113	2.22	20 (32%)
24	CLA	b	617	-	55,73,73	1.93	12 (21%)	61,113,113	2.06	17 (27%)
24	CLA	b	618	-	55,73,73	1.96	12 (21%)	61,113,113	2.10	17 (27%)
24	CLA	b	619	-	55,73,73	1.92	12 (21%)	61,113,113	2.28	23 (37%)
24	CLA	b	620	-	55,73,73	1.94	12 (21%)	61,113,113	2.11	17 (27%)
24	CLA	b	621	-	55,73,73	1.95	12 (21%)	61,113,113	2.20	17 (27%)
26	BCR	b	622	-	41,41,41	1.10	1 (2%)	56,56,56	1.40	7 (12%)
26	BCR	b	623	-	41,41,41	1.04	1 (2%)	56,56,56	1.14	4 (7%)
26	BCR	b	624	-	41,41,41	0.95	1 (2%)	56,56,56	1.26	7 (12%)
34	LMG	b	625	-	51,51,55	0.87	2 (3%)	59,59,63	1.03	2 (3%)
30	LMT	b	626	-	25,25,36	0.48	0	30,30,47	0.66	0
35	HTG	b	627	-	19,19,19	0.80	1 (5%)	22,24,24	1.50	3 (13%)
35	HTG	b	628	-	19,19,19	1.03	2 (10%)	22,24,24	2.18	3 (13%)
28	GOL	b	629	-	5,5,5	0.36	0	5,5,5	0.27	0
28	GOL	b	630	-	5,5,5	0.30	0	5,5,5	0.17	0
28	GOL	b	631	-	5,5,5	0.31	0	5,5,5	0.48	0
28	GOL	b	632	-	5,5,5	0.41	0	5,5,5	0.57	0
28	GOL	b	633	-	5,5,5	0.35	0	5,5,5	0.36	0
34	LMG	c	501	-	51,51,55	0.85	2 (3%)	59,59,63	1.27	6 (10%)
24	CLA	c	503	-	55,73,73	1.94	12 (21%)	61,113,113	2.21	19 (31%)
24	CLA	c	504	-	55,73,73	1.87	12 (21%)	61,113,113	2.12	16 (26%)
24	CLA	c	505	-	55,73,73	1.87	12 (21%)	61,113,113	2.10	19 (31%)
24	CLA	c	506	40	55,73,73	1.94	12 (21%)	61,113,113	2.16	21 (34%)
24	CLA	c	507	-	55,73,73	1.85	12 (21%)	61,113,113	2.13	15 (24%)
24	CLA	c	508	-	55,73,73	1.88	12 (21%)	61,113,113	2.10	21 (34%)
24	CLA	c	509	40	55,73,73	1.91	12 (21%)	61,113,113	2.25	18 (29%)
24	CLA	c	510	-	55,73,73	2.01	12 (21%)	61,113,113	2.16	20 (32%)
24	CLA	c	511	-	55,73,73	2.01	12 (21%)	61,113,113	2.20	18 (29%)
24	CLA	c	512	-	55,73,73	1.94	12 (21%)	61,113,113	2.09	18 (29%)
24	CLA	c	513	3	55,73,73	1.90	11 (20%)	61,113,113	2.08	19 (31%)
24	CLA	c	514	-	55,73,73	1.93	12 (21%)	61,113,113	2.18	21 (34%)
24	CLA	c	515	-	55,73,73	1.94	12 (21%)	61,113,113	2.06	19 (31%)
26	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	9 (16%)
36	DGD	c	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.10	5 (6%)
36	DGD	c	518	-	63,63,67	0.87	2 (3%)	77,77,81	0.99	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	3 (3%)
34	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	0.93	2 (3%)
34	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	4 (6%)
35	HTG	c	522	-	19,19,19	0.93	2 (10%)	22,24,24	1.85	2 (9%)
35	HTG	c	523	-	19,19,19	0.97	2 (10%)	22,24,24	1.69	2 (9%)
28	GOL	c	524	-	5,5,5	0.28	0	5,5,5	0.33	0
28	GOL	c	525	-	5,5,5	0.34	0	5,5,5	0.60	0
26	BCR	c	526	-	41,41,41	1.02	1 (2%)	56,56,56	1.52	11 (19%)
28	GOL	c	527	-	5,5,5	0.39	0	5,5,5	0.29	0
24	CLA	d	401	40	55,73,73	1.95	11 (20%)	61,113,113	2.18	20 (32%)
24	CLA	d	402	-	55,73,73	1.92	12 (21%)	61,113,113	2.26	22 (36%)
25	PHO	d	403	-	67,69,69	2.12	15 (22%)	84,99,99	1.96	20 (23%)
24	CLA	d	404	-	55,73,73	1.88	12 (21%)	61,113,113	2.04	20 (32%)
26	BCR	d	405	-	41,41,41	1.01	1 (2%)	56,56,56	1.82	13 (23%)
32	PL9	d	406	-	55,55,55	0.74	1 (1%)	68,69,69	1.63	19 (27%)
36	DGD	d	407	-	63,63,67	0.90	2 (3%)	77,77,81	1.07	6 (7%)
37	LHG	d	408	-	48,48,48	0.85	2 (4%)	49,54,54	1.02	5 (10%)
37	LHG	d	409	-	48,48,48	0.87	2 (4%)	49,54,54	1.11	4 (8%)
37	LHG	d	410	-	48,48,48	0.91	2 (4%)	49,54,54	0.99	3 (6%)
35	HTG	d	411	-	16,16,19	1.13	2 (12%)	19,21,24	1.97	1 (5%)
37	LHG	e	101	-	41,41,48	1.00	2 (4%)	42,47,54	1.07	2 (4%)
38	HEM	e	102	5,6	30,50,50	2.24	7 (23%)	24,82,82	2.59	10 (41%)
27	SQD	f	101	-	42,43,54	1.57	3 (7%)	50,54,65	1.56	7 (14%)
30	LMT	f	102	-	36,36,36	0.46	0	47,47,47	0.78	0
28	GOL	f	104	33	5,5,5	0.31	0	5,5,5	0.22	0
26	BCR	h	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.34	8 (14%)
36	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.01	7 (9%)
34	LMG	j	101	39	51,51,55	0.90	2 (3%)	59,59,63	0.99	3 (5%)
26	BCR	k	103	-	41,41,41	1.01	1 (2%)	56,56,56	1.36	4 (7%)
27	SQD	l	101	-	53,54,54	1.27	3 (5%)	61,65,65	1.52	8 (13%)
37	LHG	l	102	-	48,48,48	0.92	2 (4%)	49,54,54	1.03	3 (6%)
30	LMT	m	102	-	36,36,36	0.48	0	47,47,47	1.04	3 (6%)
30	LMT	m	103	-	36,36,36	0.54	1 (2%)	47,47,47	1.08	4 (8%)
26	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	8 (14%)
28	GOL	t	102	-	5,5,5	0.31	0	5,5,5	0.34	0
28	GOL	v	201	-	5,5,5	0.32	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	HEM	v	202	16	30,50,50	2.16	7 (23%)	24,82,82	2.27	10 (41%)
28	GOL	v	203	-	5,5,5	0.22	0	5,5,5	0.47	0
28	GOL	v	204	-	5,5,5	0.30	0	5,5,5	0.35	0
28	GOL	v	205	-	5,5,5	0.32	0	5,5,5	0.39	0
26	BCR	y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.57	11 (19%)
34	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.20	5 (10%)

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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	406	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	A	407	-	-	0/53/103/103	0/1/6/6
25	PHO	A	408	-	-	0/53/103/103	0/1/6/6
24	CLA	A	409	-	2/2/20/25	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
28	GOL	A	412	-	-	0/4/4/4	0/0/0/0
28	GOL	A	413	-	-	0/4/4/4	0/0/0/0
28	GOL	A	414	-	-	0/4/4/4	0/0/0/0
27	SQD	A	416	-	-	0/49/69/69	0/1/1/1
30	LMT	A	417	-	-	0/19/59/61	0/2/2/2
31	OEX	A	418	1,3,40	-	0/0/68/68	0/0/6/6
32	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	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	-	3/3/20/25	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	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	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
34	LMG	B	621	-	-	0/46/66/70	0/1/1/1
35	HTG	B	622	-	-	0/10/30/30	0/1/1/1
35	HTG	B	623	-	-	0/10/30/30	0/1/1/1
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
28	GOL	B	625	-	-	0/4/4/4	0/0/0/0
28	GOL	B	626	-	-	0/4/4/4	0/0/0/0
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
35	HTG	B	630	-	-	0/10/30/30	0/1/1/1
35	HTG	B	631	-	-	0/10/30/30	0/1/1/1
28	GOL	B	633	-	-	0/4/4/4	0/0/0/0
30	LMT	B	634	-	-	0/17/37/61	0/1/1/2
28	GOL	B	635	-	-	0/4/4/4	0/0/0/0
34	LMG	C	501	-	-	0/46/66/70	0/1/1/1
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	-	2/2/20/25	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
35	HTG	C	523	-	-	0/10/30/30	0/1/1/1
28	GOL	C	524	-	-	0/4/4/4	0/0/0/0
28	GOL	C	525	-	-	0/4/4/4	0/0/0/0
24	CLA	D	401	40	3/3/20/25	0/37/135/135	0/0/9/9
30	LMT	D	402	-	-	0/21/61/61	0/2/2/2
24	CLA	D	403	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	405	-	-	0/29/63/63	0/2/2/2
32	PL9	D	406	-	-	0/53/73/73	0/1/1/1
36	DGD	D	407	-	-	1/51/91/95	0/2/2/2
37	LHG	D	408	-	-	0/53/53/53	0/0/0/0
37	LHG	D	409	-	-	0/53/53/53	0/0/0/0
37	LHG	D	410	-	-	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
30	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	-	-	0/38/58/69	0/1/1/1
28	GOL	F	103	33	-	0/4/4/4	0/0/0/0
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
30	LMT	I	102	-	-	0/21/61/61	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
37	LHG	L	101	-	-	0/53/53/53	0/0/0/0
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
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
28	GOL	V	201	-	-	0/4/4/4	0/0/0/0
38	HEM	V	203	16	-	0/10/54/54	0/0/8/8
35	HTG	V	204	-	-	0/10/30/30	0/1/1/1
28	GOL	V	205	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	V	206	-	-	0/4/4/4	0/0/0/0
28	GOL	V	207	-	-	0/4/4/4	0/0/0/0
28	GOL	V	208	-	-	0/4/4/4	0/0/0/0
26	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
34	LMG	Z	101	-	-	1/31/51/70	0/1/1/1
30	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
28	GOL	a	412	-	-	0/4/4/4	0/0/0/0
28	GOL	a	413	-	-	0/4/4/4	0/0/0/0
31	OEX	a	415	1,3,40	-	0/0/68/68	0/0/6/6
32	PL9	a	416	-	-	0/53/73/73	0/1/1/1
30	LMT	a	417	-	-	0/21/61/61	0/2/2/2
23	BCT	a	418	21	-	0/0/0/0	0/0/0/0
27	SQD	b	601	-	-	1/49/69/69	0/1/1/1
30	LMT	b	602	-	-	0/17/37/61	0/1/1/2
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
35	HTG	b	604	-	-	0/10/30/30	0/1/1/1
24	CLA	b	606	40	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	-	2/2/20/25	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	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	40	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	40	3/3/20/25	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	-	3/3/20/25	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	621	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
34	LMG	b	625	-	-	0/46/66/70	0/1/1/1
30	LMT	b	626	-	-	0/17/37/61	0/1/1/2
35	HTG	b	627	-	-	0/10/30/30	0/1/1/1
35	HTG	b	628	-	-	0/10/30/30	0/1/1/1
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
34	LMG	c	501	-	-	0/46/66/70	0/1/1/1
24	CLA	c	503	-	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	509	40	3/3/20/25	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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	514	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	515	-	2/2/20/25	0/37/135/135	0/0/9/9
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
35	HTG	c	522	-	-	0/10/30/30	0/1/1/1
35	HTG	c	523	-	-	0/10/30/30	0/1/1/1
28	GOL	c	524	-	-	0/4/4/4	0/0/0/0
28	GOL	c	525	-	-	0/4/4/4	0/0/0/0
26	BCR	c	526	-	-	0/29/63/63	0/2/2/2
28	GOL	c	527	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	401	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	d	402	-	1/1/20/25	0/37/135/135	0/0/9/9
25	PHO	d	403	-	-	0/53/103/103	0/1/6/6
24	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	d	405	-	-	0/29/63/63	0/2/2/2
32	PL9	d	406	-	-	0/53/73/73	0/1/1/1
36	DGD	d	407	-	-	0/51/91/95	0/2/2/2
37	LHG	d	408	-	-	0/53/53/53	0/0/0/0
37	LHG	d	409	-	-	0/53/53/53	0/0/0/0
37	LHG	d	410	-	-	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
38	HEM	e	102	5,6	-	0/10/54/54	0/0/8/8
27	SQD	f	101	-	-	2/38/58/69	0/1/1/1
30	LMT	f	102	-	-	0/21/61/61	0/2/2/2
28	GOL	f	104	33	-	0/4/4/4	0/0/0/0
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	103	-	-	0/29/63/63	0/2/2/2
27	SQD	l	101	-	-	0/49/69/69	0/1/1/1
37	LHG	l	102	-	-	0/53/53/53	0/0/0/0
30	LMT	m	102	-	-	0/21/61/61	0/2/2/2
30	LMT	m	103	-	-	0/21/61/61	0/2/2/2
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
28	GOL	t	102	-	-	0/4/4/4	0/0/0/0
28	GOL	v	201	-	-	0/4/4/4	0/0/0/0
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 (1069) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	416	SQD	C6-S	-7.63	1.66	1.77
27	a	402	SQD	C6-S	-7.59	1.66	1.77
27	A	411	SQD	C6-S	-7.59	1.66	1.77
27	f	101	SQD	C6-S	-7.57	1.66	1.77
27	a	411	SQD	C6-S	-7.13	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	601	SQD	C6-S	-6.83	1.67	1.77
38	E	103	HEM	C2D-C3D	-6.68	1.34	1.54
38	V	203	HEM	C2D-C3D	-6.66	1.34	1.54
38	e	102	HEM	C2D-C3D	-6.66	1.34	1.54
38	v	202	HEM	C2D-C3D	-6.56	1.34	1.54
27	l	101	SQD	C6-S	-6.52	1.68	1.77
38	E	103	HEM	C2C-C1C	-6.39	1.40	1.52
27	F	101	SQD	C6-S	-6.30	1.68	1.77
38	e	102	HEM	C2C-C1C	-6.27	1.40	1.52
38	v	202	HEM	C2C-C1C	-5.96	1.41	1.52
38	V	203	HEM	C2C-C1C	-5.76	1.41	1.52
26	c	526	BCR	C23-C22	-4.87	1.35	1.45
26	C	515	BCR	C23-C22	-4.68	1.35	1.45
26	d	405	BCR	C23-C22	-4.66	1.35	1.45
26	y	101	BCR	C23-C22	-4.65	1.35	1.45
26	C	516	BCR	C23-C22	-4.62	1.35	1.45
26	B	620	BCR	C23-C22	-4.56	1.35	1.45
26	b	624	BCR	C23-C22	-4.52	1.35	1.45
26	k	103	BCR	C23-C22	-4.50	1.35	1.45
26	D	405	BCR	C23-C22	-4.50	1.35	1.45
26	a	410	BCR	C23-C22	-4.48	1.36	1.45
26	h	101	BCR	C23-C22	-4.46	1.36	1.45
26	T	102	BCR	C23-C22	-4.42	1.36	1.45
26	c	516	BCR	C23-C22	-4.37	1.36	1.45
26	b	623	BCR	C23-C22	-4.35	1.36	1.45
26	t	101	BCR	C23-C22	-4.34	1.36	1.45
26	H	101	BCR	C23-C22	-4.33	1.36	1.45
26	Y	101	BCR	C23-C22	-4.32	1.36	1.45
35	B	622	HTG	C1'-S1	-4.29	1.75	1.81
26	b	622	BCR	C23-C22	-4.27	1.36	1.45
26	B	618	BCR	C23-C22	-4.24	1.36	1.45
26	K	101	BCR	C23-C22	-4.22	1.36	1.45
26	A	410	BCR	C23-C22	-4.20	1.36	1.45
26	B	619	BCR	C23-C22	-4.18	1.36	1.45
38	E	103	HEM	C3B-C4B	-3.79	1.48	1.51
38	E	103	HEM	C3D-C4D	-3.78	1.46	1.51
35	d	411	HTG	C1'-S1	-3.77	1.76	1.81
35	b	603	HTG	C1'-S1	-3.74	1.76	1.81
35	O	303	HTG	C1'-S1	-3.65	1.76	1.81
35	b	628	HTG	C1'-S1	-3.57	1.76	1.81
38	e	102	HEM	C3D-C4D	-3.53	1.47	1.51
38	v	202	HEM	C3D-C4D	-3.46	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	624	HTG	C1'-S1	-3.44	1.76	1.81
25	A	407	PHO	C4A-NA	-3.41	1.26	1.34
35	c	523	HTG	C1'-S1	-3.40	1.76	1.81
25	d	403	PHO	C4A-NA	-3.38	1.26	1.34
25	A	408	PHO	C4A-NA	-3.34	1.27	1.34
35	B	631	HTG	C1'-S1	-3.33	1.76	1.81
35	D	411	HTG	C1'-S1	-3.32	1.76	1.81
35	C	523	HTG	C1'-S1	-3.27	1.76	1.81
35	b	604	HTG	C1'-S1	-3.26	1.76	1.81
35	B	630	HTG	C1'-S1	-3.25	1.77	1.81
38	V	203	HEM	C3B-C4B	-3.22	1.49	1.51
38	V	203	HEM	C3D-C4D	-3.18	1.47	1.51
35	C	522	HTG	C1'-S1	-3.16	1.77	1.81
35	V	204	HTG	C1'-S1	-3.12	1.77	1.81
35	c	522	HTG	C1'-S1	-3.10	1.77	1.81
35	B	623	HTG	C1'-S1	-3.07	1.77	1.81
38	v	202	HEM	C3B-C4B	-3.02	1.49	1.51
35	b	627	HTG	C1'-S1	-2.96	1.77	1.81
25	a	408	PHO	C4A-NA	-2.91	1.28	1.34
38	e	102	HEM	C3B-C4B	-2.89	1.49	1.51
38	V	203	HEM	C2B-C1B	-2.81	1.42	1.51
38	E	103	HEM	C2B-C1B	-2.79	1.42	1.51
38	v	202	HEM	C2B-C1B	-2.78	1.42	1.51
38	e	102	HEM	C2B-C1B	-2.58	1.43	1.51
35	D	411	HTG	C1-S1	-2.43	1.76	1.80
35	C	522	HTG	C1-S1	-2.31	1.76	1.80
35	c	522	HTG	C1-S1	-2.29	1.77	1.80
35	b	628	HTG	C1-S1	-2.25	1.77	1.80
35	c	523	HTG	C1-S1	-2.21	1.77	1.80
35	B	631	HTG	C1-S1	-2.19	1.77	1.80
35	d	411	HTG	C1-S1	-2.18	1.77	1.80
35	V	204	HTG	C1-S1	-2.17	1.77	1.80
24	a	409	CLA	C1C-NC	-2.13	1.34	1.37
35	b	604	HTG	C1-S1	-2.05	1.77	1.80
25	A	407	PHO	C1A-NA	-2.02	1.33	1.37
25	d	403	PHO	C4D-CHA	2.00	1.50	1.44
24	B	617	CLA	C1C-C2C	2.01	1.48	1.44
24	b	619	CLA	C1C-C2C	2.02	1.48	1.44
25	A	407	PHO	C4C-C3C	2.04	1.49	1.45
24	c	512	CLA	C4C-C3C	2.05	1.48	1.45
24	b	620	CLA	C1C-C2C	2.06	1.48	1.44
25	a	408	PHO	C1C-C2C	2.06	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C1C-C2C	2.07	1.48	1.44
24	B	610	CLA	C1C-C2C	2.10	1.48	1.44
24	b	611	CLA	C4C-C3C	2.12	1.48	1.45
24	C	514	CLA	C4C-C3C	2.14	1.48	1.45
36	D	407	DGD	O3G-C1D	2.15	1.44	1.40
24	B	604	CLA	C4C-C3C	2.15	1.48	1.45
24	C	514	CLA	C1C-C2C	2.15	1.48	1.44
24	b	621	CLA	C1C-C2C	2.16	1.48	1.44
32	D	406	PL9	C2-C3	2.16	1.40	1.34
24	b	617	CLA	C4C-C3C	2.16	1.48	1.45
24	D	404	CLA	C4C-C3C	2.17	1.48	1.45
24	B	606	CLA	C4C-C3C	2.18	1.49	1.45
24	b	616	CLA	C4C-C3C	2.18	1.49	1.45
24	A	406	CLA	C4C-C3C	2.18	1.49	1.45
24	B	607	CLA	C4C-C3C	2.20	1.49	1.45
30	m	103	LMT	O1'-C1'	2.20	1.44	1.40
24	c	504	CLA	C1C-C2C	2.21	1.49	1.44
24	b	616	CLA	C1C-C2C	2.21	1.49	1.44
24	b	614	CLA	C1C-C2C	2.22	1.49	1.44
24	B	616	CLA	C1C-C2C	2.22	1.49	1.44
24	C	508	CLA	C4C-C3C	2.22	1.49	1.45
32	a	416	PL9	C2-C3	2.22	1.40	1.34
24	c	504	CLA	C4C-C3C	2.22	1.49	1.45
24	B	602	CLA	C4C-C3C	2.23	1.49	1.45
24	a	406	CLA	C1C-C2C	2.24	1.49	1.44
32	D	406	PL9	C6-C5	2.24	1.48	1.35
24	C	511	CLA	C4C-C3C	2.24	1.49	1.45
24	A	409	CLA	C4C-C3C	2.25	1.49	1.45
24	d	401	CLA	C4C-C3C	2.25	1.49	1.45
24	B	617	CLA	C4C-C3C	2.25	1.49	1.45
24	C	512	CLA	C1C-C2C	2.25	1.49	1.44
24	B	611	CLA	C1C-C2C	2.26	1.49	1.44
24	c	505	CLA	C4C-C3C	2.26	1.49	1.45
24	b	608	CLA	C4C-C3C	2.27	1.49	1.45
24	B	605	CLA	C4C-C3C	2.27	1.49	1.45
24	c	503	CLA	C1C-C2C	2.27	1.49	1.44
32	d	406	PL9	C6-C5	2.28	1.48	1.35
24	a	409	CLA	C1C-C2C	2.28	1.49	1.44
30	M	101	LMT	O1'-C1'	2.29	1.44	1.40
24	C	507	CLA	C1C-C2C	2.29	1.49	1.44
32	A	419	PL9	C6-C5	2.29	1.48	1.35
24	B	617	CLA	C4B-CHC	2.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C4C-C3C	2.32	1.49	1.45
24	b	610	CLA	C4C-C3C	2.32	1.49	1.45
24	C	512	CLA	C4C-C3C	2.33	1.49	1.45
24	B	615	CLA	C1C-C2C	2.33	1.49	1.44
24	b	620	CLA	C4C-C3C	2.34	1.49	1.45
24	a	407	CLA	C4C-C3C	2.34	1.49	1.45
24	C	507	CLA	C4C-C3C	2.35	1.49	1.45
32	a	416	PL9	C6-C5	2.35	1.49	1.35
24	A	406	CLA	C4B-CHC	2.35	1.46	1.39
24	d	404	CLA	C4C-C3C	2.35	1.49	1.45
36	h	102	DGD	O5D-C1E	2.36	1.44	1.40
24	c	509	CLA	C4C-C3C	2.37	1.49	1.45
24	c	513	CLA	C4C-C3C	2.37	1.49	1.45
38	E	103	HEM	FE-NB	2.37	2.10	1.97
24	c	515	CLA	C1C-C2C	2.37	1.49	1.44
24	C	505	CLA	C1C-C2C	2.38	1.49	1.44
24	B	609	CLA	C4C-C3C	2.38	1.49	1.45
24	b	612	CLA	C1C-C2C	2.38	1.49	1.44
24	B	608	CLA	C1C-C2C	2.38	1.49	1.44
24	d	402	CLA	C4C-C3C	2.38	1.49	1.45
24	d	401	CLA	C4B-CHC	2.39	1.46	1.39
36	H	102	DGD	O5D-C1E	2.40	1.44	1.40
24	b	612	CLA	CHD-C4C	2.40	1.46	1.41
24	b	613	CLA	C4C-C3C	2.40	1.49	1.45
24	C	506	CLA	C1C-C2C	2.40	1.49	1.44
24	b	606	CLA	C1C-C2C	2.40	1.49	1.44
24	b	617	CLA	CHD-C4C	2.41	1.46	1.41
24	D	401	CLA	C1C-C2C	2.41	1.49	1.44
24	B	605	CLA	C1C-C2C	2.42	1.49	1.44
24	b	613	CLA	C1C-C2C	2.42	1.49	1.44
24	B	616	CLA	C4C-C3C	2.42	1.49	1.45
24	b	607	CLA	C4C-C3C	2.43	1.49	1.45
24	B	612	CLA	C4C-C3C	2.43	1.49	1.45
24	B	602	CLA	C1C-C2C	2.43	1.49	1.44
24	B	609	CLA	C1C-C2C	2.43	1.49	1.44
24	C	513	CLA	C4C-C3C	2.43	1.49	1.45
24	c	511	CLA	C4C-C3C	2.44	1.49	1.45
24	a	409	CLA	C4B-CHC	2.46	1.46	1.39
24	C	507	CLA	C4B-CHC	2.46	1.46	1.39
24	c	506	CLA	C4C-C3C	2.46	1.49	1.45
24	B	609	CLA	C4B-CHC	2.46	1.46	1.39
34	Z	101	LMG	O8-C28	2.46	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	C4C-C3C	2.47	1.49	1.45
24	b	609	CLA	CHD-C4C	2.47	1.47	1.41
24	b	618	CLA	C4C-C3C	2.47	1.49	1.45
24	a	407	CLA	C1C-C2C	2.47	1.49	1.44
24	B	608	CLA	C4C-C3C	2.47	1.49	1.45
24	b	614	CLA	C4C-C3C	2.48	1.49	1.45
24	b	607	CLA	C1C-C2C	2.48	1.49	1.44
24	b	621	CLA	C4B-CHC	2.48	1.46	1.39
24	C	509	CLA	C1C-C2C	2.48	1.49	1.44
24	B	613	CLA	C1C-C2C	2.48	1.49	1.44
38	v	202	HEM	FE-NB	2.48	2.10	1.97
24	C	502	CLA	C4C-C3C	2.49	1.49	1.45
24	c	514	CLA	C1C-C2C	2.49	1.49	1.44
24	C	512	CLA	C4B-CHC	2.49	1.46	1.39
24	c	514	CLA	C4C-C3C	2.50	1.49	1.45
24	C	511	CLA	C1C-C2C	2.50	1.49	1.44
24	c	511	CLA	C1C-C2C	2.50	1.49	1.44
24	c	509	CLA	C1C-C2C	2.51	1.49	1.44
24	a	406	CLA	C4B-CHC	2.51	1.46	1.39
24	C	504	CLA	C4C-C3C	2.51	1.49	1.45
24	C	504	CLA	C1C-C2C	2.52	1.49	1.44
24	c	508	CLA	C4B-CHC	2.52	1.46	1.39
24	B	603	CLA	C1C-C2C	2.52	1.49	1.44
24	B	605	CLA	CHD-C4C	2.52	1.47	1.41
24	B	606	CLA	C1C-C2C	2.53	1.49	1.44
24	c	504	CLA	C4B-CHC	2.54	1.46	1.39
24	B	614	CLA	C1C-C2C	2.54	1.49	1.44
24	d	402	CLA	C1C-C2C	2.54	1.49	1.44
24	b	619	CLA	C4B-CHC	2.54	1.46	1.39
24	A	409	CLA	C1C-C2C	2.54	1.49	1.44
24	b	617	CLA	C1C-C2C	2.55	1.49	1.44
24	c	513	CLA	C4B-CHC	2.55	1.46	1.39
24	c	503	CLA	C4B-CHC	2.55	1.46	1.39
24	b	610	CLA	C1C-C2C	2.55	1.49	1.44
24	c	510	CLA	C4C-C3C	2.55	1.49	1.45
24	B	611	CLA	C4C-C3C	2.55	1.49	1.45
24	c	515	CLA	C1B-CHB	2.55	1.46	1.39
24	c	515	CLA	C4C-C3C	2.57	1.49	1.45
24	B	615	CLA	C4B-CHC	2.57	1.46	1.39
24	C	510	CLA	C1C-C2C	2.57	1.49	1.44
24	C	502	CLA	CHD-C4C	2.57	1.47	1.41
24	B	603	CLA	C4C-C3C	2.58	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C4C-C3C	2.59	1.49	1.45
24	D	404	CLA	CHD-C4C	2.60	1.47	1.41
24	c	506	CLA	CHD-C4C	2.60	1.47	1.41
24	C	505	CLA	C4B-CHC	2.60	1.47	1.39
24	D	401	CLA	C4B-CHC	2.60	1.47	1.39
24	C	502	CLA	C1C-C2C	2.60	1.49	1.44
24	D	401	CLA	C1B-CHB	2.61	1.47	1.39
24	A	405	CLA	CHD-C4C	2.61	1.47	1.41
24	c	506	CLA	C4B-CHC	2.62	1.47	1.39
24	B	612	CLA	C1B-CHB	2.62	1.47	1.39
24	c	507	CLA	C1C-C2C	2.63	1.49	1.44
24	d	401	CLA	CHD-C4C	2.63	1.47	1.41
24	B	609	CLA	C1B-CHB	2.63	1.47	1.39
24	b	619	CLA	C1B-CHB	2.64	1.47	1.39
24	B	612	CLA	C1C-C2C	2.64	1.49	1.44
24	c	512	CLA	C1C-C2C	2.64	1.49	1.44
24	b	618	CLA	C4B-CHC	2.64	1.47	1.39
24	b	619	CLA	C4C-C3C	2.65	1.49	1.45
24	C	513	CLA	C1C-C2C	2.65	1.49	1.44
24	B	613	CLA	CHD-C4C	2.66	1.47	1.41
24	B	602	CLA	C1B-CHB	2.66	1.47	1.39
24	C	505	CLA	C4C-C3C	2.66	1.49	1.45
24	b	614	CLA	C4B-CHC	2.67	1.47	1.39
24	c	506	CLA	C1B-CHB	2.67	1.47	1.39
24	C	503	CLA	C1C-C2C	2.67	1.49	1.44
24	C	502	CLA	C4B-CHC	2.67	1.47	1.39
24	b	618	CLA	CHD-C4C	2.67	1.47	1.41
24	B	603	CLA	C4B-CHC	2.67	1.47	1.39
24	b	620	CLA	C1B-CHB	2.68	1.47	1.39
24	D	404	CLA	C1B-CHB	2.68	1.47	1.39
24	C	513	CLA	C4B-CHC	2.68	1.47	1.39
24	C	514	CLA	C4B-CHC	2.68	1.47	1.39
38	V	203	HEM	FE-NB	2.69	2.11	1.97
24	B	613	CLA	C4B-CHC	2.69	1.47	1.39
24	a	409	CLA	C1B-CHB	2.69	1.47	1.39
24	B	607	CLA	CHD-C4C	2.69	1.47	1.41
24	C	508	CLA	C1C-C2C	2.69	1.50	1.44
24	c	514	CLA	C1B-CHB	2.69	1.47	1.39
24	b	610	CLA	C1B-CHB	2.70	1.47	1.39
24	C	513	CLA	C1B-CHB	2.70	1.47	1.39
24	B	617	CLA	CHD-C4C	2.70	1.47	1.41
24	b	609	CLA	C4C-C3C	2.70	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C4B-CHC	2.70	1.47	1.39
24	C	503	CLA	C4C-C3C	2.71	1.49	1.45
24	c	508	CLA	C1B-CHB	2.71	1.47	1.39
24	c	509	CLA	CHD-C4C	2.71	1.47	1.41
24	a	407	CLA	C1B-CHB	2.71	1.47	1.39
24	A	405	CLA	C1C-C2C	2.71	1.50	1.44
24	c	503	CLA	CHD-C4C	2.71	1.47	1.41
24	B	603	CLA	C1B-CHB	2.71	1.47	1.39
24	B	616	CLA	C4B-CHC	2.71	1.47	1.39
24	c	509	CLA	C4B-CHC	2.72	1.47	1.39
24	b	611	CLA	C1C-C2C	2.72	1.50	1.44
24	b	620	CLA	C4B-CHC	2.72	1.47	1.39
24	B	604	CLA	CHD-C4C	2.72	1.47	1.41
24	D	401	CLA	C4C-C3C	2.72	1.49	1.45
24	d	402	CLA	C4B-CHC	2.73	1.47	1.39
24	b	611	CLA	C1B-CHB	2.73	1.47	1.39
24	d	404	CLA	C1C-C2C	2.73	1.50	1.44
24	A	405	CLA	C4B-CHC	2.73	1.47	1.39
24	C	508	CLA	C1B-CHB	2.74	1.47	1.39
24	B	603	CLA	CHD-C4C	2.74	1.47	1.41
24	b	618	CLA	C1C-C2C	2.74	1.50	1.44
24	b	612	CLA	C1B-CHB	2.74	1.47	1.39
24	D	404	CLA	C1C-C2C	2.75	1.50	1.44
24	B	615	CLA	C1B-CHB	2.75	1.47	1.39
38	e	102	HEM	FE-NB	2.75	2.12	1.97
24	B	616	CLA	CHD-C4C	2.75	1.47	1.41
24	c	505	CLA	C1C-C2C	2.75	1.50	1.44
24	d	404	CLA	C1B-CHB	2.75	1.47	1.39
24	c	505	CLA	CHD-C4C	2.76	1.47	1.41
24	B	608	CLA	CHD-C4C	2.76	1.47	1.41
24	b	615	CLA	C4C-C3C	2.76	1.50	1.45
24	B	610	CLA	CHD-C4C	2.76	1.47	1.41
24	D	403	CLA	C4C-C3C	2.77	1.50	1.45
24	C	502	CLA	C1B-CHB	2.77	1.47	1.39
24	c	510	CLA	CHD-C4C	2.77	1.47	1.41
24	b	613	CLA	C1B-CHB	2.77	1.47	1.39
24	b	607	CLA	CHD-C4C	2.77	1.47	1.41
24	b	612	CLA	C4B-CHC	2.78	1.47	1.39
24	B	606	CLA	CHD-C4C	2.78	1.47	1.41
24	C	504	CLA	CHD-C4C	2.79	1.47	1.41
24	C	504	CLA	C1B-CHB	2.79	1.47	1.39
24	C	513	CLA	CHD-C4C	2.79	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C4B-CHC	2.79	1.47	1.39
24	C	506	CLA	C4B-CHC	2.80	1.47	1.39
24	B	610	CLA	C4B-CHC	2.80	1.47	1.39
24	B	614	CLA	C4B-CHC	2.80	1.47	1.39
24	B	607	CLA	C1B-CHB	2.80	1.47	1.39
24	D	401	CLA	CHD-C4C	2.81	1.47	1.41
24	b	611	CLA	CHD-C4C	2.81	1.47	1.41
24	b	608	CLA	C1C-C2C	2.82	1.50	1.44
24	B	607	CLA	C4B-CHC	2.82	1.47	1.39
24	C	514	CLA	CHD-C4C	2.82	1.47	1.41
24	c	510	CLA	C1B-CHB	2.82	1.47	1.39
24	B	609	CLA	CHD-C4C	2.82	1.47	1.41
24	b	621	CLA	C4C-C3C	2.82	1.50	1.45
24	B	605	CLA	C4B-CHC	2.82	1.47	1.39
24	D	403	CLA	C4B-CHC	2.82	1.47	1.39
24	c	506	CLA	C1C-C2C	2.83	1.50	1.44
24	B	602	CLA	CHD-C4C	2.83	1.47	1.41
24	c	515	CLA	C4B-CHC	2.83	1.47	1.39
24	a	406	CLA	C4C-C3C	2.83	1.50	1.45
24	A	409	CLA	C1B-CHB	2.83	1.47	1.39
24	D	404	CLA	C4B-CHC	2.83	1.47	1.39
25	d	403	PHO	C3B-C4B	2.83	1.49	1.43
24	C	504	CLA	C4B-CHC	2.83	1.47	1.39
24	B	615	CLA	CHD-C4C	2.83	1.47	1.41
24	b	620	CLA	CHD-C4C	2.83	1.47	1.41
24	c	507	CLA	C4B-CHC	2.83	1.47	1.39
24	C	506	CLA	C4C-C3C	2.84	1.50	1.45
24	D	403	CLA	C1C-C2C	2.84	1.50	1.44
24	B	616	CLA	C1B-CHB	2.84	1.47	1.39
24	c	507	CLA	C1B-CHB	2.84	1.47	1.39
24	c	511	CLA	C4B-CHC	2.84	1.47	1.39
24	B	612	CLA	CHD-C4C	2.85	1.47	1.41
24	c	512	CLA	C4B-CHC	2.85	1.47	1.39
24	A	409	CLA	CHD-C4C	2.85	1.47	1.41
24	C	510	CLA	C4C-C3C	2.85	1.50	1.45
24	C	509	CLA	C4C-C3C	2.85	1.50	1.45
24	b	607	CLA	C1B-CHB	2.86	1.47	1.39
24	C	506	CLA	CHD-C4C	2.86	1.47	1.41
24	C	507	CLA	CHD-C4C	2.86	1.47	1.41
24	B	614	CLA	CHD-C4C	2.87	1.47	1.41
24	b	608	CLA	C1B-CHB	2.87	1.47	1.39
24	B	604	CLA	C1C-C2C	2.87	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	C1B-CHB	2.87	1.47	1.39
24	b	613	CLA	CHD-C4C	2.87	1.47	1.41
25	A	407	PHO	C3B-C4B	2.89	1.49	1.43
25	A	407	PHO	CHC-C4B	2.89	1.47	1.40
24	c	505	CLA	C1B-CHB	2.89	1.47	1.39
24	C	510	CLA	C4B-CHC	2.89	1.47	1.39
24	B	606	CLA	C4B-CHC	2.89	1.47	1.39
24	B	606	CLA	C1B-CHB	2.89	1.47	1.39
24	b	610	CLA	CHD-C4C	2.89	1.48	1.41
24	C	508	CLA	CHD-C4C	2.89	1.48	1.41
24	b	607	CLA	C4B-CHC	2.90	1.47	1.39
24	b	616	CLA	CHD-C4C	2.90	1.48	1.41
24	B	614	CLA	C4C-C3C	2.90	1.50	1.45
24	B	607	CLA	C1C-C2C	2.91	1.50	1.44
24	c	511	CLA	C1B-CHB	2.91	1.47	1.39
25	a	408	PHO	CHD-C4C	2.91	1.47	1.40
24	C	511	CLA	C4B-CHC	2.91	1.47	1.39
24	C	503	CLA	C4B-CHC	2.91	1.47	1.39
24	d	402	CLA	C1B-CHB	2.91	1.47	1.39
24	b	606	CLA	C4B-CHC	2.92	1.47	1.39
24	B	611	CLA	C1B-CHB	2.92	1.47	1.39
24	D	403	CLA	CHD-C4C	2.92	1.48	1.41
24	B	602	CLA	C4B-CHC	2.92	1.47	1.39
24	a	407	CLA	C4B-CHC	2.92	1.47	1.39
24	b	615	CLA	C1C-C2C	2.93	1.50	1.44
24	B	604	CLA	C1B-CHB	2.93	1.47	1.39
24	B	614	CLA	C1B-CHB	2.93	1.47	1.39
24	c	512	CLA	CHD-C4C	2.93	1.48	1.41
24	B	613	CLA	C4C-C3C	2.94	1.50	1.45
24	c	507	CLA	C4C-C3C	2.94	1.50	1.45
24	B	611	CLA	CHD-C4C	2.94	1.48	1.41
24	b	615	CLA	CHD-C4C	2.94	1.48	1.41
24	b	608	CLA	C4B-CHC	2.95	1.48	1.39
24	a	409	CLA	CHD-C4C	2.95	1.48	1.41
24	c	514	CLA	C4B-CHC	2.95	1.48	1.39
24	b	614	CLA	CHD-C4C	2.95	1.48	1.41
24	b	617	CLA	C4B-CHC	2.96	1.48	1.39
24	b	610	CLA	C4B-CHC	2.97	1.48	1.39
24	A	405	CLA	C4C-C3C	2.97	1.50	1.45
24	b	616	CLA	C4B-CHC	2.97	1.48	1.39
24	b	611	CLA	C4B-CHC	2.98	1.48	1.39
24	d	404	CLA	CHD-C4C	2.98	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	CHD-C4C	2.99	1.48	1.41
24	B	612	CLA	C4B-CHC	2.99	1.48	1.39
24	c	504	CLA	C1B-CHB	2.99	1.48	1.39
24	C	510	CLA	CHD-C4C	2.99	1.48	1.41
24	C	511	CLA	CHD-C4C	2.99	1.48	1.41
24	C	512	CLA	C1B-CHB	2.99	1.48	1.39
24	B	613	CLA	C1B-CHB	3.00	1.48	1.39
25	d	403	PHO	CHC-C4B	3.00	1.47	1.40
24	c	504	CLA	CHD-C4C	3.00	1.48	1.41
25	A	407	PHO	CHD-C4C	3.00	1.47	1.40
24	b	613	CLA	C4B-CHC	3.01	1.48	1.39
24	c	505	CLA	C4B-CHC	3.01	1.48	1.39
24	C	503	CLA	CHD-C4C	3.01	1.48	1.41
24	C	509	CLA	CHD-C4C	3.01	1.48	1.41
24	C	509	CLA	C1B-CHB	3.02	1.48	1.39
24	C	506	CLA	C1B-CHB	3.02	1.48	1.39
24	d	404	CLA	C4B-CHC	3.02	1.48	1.39
24	C	514	CLA	C1B-CHB	3.03	1.48	1.39
24	b	615	CLA	C4B-CHC	3.03	1.48	1.39
24	d	401	CLA	C1B-CHB	3.03	1.48	1.39
24	C	511	CLA	C1B-CHB	3.04	1.48	1.39
24	b	616	CLA	C1B-CHB	3.04	1.48	1.39
24	c	509	CLA	C1B-CHB	3.04	1.48	1.39
24	b	614	CLA	C1B-CHB	3.04	1.48	1.39
24	C	508	CLA	C4B-CHC	3.04	1.48	1.39
24	b	608	CLA	CHD-C4C	3.04	1.48	1.41
24	c	510	CLA	C4B-CHC	3.04	1.48	1.39
24	b	621	CLA	C1B-CHB	3.05	1.48	1.39
25	A	408	PHO	CHD-C4C	3.06	1.48	1.40
24	c	514	CLA	CHD-C4C	3.06	1.48	1.41
24	B	617	CLA	C1B-CHB	3.08	1.48	1.39
24	c	513	CLA	C1B-CHB	3.08	1.48	1.39
24	A	405	CLA	C1B-CHB	3.08	1.48	1.39
24	c	510	CLA	C1C-C2C	3.08	1.50	1.44
24	B	605	CLA	C1B-CHB	3.08	1.48	1.39
24	b	606	CLA	CHD-C4C	3.09	1.48	1.41
25	d	403	PHO	CHD-C4C	3.10	1.48	1.40
24	b	617	CLA	C1B-CHB	3.10	1.48	1.39
24	A	406	CLA	C1B-CHB	3.10	1.48	1.39
24	C	503	CLA	C1B-CHB	3.11	1.48	1.39
24	C	512	CLA	CHD-C4C	3.11	1.48	1.41
24	c	507	CLA	CHD-C4C	3.11	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C1B-CHB	3.12	1.48	1.39
24	b	621	CLA	CHD-C4C	3.12	1.48	1.41
24	b	609	CLA	C1B-CHB	3.12	1.48	1.39
24	b	618	CLA	C1B-CHB	3.12	1.48	1.39
24	B	605	CLA	C3D-C2D	3.13	1.47	1.40
25	A	408	PHO	C3B-C4B	3.13	1.50	1.43
24	d	402	CLA	CHD-C4C	3.13	1.48	1.41
24	c	508	CLA	CHD-C4C	3.14	1.48	1.41
24	B	608	CLA	C4B-CHC	3.14	1.48	1.39
24	b	615	CLA	C1B-CHB	3.14	1.48	1.39
24	B	610	CLA	C1B-CHB	3.14	1.48	1.39
24	C	510	CLA	C1B-CHB	3.16	1.48	1.39
24	a	407	CLA	CHD-C4C	3.16	1.48	1.41
24	a	406	CLA	C1B-CHB	3.16	1.48	1.39
24	c	515	CLA	CHD-C4C	3.17	1.48	1.41
38	E	103	HEM	FE-NC	3.17	2.08	1.95
24	C	505	CLA	CHD-C4C	3.17	1.48	1.41
24	c	513	CLA	CHD-C4C	3.18	1.48	1.41
37	d	408	LHG	O7-C7	3.19	1.43	1.34
24	b	609	CLA	C4B-CHC	3.19	1.48	1.39
24	c	511	CLA	CHD-C4C	3.19	1.48	1.41
24	A	409	CLA	C4B-CHC	3.20	1.48	1.39
24	c	503	CLA	C1B-CHB	3.20	1.48	1.39
25	d	403	PHO	OBD-CAD	3.21	1.28	1.22
24	B	608	CLA	C1B-CHB	3.22	1.48	1.39
37	D	408	LHG	O7-C7	3.24	1.44	1.34
24	B	605	CLA	OBD-CAD	3.24	1.27	1.22
24	B	611	CLA	C4B-CHC	3.25	1.48	1.39
24	b	619	CLA	CHD-C4C	3.26	1.48	1.41
24	D	403	CLA	C1B-CHB	3.26	1.48	1.39
37	D	409	LHG	O7-C7	3.28	1.44	1.34
24	A	406	CLA	CHD-C4C	3.29	1.48	1.41
24	C	505	CLA	C1B-CHB	3.30	1.48	1.39
25	a	408	PHO	CHB-C4A	3.32	1.46	1.40
24	b	609	CLA	C1C-C2C	3.35	1.51	1.44
24	c	512	CLA	C1B-CHB	3.35	1.49	1.39
25	a	408	PHO	OBD-CAD	3.36	1.28	1.22
25	a	408	PHO	C3B-C4B	3.37	1.51	1.43
36	C	519	DGD	O2G-C1B	3.39	1.44	1.34
37	d	409	LHG	O7-C7	3.40	1.44	1.34
38	v	202	HEM	FE-NC	3.42	2.09	1.95
38	e	102	HEM	FE-NC	3.42	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	409	LHG	O8-C23	3.42	1.43	1.33
24	a	406	CLA	O2A-CGA	3.44	1.43	1.33
25	a	408	PHO	C3D-C2D	3.44	1.48	1.38
24	c	507	CLA	C3D-C2D	3.45	1.48	1.40
24	d	402	CLA	OBD-CAD	3.45	1.27	1.22
38	V	203	HEM	FE-NC	3.47	2.09	1.95
34	b	625	LMG	O7-C10	3.48	1.44	1.34
25	A	408	PHO	OBD-CAD	3.49	1.28	1.22
37	L	101	LHG	O7-C7	3.50	1.44	1.34
36	c	518	DGD	O2G-C1B	3.50	1.44	1.34
34	J	101	LMG	O7-C10	3.52	1.44	1.34
25	A	408	PHO	CHB-C4A	3.53	1.47	1.40
34	c	501	LMG	O7-C10	3.54	1.44	1.34
25	A	408	PHO	CHC-C4B	3.55	1.49	1.40
37	D	408	LHG	O8-C23	3.55	1.44	1.33
24	C	509	CLA	OBD-CAD	3.56	1.27	1.22
24	b	617	CLA	C3D-C2D	3.57	1.48	1.40
24	B	603	CLA	O2A-CGA	3.57	1.44	1.33
25	A	408	PHO	O2A-CGA	3.58	1.44	1.33
25	a	408	PHO	CHC-C4B	3.58	1.49	1.40
24	b	608	CLA	C3D-C2D	3.58	1.48	1.40
24	d	401	CLA	CHC-C1C	3.58	1.46	1.35
24	c	503	CLA	C3D-C2D	3.58	1.48	1.40
24	A	405	CLA	O2A-CGA	3.59	1.44	1.33
24	b	612	CLA	O2A-CGA	3.60	1.44	1.33
36	h	102	DGD	O2G-C1B	3.60	1.45	1.34
24	B	615	CLA	C3D-C2D	3.60	1.48	1.40
24	C	508	CLA	C3D-C2D	3.60	1.48	1.40
34	J	101	LMG	O8-C28	3.61	1.44	1.33
24	B	617	CLA	C3D-C2D	3.62	1.48	1.40
24	c	507	CLA	O2A-CGA	3.62	1.44	1.33
24	b	610	CLA	C3D-C2D	3.64	1.48	1.40
24	c	512	CLA	C3D-C2D	3.65	1.48	1.40
24	B	602	CLA	OBD-CAD	3.66	1.27	1.22
24	B	606	CLA	C3D-C2D	3.66	1.48	1.40
24	B	606	CLA	CHC-C1C	3.67	1.46	1.35
27	A	411	SQD	O47-C7	3.67	1.45	1.34
34	j	101	LMG	O7-C10	3.68	1.45	1.34
36	C	517	DGD	O1G-C1A	3.68	1.44	1.33
27	a	411	SQD	O47-C7	3.68	1.45	1.34
24	c	513	CLA	C3D-C2D	3.68	1.49	1.40
24	C	506	CLA	C3D-C2D	3.69	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	518	DGD	O2G-C1B	3.69	1.45	1.34
36	c	517	DGD	O1G-C1A	3.69	1.44	1.33
24	B	613	CLA	C3D-C2D	3.70	1.49	1.40
25	A	407	PHO	CHB-C4A	3.71	1.47	1.40
24	B	615	CLA	O2A-CGA	3.71	1.44	1.33
24	B	613	CLA	OBD-CAD	3.71	1.28	1.22
25	A	407	PHO	C3D-C2D	3.71	1.49	1.38
24	A	406	CLA	O2A-CGA	3.72	1.44	1.33
37	d	410	LHG	O7-C7	3.72	1.45	1.34
24	C	507	CLA	OBD-CAD	3.73	1.28	1.22
36	c	519	DGD	O2G-C1B	3.73	1.45	1.34
36	c	517	DGD	O2G-C1B	3.73	1.45	1.34
24	C	512	CLA	C3D-C2D	3.74	1.49	1.40
36	C	519	DGD	O1G-C1A	3.74	1.44	1.33
27	A	411	SQD	O48-C23	3.75	1.44	1.33
24	A	409	CLA	O2A-CGA	3.75	1.44	1.33
24	d	402	CLA	CHC-C1C	3.75	1.47	1.35
24	b	609	CLA	C3D-C2D	3.76	1.49	1.40
37	L	101	LHG	O8-C23	3.76	1.44	1.33
24	b	607	CLA	O2A-CGA	3.77	1.44	1.33
24	b	615	CLA	O2A-CGA	3.77	1.44	1.33
24	b	606	CLA	OBD-CAD	3.77	1.28	1.22
24	a	406	CLA	CHC-C1C	3.77	1.47	1.35
25	A	407	PHO	O2A-CGA	3.77	1.44	1.33
24	D	404	CLA	O2A-CGA	3.77	1.44	1.33
24	B	614	CLA	C3D-C2D	3.78	1.49	1.40
24	D	403	CLA	C3D-C2D	3.78	1.49	1.40
24	B	606	CLA	OBD-CAD	3.78	1.28	1.22
37	d	408	LHG	O8-C23	3.78	1.44	1.33
24	B	609	CLA	OBD-CAD	3.79	1.28	1.22
24	B	608	CLA	C3D-C2D	3.79	1.49	1.40
24	b	614	CLA	CHC-C1C	3.80	1.47	1.35
24	B	605	CLA	O2A-CGA	3.80	1.44	1.33
24	B	614	CLA	CHC-C1C	3.80	1.47	1.35
24	a	409	CLA	CHC-C1C	3.81	1.47	1.35
24	B	617	CLA	CHC-C1C	3.81	1.47	1.35
24	b	618	CLA	CHC-C1C	3.81	1.47	1.35
24	b	618	CLA	C3D-C2D	3.81	1.49	1.40
24	a	406	CLA	C3D-C2D	3.81	1.49	1.40
24	C	503	CLA	OBD-CAD	3.81	1.28	1.22
24	C	507	CLA	CHC-C1C	3.82	1.47	1.35
34	B	621	LMG	O7-C10	3.82	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	517	DGD	O2G-C1B	3.82	1.45	1.34
24	D	403	CLA	CHC-C1C	3.83	1.47	1.35
24	c	508	CLA	OBD-CAD	3.83	1.28	1.22
34	c	520	LMG	O7-C10	3.83	1.45	1.34
24	B	603	CLA	C3D-C2D	3.83	1.49	1.40
37	D	410	LHG	O8-C23	3.83	1.44	1.33
24	D	404	CLA	C3D-C2D	3.83	1.49	1.40
24	d	404	CLA	C3D-C2D	3.83	1.49	1.40
24	C	514	CLA	C3D-C2D	3.83	1.49	1.40
34	C	520	LMG	O7-C10	3.83	1.45	1.34
27	a	402	SQD	O47-C7	3.83	1.45	1.34
24	b	609	CLA	CHC-C1C	3.84	1.47	1.35
27	a	411	SQD	O48-C23	3.84	1.44	1.33
24	c	505	CLA	OBD-CAD	3.84	1.28	1.22
37	l	102	LHG	O7-C7	3.84	1.45	1.34
24	C	510	CLA	CHC-C1C	3.84	1.47	1.35
24	B	610	CLA	C3D-C2D	3.84	1.49	1.40
24	c	503	CLA	CHC-C1C	3.84	1.47	1.35
24	c	508	CLA	C3D-C2D	3.84	1.49	1.40
24	a	407	CLA	C3D-C2D	3.84	1.49	1.40
24	B	614	CLA	O2A-CGA	3.84	1.44	1.33
36	H	102	DGD	O1G-C1A	3.84	1.44	1.33
34	j	101	LMG	O8-C28	3.84	1.44	1.33
24	b	613	CLA	C3D-C2D	3.85	1.49	1.40
24	C	511	CLA	CHC-C1C	3.85	1.47	1.35
24	b	612	CLA	OBD-CAD	3.85	1.28	1.22
24	b	611	CLA	C3D-C2D	3.85	1.49	1.40
25	d	403	PHO	C3D-C2D	3.85	1.49	1.38
24	b	612	CLA	CHC-C1C	3.85	1.47	1.35
24	c	508	CLA	CHC-C1C	3.86	1.47	1.35
24	B	612	CLA	O2A-CGA	3.86	1.44	1.33
24	a	409	CLA	C3D-C2D	3.86	1.49	1.40
24	c	505	CLA	O2A-CGA	3.86	1.44	1.33
25	A	408	PHO	CHD-C1D	3.86	1.46	1.38
36	H	102	DGD	O2G-C1B	3.86	1.45	1.34
24	C	513	CLA	OBD-CAD	3.86	1.28	1.22
24	c	513	CLA	O2A-CGA	3.86	1.45	1.33
24	C	502	CLA	CHC-C1C	3.87	1.47	1.35
24	c	505	CLA	C3D-C2D	3.87	1.49	1.40
24	c	511	CLA	C3D-C2D	3.87	1.49	1.40
24	b	621	CLA	CHC-C1C	3.87	1.47	1.35
37	E	101	LHG	O7-C7	3.87	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	CLA	CHC-C1C	3.88	1.47	1.35
24	b	620	CLA	O2A-CGA	3.88	1.45	1.33
24	b	620	CLA	CHC-C1C	3.88	1.47	1.35
25	d	403	PHO	CHB-C4A	3.89	1.47	1.40
24	c	509	CLA	OBD-CAD	3.89	1.28	1.22
25	A	408	PHO	C3D-C2D	3.89	1.49	1.38
24	B	611	CLA	CHC-C1C	3.89	1.47	1.35
24	b	614	CLA	C3D-C2D	3.89	1.49	1.40
24	b	619	CLA	CHC-C1C	3.89	1.47	1.35
24	c	509	CLA	C3D-C2D	3.89	1.49	1.40
24	d	402	CLA	C3D-C2D	3.90	1.49	1.40
27	l	101	SQD	O47-C7	3.90	1.46	1.34
24	c	515	CLA	C3D-C2D	3.90	1.49	1.40
24	C	504	CLA	C3D-C2D	3.91	1.49	1.40
24	b	621	CLA	C3D-C2D	3.91	1.49	1.40
24	c	509	CLA	CHC-C1C	3.91	1.47	1.35
24	b	613	CLA	CHC-C1C	3.91	1.47	1.35
37	D	410	LHG	O7-C7	3.91	1.46	1.34
24	b	618	CLA	OBD-CAD	3.91	1.28	1.22
24	B	607	CLA	OBD-CAD	3.92	1.28	1.22
24	c	506	CLA	O2A-CGA	3.92	1.45	1.33
24	B	602	CLA	C3D-C2D	3.92	1.49	1.40
24	c	512	CLA	OBD-CAD	3.92	1.28	1.22
24	B	608	CLA	CHC-C1C	3.92	1.47	1.35
24	b	611	CLA	O2A-CGA	3.92	1.45	1.33
27	l	101	SQD	O48-C23	3.92	1.45	1.33
24	c	504	CLA	OBD-CAD	3.92	1.28	1.22
34	z	101	LMG	O7-C10	3.92	1.46	1.34
24	C	509	CLA	CHC-C1C	3.92	1.47	1.35
24	B	611	CLA	O2A-CGA	3.92	1.45	1.33
24	B	604	CLA	C3D-C2D	3.93	1.49	1.40
25	a	408	PHO	O2A-CGA	3.93	1.45	1.33
24	B	611	CLA	C3D-C2D	3.94	1.49	1.40
37	e	101	LHG	O7-C7	3.94	1.46	1.34
24	B	613	CLA	O2A-CGA	3.94	1.45	1.33
24	C	511	CLA	O2A-CGA	3.94	1.45	1.33
24	A	406	CLA	C3D-C2D	3.94	1.49	1.40
24	c	513	CLA	CHC-C1C	3.95	1.47	1.35
24	D	401	CLA	O2A-CGA	3.95	1.45	1.33
24	c	506	CLA	CHC-C1C	3.95	1.47	1.35
24	c	504	CLA	CHC-C1C	3.95	1.47	1.35
34	B	621	LMG	O8-C28	3.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	CHC-C1C	3.96	1.47	1.35
27	b	601	SQD	O48-C23	3.96	1.45	1.33
34	c	501	LMG	O8-C28	3.96	1.45	1.33
24	B	604	CLA	CHC-C1C	3.96	1.47	1.35
24	B	607	CLA	O2A-CGA	3.96	1.45	1.33
36	h	102	DGD	O1G-C1A	3.96	1.45	1.33
24	b	612	CLA	C3D-C2D	3.96	1.49	1.40
24	b	618	CLA	O2A-CGA	3.96	1.45	1.33
24	C	504	CLA	CHC-C1C	3.96	1.47	1.35
24	c	514	CLA	C3D-C2D	3.96	1.49	1.40
27	A	416	SQD	O47-C7	3.96	1.46	1.34
24	c	511	CLA	CHC-C1C	3.96	1.47	1.35
25	d	403	PHO	O2A-CGA	3.97	1.45	1.33
24	B	609	CLA	CHC-C1C	3.97	1.47	1.35
34	Z	101	LMG	O7-C10	3.97	1.46	1.34
24	B	607	CLA	C3D-C2D	3.97	1.49	1.40
24	C	503	CLA	O2A-CGA	3.97	1.45	1.33
24	C	514	CLA	CHC-C1C	3.98	1.47	1.35
24	C	505	CLA	C3D-C2D	3.98	1.49	1.40
24	C	505	CLA	O2A-CGA	3.98	1.45	1.33
24	B	611	CLA	OBD-CAD	3.99	1.28	1.22
24	d	404	CLA	OBD-CAD	3.99	1.28	1.22
24	C	513	CLA	C3D-C2D	3.99	1.49	1.40
37	d	410	LHG	O8-C23	3.99	1.45	1.33
25	A	407	PHO	OBD-CAD	3.99	1.29	1.22
24	b	610	CLA	CHC-C1C	3.99	1.47	1.35
24	B	607	CLA	CHC-C1C	4.00	1.47	1.35
24	b	608	CLA	O2A-CGA	4.00	1.45	1.33
24	c	506	CLA	C3D-C2D	4.00	1.49	1.40
24	C	512	CLA	CHC-C1C	4.00	1.47	1.35
24	C	512	CLA	O2A-CGA	4.00	1.45	1.33
24	b	617	CLA	OBD-CAD	4.00	1.28	1.22
24	B	603	CLA	CHC-C1C	4.00	1.47	1.35
37	d	409	LHG	O8-C23	4.00	1.45	1.33
24	b	609	CLA	O2A-CGA	4.01	1.45	1.33
24	a	409	CLA	OBD-CAD	4.01	1.28	1.22
24	B	605	CLA	CHC-C1C	4.01	1.47	1.35
24	c	512	CLA	CHC-C1C	4.01	1.47	1.35
24	b	621	CLA	O2A-CGA	4.01	1.45	1.33
24	a	406	CLA	OBD-CAD	4.02	1.28	1.22
24	B	612	CLA	CHC-C1C	4.02	1.47	1.35
24	C	506	CLA	CHC-C1C	4.02	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	CHC-C1C	4.02	1.47	1.35
24	B	617	CLA	O2A-CGA	4.02	1.45	1.33
24	b	616	CLA	OBD-CAD	4.02	1.28	1.22
24	C	510	CLA	C3D-C2D	4.02	1.49	1.40
24	b	619	CLA	O2A-CGA	4.02	1.45	1.33
24	c	507	CLA	CHC-C1C	4.02	1.47	1.35
24	b	614	CLA	O2A-CGA	4.03	1.45	1.33
24	c	514	CLA	OBD-CAD	4.03	1.28	1.22
24	b	606	CLA	C3D-C2D	4.03	1.49	1.40
24	b	610	CLA	O2A-CGA	4.03	1.45	1.33
24	d	404	CLA	O2A-CGA	4.03	1.45	1.33
24	C	505	CLA	CHC-C1C	4.03	1.48	1.35
24	b	615	CLA	C3D-C2D	4.04	1.49	1.40
27	b	601	SQD	O47-C7	4.04	1.46	1.34
24	A	406	CLA	CHC-C1C	4.04	1.48	1.35
37	l	102	LHG	O8-C23	4.04	1.45	1.33
36	c	518	DGD	O1G-C1A	4.04	1.45	1.33
24	C	511	CLA	C3D-C2D	4.04	1.49	1.40
24	C	504	CLA	O2A-CGA	4.04	1.45	1.33
24	c	512	CLA	O2A-CGA	4.04	1.45	1.33
24	D	404	CLA	CHC-C1C	4.04	1.48	1.35
24	B	605	CLA	O2D-CGD	4.04	1.43	1.33
24	B	604	CLA	OBD-CAD	4.04	1.28	1.22
24	c	511	CLA	O2A-CGA	4.04	1.45	1.33
24	b	619	CLA	C3D-C2D	4.05	1.49	1.40
24	b	611	CLA	OBD-CAD	4.05	1.28	1.22
24	d	404	CLA	CHC-C1C	4.05	1.48	1.35
27	F	101	SQD	O48-C23	4.06	1.45	1.33
24	b	621	CLA	OBD-CAD	4.06	1.28	1.22
34	b	625	LMG	O8-C28	4.06	1.45	1.33
24	A	405	CLA	CHC-C1C	4.06	1.48	1.35
24	B	610	CLA	O2A-CGA	4.06	1.45	1.33
24	C	514	CLA	O2A-CGA	4.06	1.45	1.33
27	f	101	SQD	O48-C23	4.06	1.45	1.33
24	b	619	CLA	OBD-CAD	4.06	1.28	1.22
24	b	616	CLA	O2A-CGA	4.07	1.45	1.33
24	C	506	CLA	O2A-CGA	4.07	1.45	1.33
34	c	521	LMG	O7-C10	4.07	1.46	1.34
24	c	504	CLA	O2A-CGA	4.08	1.45	1.33
24	b	606	CLA	CHC-C1C	4.08	1.48	1.35
24	C	509	CLA	O2A-CGA	4.08	1.45	1.33
24	C	507	CLA	O2A-CGA	4.08	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	521	LMG	O8-C28	4.08	1.45	1.33
24	b	608	CLA	OBD-CAD	4.09	1.28	1.22
34	C	521	LMG	O8-C28	4.09	1.45	1.33
24	C	502	CLA	C3D-C2D	4.09	1.49	1.40
24	c	510	CLA	CHC-C1C	4.09	1.48	1.35
24	A	409	CLA	CHC-C1C	4.09	1.48	1.35
24	b	615	CLA	CHC-C1C	4.10	1.48	1.35
24	A	405	CLA	C3D-C2D	4.10	1.50	1.40
24	B	615	CLA	CHC-C1C	4.10	1.48	1.35
34	C	521	LMG	O7-C10	4.10	1.46	1.34
24	B	609	CLA	O2A-CGA	4.10	1.45	1.33
24	b	613	CLA	OBD-CAD	4.11	1.28	1.22
24	c	504	CLA	C3D-C2D	4.11	1.50	1.40
24	C	502	CLA	OBD-CAD	4.11	1.28	1.22
27	F	101	SQD	O47-C7	4.11	1.46	1.34
24	B	608	CLA	O2A-CGA	4.12	1.45	1.33
24	C	503	CLA	CHC-C1C	4.12	1.48	1.35
24	c	514	CLA	CHC-C1C	4.12	1.48	1.35
24	c	508	CLA	O2A-CGA	4.13	1.45	1.33
24	B	612	CLA	C3D-C2D	4.13	1.50	1.40
24	C	502	CLA	O2A-CGA	4.13	1.45	1.33
24	B	612	CLA	OBD-CAD	4.13	1.28	1.22
24	b	610	CLA	O2D-CGD	4.13	1.43	1.33
24	B	616	CLA	CHC-C1C	4.13	1.48	1.35
24	B	602	CLA	CHC-C1C	4.13	1.48	1.35
36	C	518	DGD	O1G-C1A	4.13	1.45	1.33
24	a	407	CLA	CHC-C1C	4.14	1.48	1.35
34	c	520	LMG	O8-C28	4.14	1.45	1.33
36	D	407	DGD	O2G-C1B	4.14	1.46	1.34
24	c	503	CLA	O2A-CGA	4.14	1.45	1.33
24	B	614	CLA	OBD-CAD	4.14	1.28	1.22
24	b	608	CLA	CHC-C1C	4.14	1.48	1.35
34	C	501	LMG	O8-C28	4.14	1.45	1.33
24	c	514	CLA	O2A-CGA	4.14	1.45	1.33
24	d	401	CLA	O2A-CGA	4.14	1.45	1.33
24	b	607	CLA	CHC-C1C	4.15	1.48	1.35
24	b	620	CLA	C3D-C2D	4.15	1.50	1.40
27	f	101	SQD	O47-C7	4.15	1.46	1.34
24	b	616	CLA	CHC-C1C	4.15	1.48	1.35
34	C	501	LMG	O7-C10	4.15	1.46	1.34
36	c	519	DGD	O1G-C1A	4.15	1.45	1.33
24	c	505	CLA	CHC-C1C	4.15	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	O2A-CGA	4.15	1.45	1.33
24	A	405	CLA	OBD-CAD	4.16	1.28	1.22
24	c	515	CLA	CHC-C1C	4.16	1.48	1.35
24	c	515	CLA	O2A-CGA	4.16	1.45	1.33
24	c	510	CLA	C3D-C2D	4.16	1.50	1.40
24	D	401	CLA	C3D-C2D	4.16	1.50	1.40
24	C	512	CLA	OBD-CAD	4.17	1.28	1.22
24	b	606	CLA	O2A-CGA	4.17	1.45	1.33
37	E	101	LHG	O8-C23	4.17	1.45	1.33
24	b	611	CLA	CHC-C1C	4.17	1.48	1.35
24	C	508	CLA	O2A-CGA	4.17	1.45	1.33
36	d	407	DGD	O2G-C1B	4.17	1.46	1.34
24	B	604	CLA	O2A-CGA	4.18	1.45	1.33
36	d	407	DGD	O1G-C1A	4.18	1.45	1.33
24	C	509	CLA	C3D-C2D	4.18	1.50	1.40
24	c	503	CLA	OBD-CAD	4.19	1.28	1.22
24	B	616	CLA	OBD-CAD	4.19	1.28	1.22
24	A	409	CLA	C3D-C2D	4.19	1.50	1.40
24	C	513	CLA	O2A-CGA	4.19	1.45	1.33
24	B	606	CLA	O2A-CGA	4.20	1.46	1.33
24	C	506	CLA	OBD-CAD	4.20	1.28	1.22
24	a	407	CLA	O2D-CGD	4.20	1.43	1.33
24	a	407	CLA	OBD-CAD	4.21	1.28	1.22
24	b	617	CLA	CHC-C1C	4.21	1.48	1.35
24	D	403	CLA	O2D-CGD	4.21	1.43	1.33
24	B	616	CLA	C3D-C2D	4.21	1.50	1.40
24	d	401	CLA	C3D-C2D	4.21	1.50	1.40
24	C	507	CLA	C3D-C2D	4.22	1.50	1.40
24	B	613	CLA	CHC-C1C	4.23	1.48	1.35
24	D	403	CLA	OBD-CAD	4.23	1.28	1.22
24	b	616	CLA	C3D-C2D	4.24	1.50	1.40
24	C	511	CLA	OBD-CAD	4.24	1.28	1.22
24	D	404	CLA	OBD-CAD	4.25	1.28	1.22
37	e	101	LHG	O8-C23	4.26	1.46	1.33
24	c	509	CLA	O2A-CGA	4.26	1.46	1.33
24	a	409	CLA	O2A-CGA	4.26	1.46	1.33
24	B	608	CLA	O2D-CGD	4.27	1.44	1.33
24	c	513	CLA	OBD-CAD	4.27	1.28	1.22
24	a	407	CLA	O2A-CGA	4.27	1.46	1.33
24	B	610	CLA	CHC-C1C	4.28	1.48	1.35
27	a	402	SQD	O48-C23	4.28	1.46	1.33
34	C	520	LMG	O8-C28	4.28	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	OBD-CAD	4.29	1.28	1.22
24	C	503	CLA	C3D-C2D	4.29	1.50	1.40
24	b	615	CLA	O2D-CGD	4.29	1.44	1.33
24	b	609	CLA	OBD-CAD	4.30	1.28	1.22
24	c	510	CLA	O2A-CGA	4.30	1.46	1.33
24	C	505	CLA	OBD-CAD	4.30	1.28	1.22
24	B	609	CLA	C3D-C2D	4.31	1.50	1.40
24	B	602	CLA	O2A-CGA	4.31	1.46	1.33
27	A	416	SQD	O48-C23	4.33	1.46	1.33
24	C	510	CLA	O2A-CGA	4.34	1.46	1.33
24	B	610	CLA	O2D-CGD	4.34	1.44	1.33
36	D	407	DGD	O1G-C1A	4.34	1.46	1.33
24	A	409	CLA	OBD-CAD	4.36	1.29	1.22
24	c	515	CLA	OBD-CAD	4.36	1.29	1.22
24	c	510	CLA	OBD-CAD	4.36	1.29	1.22
24	C	508	CLA	OBD-CAD	4.37	1.29	1.22
24	b	610	CLA	OBD-CAD	4.37	1.29	1.22
24	b	607	CLA	OBD-CAD	4.38	1.29	1.22
24	b	615	CLA	OBD-CAD	4.38	1.29	1.22
24	b	607	CLA	C3D-C2D	4.39	1.50	1.40
24	B	616	CLA	O2A-CGA	4.39	1.46	1.33
24	d	401	CLA	O2D-CGD	4.40	1.44	1.33
24	B	603	CLA	OBD-CAD	4.40	1.29	1.22
24	b	613	CLA	O2A-CGA	4.40	1.46	1.33
34	z	101	LMG	O8-C28	4.41	1.46	1.33
24	d	402	CLA	O2D-CGD	4.43	1.44	1.33
24	C	504	CLA	OBD-CAD	4.43	1.29	1.22
24	C	505	CLA	O2D-CGD	4.44	1.44	1.33
24	c	507	CLA	O2D-CGD	4.44	1.44	1.33
24	c	506	CLA	OBD-CAD	4.44	1.29	1.22
24	B	612	CLA	O2D-CGD	4.46	1.44	1.33
24	c	504	CLA	O2D-CGD	4.47	1.44	1.33
24	C	504	CLA	O2D-CGD	4.47	1.44	1.33
24	B	611	CLA	O2D-CGD	4.48	1.44	1.33
24	D	403	CLA	O2A-CGA	4.48	1.46	1.33
24	C	511	CLA	O2D-CGD	4.49	1.44	1.33
24	b	609	CLA	C3C-C2C	4.50	1.46	1.36
25	A	408	PHO	O2D-CGD	4.50	1.44	1.33
24	c	510	CLA	O2D-CGD	4.51	1.44	1.33
24	C	502	CLA	O2D-CGD	4.52	1.44	1.33
24	C	503	CLA	O2D-CGD	4.52	1.44	1.33
24	B	605	CLA	C3C-C2C	4.54	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	OBD-CAD	4.54	1.29	1.22
24	A	405	CLA	O2D-CGD	4.55	1.44	1.33
24	d	402	CLA	O2A-CGA	4.56	1.47	1.33
24	c	507	CLA	OBD-CAD	4.57	1.29	1.22
24	D	404	CLA	O2D-CGD	4.59	1.44	1.33
24	c	508	CLA	O2D-CGD	4.59	1.44	1.33
25	A	407	PHO	O2D-CGD	4.61	1.45	1.33
24	c	505	CLA	O2D-CGD	4.61	1.45	1.33
24	B	610	CLA	OBD-CAD	4.61	1.29	1.22
24	C	508	CLA	O2D-CGD	4.61	1.45	1.33
24	C	514	CLA	O2D-CGD	4.62	1.45	1.33
24	b	612	CLA	O2D-CGD	4.62	1.45	1.33
24	b	608	CLA	O2D-CGD	4.62	1.45	1.33
25	a	408	PHO	CHD-C1D	4.62	1.47	1.38
24	c	511	CLA	OBD-CAD	4.63	1.29	1.22
24	B	617	CLA	OBD-CAD	4.63	1.29	1.22
24	B	613	CLA	O2D-CGD	4.63	1.45	1.33
24	D	401	CLA	O2D-CGD	4.64	1.45	1.33
24	b	620	CLA	OBD-CAD	4.64	1.29	1.22
24	B	603	CLA	O2D-CGD	4.64	1.45	1.33
24	c	509	CLA	O2D-CGD	4.65	1.45	1.33
24	b	611	CLA	O2D-CGD	4.66	1.45	1.33
24	b	619	CLA	O2D-CGD	4.66	1.45	1.33
24	C	513	CLA	O2D-CGD	4.66	1.45	1.33
24	B	609	CLA	O2D-CGD	4.67	1.45	1.33
24	B	614	CLA	O2D-CGD	4.68	1.45	1.33
24	C	506	CLA	O2D-CGD	4.69	1.45	1.33
24	C	514	CLA	OBD-CAD	4.69	1.29	1.22
24	B	616	CLA	C3C-C2C	4.70	1.46	1.36
24	d	404	CLA	O2D-CGD	4.70	1.45	1.33
24	A	409	CLA	O2D-CGD	4.70	1.45	1.33
24	a	409	CLA	O2D-CGD	4.72	1.45	1.33
24	B	604	CLA	O2D-CGD	4.72	1.45	1.33
24	d	401	CLA	OBD-CAD	4.73	1.29	1.22
24	b	620	CLA	O2D-CGD	4.73	1.45	1.33
24	c	503	CLA	O2D-CGD	4.74	1.45	1.33
24	B	615	CLA	O2D-CGD	4.75	1.45	1.33
24	A	406	CLA	O2D-CGD	4.75	1.45	1.33
24	b	617	CLA	O2D-CGD	4.75	1.45	1.33
25	A	408	PHO	CHB-C1B	4.75	1.48	1.38
24	D	403	CLA	C3C-C2C	4.76	1.47	1.36
25	d	403	PHO	O2D-CGD	4.76	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	O2D-CGD	4.76	1.45	1.33
24	C	509	CLA	O2D-CGD	4.76	1.45	1.33
24	C	512	CLA	O2D-CGD	4.76	1.45	1.33
25	d	403	PHO	CHD-C1D	4.77	1.48	1.38
24	c	513	CLA	O2D-CGD	4.79	1.45	1.33
24	b	619	CLA	C3C-C2C	4.79	1.47	1.36
24	c	514	CLA	O2D-CGD	4.80	1.45	1.33
25	A	407	PHO	CHC-C1C	4.81	1.48	1.38
24	b	607	CLA	O2D-CGD	4.81	1.45	1.33
24	b	609	CLA	O2D-CGD	4.82	1.45	1.33
24	C	514	CLA	C3C-C2C	4.82	1.47	1.36
24	c	512	CLA	O2D-CGD	4.82	1.45	1.33
24	B	616	CLA	O2D-CGD	4.83	1.45	1.33
25	a	408	PHO	O2D-CGD	4.84	1.45	1.33
24	C	507	CLA	O2D-CGD	4.84	1.45	1.33
24	B	608	CLA	OBD-CAD	4.84	1.29	1.22
24	B	608	CLA	C3C-C2C	4.85	1.47	1.36
24	a	406	CLA	O2D-CGD	4.85	1.45	1.33
24	B	607	CLA	O2D-CGD	4.86	1.45	1.33
24	d	404	CLA	C3C-C2C	4.86	1.47	1.36
24	b	613	CLA	O2D-CGD	4.86	1.45	1.33
25	A	407	PHO	CHD-C1D	4.86	1.48	1.38
24	b	614	CLA	OBD-CAD	4.87	1.29	1.22
24	c	515	CLA	O2D-CGD	4.89	1.45	1.33
24	A	405	CLA	C3C-C2C	4.90	1.47	1.36
25	A	408	PHO	CHC-C1C	4.90	1.48	1.38
24	C	502	CLA	C3C-C2C	4.90	1.47	1.36
24	b	621	CLA	O2D-CGD	4.91	1.45	1.33
24	D	401	CLA	OBD-CAD	4.92	1.29	1.22
24	b	618	CLA	O2D-CGD	4.92	1.45	1.33
24	B	617	CLA	O2D-CGD	4.92	1.45	1.33
24	c	506	CLA	O2D-CGD	4.94	1.45	1.33
24	C	508	CLA	C3C-C2C	4.94	1.47	1.36
24	c	511	CLA	O2D-CGD	4.95	1.45	1.33
24	b	610	CLA	C3C-C2C	4.95	1.47	1.36
24	B	606	CLA	C3C-C2C	4.95	1.47	1.36
24	B	602	CLA	O2D-CGD	4.97	1.45	1.33
24	B	615	CLA	C3C-C2C	4.98	1.47	1.36
24	b	611	CLA	C3C-C2C	4.99	1.47	1.36
24	b	621	CLA	C3C-C2C	5.00	1.47	1.36
24	B	617	CLA	C3C-C2C	5.00	1.47	1.36
24	b	606	CLA	O2D-CGD	5.01	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C3C-C2C	5.02	1.47	1.36
24	B	606	CLA	O2D-CGD	5.02	1.46	1.33
24	C	510	CLA	O2D-CGD	5.02	1.46	1.33
24	B	614	CLA	C3C-C2C	5.03	1.47	1.36
25	a	408	PHO	CHB-C1B	5.03	1.48	1.38
24	b	616	CLA	C3C-C2C	5.03	1.47	1.36
24	c	508	CLA	C3C-C2C	5.04	1.47	1.36
25	d	403	PHO	CHB-C1B	5.04	1.48	1.38
24	C	512	CLA	C3C-C2C	5.05	1.47	1.36
24	d	401	CLA	C3C-C2C	5.06	1.47	1.36
24	B	613	CLA	C3C-C2C	5.07	1.47	1.36
24	a	407	CLA	C3C-C2C	5.07	1.47	1.36
24	c	513	CLA	C3C-C2C	5.08	1.47	1.36
24	c	507	CLA	C3C-C2C	5.08	1.47	1.36
24	b	612	CLA	C3C-C2C	5.08	1.47	1.36
24	B	603	CLA	C3C-C2C	5.09	1.47	1.36
24	A	406	CLA	C3C-C2C	5.10	1.47	1.36
24	D	401	CLA	C3C-C2C	5.10	1.47	1.36
24	c	515	CLA	C3C-C2C	5.10	1.47	1.36
24	b	614	CLA	O2D-CGD	5.10	1.46	1.33
24	c	505	CLA	C3C-C2C	5.11	1.47	1.36
24	b	608	CLA	C3C-C2C	5.11	1.47	1.36
24	B	610	CLA	C3C-C2C	5.11	1.47	1.36
24	b	615	CLA	C3C-C2C	5.13	1.47	1.36
24	C	507	CLA	C3C-C2C	5.14	1.47	1.36
24	c	507	CLA	C3B-C2B	5.14	1.47	1.40
24	A	406	CLA	OBD-CAD	5.14	1.30	1.22
24	C	505	CLA	C3C-C2C	5.15	1.47	1.36
24	b	614	CLA	C3C-C2C	5.17	1.47	1.36
25	A	407	PHO	CHB-C1B	5.17	1.48	1.38
24	C	511	CLA	C3C-C2C	5.17	1.47	1.36
24	B	616	CLA	C3B-C2B	5.17	1.47	1.40
24	B	604	CLA	C3C-C2C	5.18	1.47	1.36
24	c	510	CLA	C3C-C2C	5.18	1.47	1.36
24	b	607	CLA	C3C-C2C	5.19	1.47	1.36
24	C	513	CLA	C3C-C2C	5.20	1.48	1.36
24	c	509	CLA	C3C-C2C	5.22	1.48	1.36
24	C	510	CLA	C3C-C2C	5.22	1.48	1.36
24	a	409	CLA	C3C-C2C	5.24	1.48	1.36
24	c	504	CLA	C3C-C2C	5.24	1.48	1.36
24	d	402	CLA	C3C-C2C	5.24	1.48	1.36
24	b	613	CLA	C3C-C2C	5.25	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	C3C-C2C	5.25	1.48	1.36
24	c	514	CLA	C3C-C2C	5.26	1.48	1.36
24	b	618	CLA	C3C-C2C	5.26	1.48	1.36
24	D	404	CLA	C3C-C2C	5.26	1.48	1.36
24	b	617	CLA	C3C-C2C	5.27	1.48	1.36
24	a	406	CLA	C3C-C2C	5.27	1.48	1.36
24	c	503	CLA	C3C-C2C	5.29	1.48	1.36
24	b	620	CLA	C3C-C2C	5.29	1.48	1.36
24	C	504	CLA	C3C-C2C	5.30	1.48	1.36
24	c	511	CLA	C3C-C2C	5.30	1.48	1.36
24	C	503	CLA	C3C-C2C	5.31	1.48	1.36
24	c	506	CLA	C3C-C2C	5.34	1.48	1.36
24	C	506	CLA	C3C-C2C	5.34	1.48	1.36
25	d	403	PHO	CHC-C1C	5.35	1.49	1.38
24	C	509	CLA	C3C-C2C	5.37	1.48	1.36
24	B	611	CLA	C3C-C2C	5.37	1.48	1.36
24	B	602	CLA	C3C-C2C	5.41	1.48	1.36
24	B	612	CLA	C3C-C2C	5.42	1.48	1.36
25	a	408	PHO	CHC-C1C	5.42	1.49	1.38
24	b	610	CLA	C3B-C2B	5.46	1.47	1.40
25	d	403	PHO	C3C-C2C	5.47	1.48	1.36
25	A	408	PHO	C3C-C2C	5.49	1.48	1.36
24	A	409	CLA	C3C-C2C	5.51	1.48	1.36
24	B	609	CLA	C3C-C2C	5.52	1.48	1.36
24	b	606	CLA	C3C-C2C	5.57	1.48	1.36
24	B	610	CLA	C3B-C2B	5.58	1.47	1.40
24	c	504	CLA	C3B-C2B	5.60	1.47	1.40
24	c	505	CLA	C3B-C2B	5.66	1.47	1.40
24	B	606	CLA	C3B-C2B	5.67	1.47	1.40
24	a	409	CLA	C3B-C2B	5.73	1.47	1.40
24	d	404	CLA	C3B-C2B	5.74	1.47	1.40
24	C	512	CLA	C3B-C2B	5.79	1.47	1.40
24	B	615	CLA	C3B-C2B	5.81	1.48	1.40
25	a	408	PHO	C3C-C2C	5.83	1.49	1.36
24	b	614	CLA	C3B-C2B	5.83	1.48	1.40
25	A	407	PHO	C3C-C2C	5.84	1.49	1.36
25	A	407	PHO	C3B-C2B	5.91	1.49	1.36
25	a	408	PHO	C3B-C2B	5.94	1.49	1.36
24	b	616	CLA	C3B-C2B	5.96	1.48	1.40
24	C	505	CLA	C3B-C2B	5.97	1.48	1.40
25	A	408	PHO	C3B-C2B	5.99	1.49	1.36
24	b	612	CLA	C3B-C2B	6.03	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	C3B-C2B	6.05	1.48	1.40
24	A	406	CLA	C3B-C2B	6.08	1.48	1.40
24	c	509	CLA	C3B-C2B	6.08	1.48	1.40
25	d	403	PHO	C3B-C2B	6.08	1.49	1.36
24	C	507	CLA	C3B-C2B	6.08	1.48	1.40
24	a	407	CLA	C3B-C2B	6.09	1.48	1.40
24	c	515	CLA	C3B-C2B	6.09	1.48	1.40
24	D	403	CLA	C3B-C2B	6.13	1.48	1.40
24	c	514	CLA	C3B-C2B	6.15	1.48	1.40
24	b	613	CLA	C3B-C2B	6.16	1.48	1.40
24	c	506	CLA	C3B-C2B	6.18	1.48	1.40
24	c	508	CLA	C3B-C2B	6.19	1.48	1.40
24	c	512	CLA	C3B-C2B	6.21	1.48	1.40
24	D	404	CLA	C3B-C2B	6.21	1.48	1.40
24	b	617	CLA	C3B-C2B	6.22	1.48	1.40
24	C	503	CLA	C3B-C2B	6.23	1.48	1.40
24	C	510	CLA	C3B-C2B	6.25	1.48	1.40
24	a	406	CLA	C3B-C2B	6.25	1.48	1.40
24	B	607	CLA	C3B-C2B	6.25	1.48	1.40
24	c	513	CLA	C3B-C2B	6.27	1.48	1.40
24	B	611	CLA	C3B-C2B	6.28	1.48	1.40
24	b	609	CLA	C3B-C2B	6.31	1.48	1.40
24	b	611	CLA	C3B-C2B	6.32	1.48	1.40
24	C	502	CLA	C3B-C2B	6.32	1.48	1.40
24	b	620	CLA	C3B-C2B	6.34	1.48	1.40
24	B	608	CLA	C3B-C2B	6.34	1.48	1.40
24	b	606	CLA	C3B-C2B	6.36	1.48	1.40
24	b	607	CLA	C3B-C2B	6.39	1.48	1.40
24	C	514	CLA	C3B-C2B	6.39	1.48	1.40
24	C	509	CLA	C3B-C2B	6.40	1.48	1.40
24	d	401	CLA	C3B-C2B	6.42	1.48	1.40
24	d	402	CLA	C3B-C2B	6.42	1.48	1.40
24	D	401	CLA	C3B-C2B	6.44	1.48	1.40
24	b	619	CLA	C3B-C2B	6.49	1.48	1.40
24	b	615	CLA	C3B-C2B	6.50	1.48	1.40
24	B	605	CLA	C3B-C2B	6.52	1.48	1.40
24	C	513	CLA	C3B-C2B	6.52	1.48	1.40
24	C	506	CLA	C3B-C2B	6.53	1.48	1.40
24	B	602	CLA	C3B-C2B	6.54	1.48	1.40
24	c	503	CLA	C3B-C2B	6.56	1.49	1.40
24	B	604	CLA	C3B-C2B	6.57	1.49	1.40
24	b	608	CLA	C3B-C2B	6.57	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3B-C2B	6.58	1.49	1.40
24	B	612	CLA	C3B-C2B	6.59	1.49	1.40
24	B	603	CLA	C3B-C2B	6.64	1.49	1.40
24	B	614	CLA	C3B-C2B	6.66	1.49	1.40
24	B	613	CLA	C3B-C2B	6.66	1.49	1.40
24	b	621	CLA	C3B-C2B	6.67	1.49	1.40
24	C	504	CLA	C3B-C2B	6.73	1.49	1.40
24	b	618	CLA	C3B-C2B	6.74	1.49	1.40
24	c	510	CLA	C3B-C2B	6.76	1.49	1.40
24	B	609	CLA	C3B-C2B	6.79	1.49	1.40
24	A	405	CLA	C3B-C2B	6.84	1.49	1.40
24	C	511	CLA	C3B-C2B	6.94	1.49	1.40
24	B	617	CLA	C3B-C2B	7.00	1.49	1.40
24	c	511	CLA	C3B-C2B	7.01	1.49	1.40

All (1991) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	616	CLA	CHD-C4C-C3C	-6.38	115.08	124.94
24	B	610	CLA	CHD-C4C-C3C	-6.37	115.09	124.94
24	b	618	CLA	CHD-C4C-C3C	-6.34	115.14	124.94
24	b	612	CLA	CHD-C4C-C3C	-6.23	115.31	124.94
24	C	508	CLA	CHD-C4C-C3C	-6.20	115.36	124.94
24	B	607	CLA	CHD-C4C-C3C	-6.19	115.37	124.94
24	b	610	CLA	CHD-C4C-C3C	-6.17	115.40	124.94
24	A	409	CLA	CHD-C4C-C3C	-6.12	115.49	124.94
24	B	605	CLA	CHD-C4C-C3C	-6.07	115.56	124.94
24	b	606	CLA	CHD-C4C-C3C	-6.06	115.57	124.94
24	B	606	CLA	CHD-C4C-C3C	-6.04	115.61	124.94
24	c	510	CLA	CHD-C4C-C3C	-6.03	115.61	124.94
24	B	604	CLA	CHD-C4C-C3C	-6.01	115.64	124.94
24	B	609	CLA	CHD-C4C-C3C	-5.95	115.75	124.94
24	b	611	CLA	CHD-C4C-C3C	-5.95	115.75	124.94
24	c	505	CLA	CHD-C4C-C3C	-5.89	115.84	124.94
24	c	509	CLA	CHD-C4C-C3C	-5.88	115.85	124.94
24	B	612	CLA	CHD-C4C-C3C	-5.86	115.88	124.94
24	b	609	CLA	CHD-C4C-C3C	-5.86	115.89	124.94
24	C	504	CLA	CHD-C4C-C3C	-5.83	115.93	124.94
24	c	512	CLA	CHD-C4C-C3C	-5.79	115.99	124.94
24	b	617	CLA	CHD-C4C-C3C	-5.79	115.99	124.94
24	d	404	CLA	CHD-C4C-C3C	-5.77	116.02	124.94
24	D	404	CLA	CHD-C4C-C3C	-5.77	116.02	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	607	CLA	CHD-C4C-C3C	-5.76	116.03	124.94
24	B	602	CLA	CHD-C4C-C3C	-5.74	116.07	124.94
24	b	615	CLA	CHD-C4C-C3C	-5.73	116.09	124.94
24	C	511	CLA	CHD-C4C-C3C	-5.73	116.09	124.94
24	B	603	CLA	CHD-C4C-C3C	-5.65	116.21	124.94
24	B	615	CLA	CHD-C4C-C3C	-5.63	116.24	124.94
24	a	407	CLA	CHD-C4C-C3C	-5.62	116.25	124.94
24	B	617	CLA	CHD-C4C-C3C	-5.61	116.27	124.94
24	C	503	CLA	CHD-C4C-C3C	-5.61	116.28	124.94
24	B	616	CLA	CHD-C4C-C3C	-5.61	116.28	124.94
24	C	512	CLA	CHD-C4C-C3C	-5.59	116.30	124.94
24	C	513	CLA	CHD-C4C-C3C	-5.59	116.30	124.94
24	D	403	CLA	CHD-C4C-C3C	-5.51	116.43	124.94
24	C	506	CLA	CHD-C4C-C3C	-5.47	116.49	124.94
24	b	614	CLA	CHD-C4C-C3C	-5.46	116.51	124.94
24	c	504	CLA	CHD-C4C-C3C	-5.44	116.53	124.94
24	B	611	CLA	CHD-C4C-C3C	-5.42	116.57	124.94
24	C	507	CLA	CHD-C4C-C3C	-5.37	116.64	124.94
24	B	608	CLA	CHD-C4C-C3C	-5.34	116.68	124.94
24	a	409	CLA	CHD-C4C-C3C	-5.34	116.68	124.94
24	b	608	CLA	CHD-C4C-C3C	-5.34	116.69	124.94
24	c	513	CLA	CHD-C4C-C3C	-5.34	116.69	124.94
24	c	514	CLA	CHD-C4C-C3C	-5.31	116.73	124.94
24	c	503	CLA	CHD-C4C-C3C	-5.31	116.73	124.94
24	c	506	CLA	CHD-C4C-C3C	-5.31	116.74	124.94
24	b	620	CLA	CHD-C4C-C3C	-5.30	116.75	124.94
26	y	101	BCR	C33-C5-C6	-5.30	119.40	124.61
24	c	511	CLA	CHD-C4C-C3C	-5.29	116.76	124.94
24	C	514	CLA	CHD-C4C-C3C	-5.29	116.77	124.94
24	c	508	CLA	CHD-C4C-C3C	-5.28	116.78	124.94
24	C	510	CLA	CHD-C4C-C3C	-5.26	116.81	124.94
24	C	502	CLA	CHD-C4C-C3C	-5.26	116.81	124.94
24	c	515	CLA	CHD-C4C-C3C	-5.26	116.81	124.94
24	b	613	CLA	CHD-C4C-C3C	-5.19	116.93	124.94
25	A	408	PHO	C3D-C2D-C1D	-5.10	97.58	105.77
24	C	509	CLA	CHD-C4C-C3C	-5.05	117.14	124.94
24	d	402	CLA	CHD-C4C-C3C	-5.04	117.15	124.94
26	Y	101	BCR	C33-C5-C6	-5.02	119.68	124.61
24	c	507	CLA	CHD-C4C-C3C	-5.02	117.19	124.94
24	B	614	CLA	CHD-C4C-C3C	-4.99	117.23	124.94
24	A	406	CLA	CHD-C4C-C3C	-4.94	117.30	124.94
25	a	408	PHO	C3D-C2D-C1D	-4.94	97.84	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	622	BCR	C33-C5-C6	-4.93	119.77	124.61
24	b	619	CLA	CHD-C4C-C3C	-4.92	117.33	124.94
26	D	405	BCR	C24-C23-C22	-4.91	118.73	126.22
26	D	405	BCR	C38-C26-C25	-4.89	119.80	124.61
24	d	401	CLA	CHD-C4C-C3C	-4.89	117.39	124.94
24	b	621	CLA	CHD-C4C-C3C	-4.85	117.44	124.94
25	d	403	PHO	C3D-C2D-C1D	-4.84	98.00	105.77
26	d	405	BCR	C38-C26-C25	-4.82	119.87	124.61
24	B	613	CLA	CHD-C4C-C3C	-4.81	117.51	124.94
24	A	405	CLA	CHD-C4C-C3C	-4.81	117.51	124.94
38	e	102	HEM	CBA-CAA-C2A	-4.76	103.99	112.53
32	A	419	PL9	C32-C33-C34	-4.76	117.42	127.76
26	H	101	BCR	C38-C26-C25	-4.73	119.96	124.61
24	D	401	CLA	CHD-C4C-C3C	-4.72	117.65	124.94
24	a	406	CLA	CHD-C4C-C3C	-4.70	117.68	124.94
24	C	505	CLA	CHD-C4C-C3C	-4.63	117.79	124.94
26	C	515	BCR	C33-C5-C6	-4.60	120.09	124.61
26	D	405	BCR	C7-C8-C9	-4.52	119.33	126.22
26	c	526	BCR	C33-C5-C6	-4.44	120.24	124.61
26	B	618	BCR	C33-C5-C6	-4.43	120.25	124.61
26	d	405	BCR	C33-C5-C6	-4.43	120.25	124.61
26	K	101	BCR	C33-C5-C6	-4.36	120.32	124.61
26	T	102	BCR	C33-C5-C6	-4.33	120.35	124.61
26	D	405	BCR	C33-C5-C6	-4.32	120.37	124.61
25	a	408	PHO	C4C-C3C-C2C	-4.28	102.04	106.81
26	k	103	BCR	C24-C23-C22	-4.25	119.73	126.22
25	A	407	PHO	C3D-C2D-C1D	-4.24	98.96	105.77
24	D	401	CLA	C1C-C2C-C3C	-4.24	101.84	106.91
24	b	609	CLA	O1D-CGD-CBD	-4.13	118.70	124.62
32	A	419	PL9	C27-C28-C29	-4.12	118.80	127.76
26	h	101	BCR	C38-C26-C25	-4.11	120.57	124.61
32	a	416	PL9	C22-C23-C24	-4.06	118.92	127.76
26	B	620	BCR	C38-C26-C25	-4.02	120.66	124.61
32	a	416	PL9	C17-C18-C19	-4.00	119.06	127.76
26	c	516	BCR	C7-C8-C9	-4.00	120.12	126.22
26	t	101	BCR	C33-C5-C6	-4.00	120.68	124.61
26	y	101	BCR	C15-C14-C13	-3.99	121.44	127.20
24	c	503	CLA	O2D-CGD-O1D	-3.97	115.60	123.79
32	A	419	PL9	C22-C23-C24	-3.95	119.17	127.76
26	C	515	BCR	C38-C26-C25	-3.95	120.73	124.61
26	d	405	BCR	C15-C14-C13	-3.95	121.50	127.20
26	Y	101	BCR	C38-C26-C25	-3.94	120.74	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	416	PL9	C32-C33-C34	-3.93	119.22	127.76
26	C	516	BCR	C7-C8-C9	-3.92	120.24	126.22
24	c	505	CLA	C1D-CHD-C4C	-3.91	116.68	122.60
26	c	516	BCR	C38-C26-C25	-3.89	120.79	124.61
24	b	609	CLA	C1C-C2C-C3C	-3.88	102.26	106.91
24	C	510	CLA	O2D-CGD-O1D	-3.88	115.77	123.79
24	C	503	CLA	O2D-CGD-O1D	-3.87	115.79	123.79
26	d	405	BCR	C7-C8-C9	-3.87	120.31	126.22
24	B	607	CLA	C1D-CHD-C4C	-3.84	116.78	122.60
24	b	610	CLA	O2D-CGD-O1D	-3.82	115.91	123.79
32	A	419	PL9	C37-C38-C39	-3.82	119.46	127.76
24	C	511	CLA	O1D-CGD-CBD	-3.81	119.16	124.62
24	A	405	CLA	C1C-C2C-C3C	-3.81	102.35	106.91
24	d	402	CLA	O2D-CGD-O1D	-3.80	115.95	123.79
24	b	608	CLA	C1D-CHD-C4C	-3.78	116.89	122.60
24	B	614	CLA	C1C-C2C-C3C	-3.77	102.40	106.91
26	C	515	BCR	C7-C8-C9	-3.76	120.48	126.22
32	a	416	PL9	C37-C38-C39	-3.75	119.60	127.76
38	V	203	HEM	C3B-CAB-CBB	-3.75	118.70	124.46
25	a	408	PHO	O1D-CGD-CBD	-3.75	119.25	124.62
25	A	407	PHO	CHC-C1C-C2C	-3.75	117.14	125.61
34	c	501	LMG	C8-O7-C10	-3.74	108.93	117.89
24	B	605	CLA	C1C-C2C-C3C	-3.73	102.44	106.91
24	C	505	CLA	C1C-C2C-C3C	-3.72	102.46	106.91
24	b	610	CLA	C1C-C2C-C3C	-3.71	102.47	106.91
24	D	401	CLA	CAA-C2A-C3A	-3.68	102.65	113.22
24	c	511	CLA	C1D-CHD-C4C	-3.67	117.04	122.60
27	a	411	SQD	C1-O5-C5	-3.67	106.62	113.75
24	C	504	CLA	C1D-CHD-C4C	-3.67	117.05	122.60
24	a	406	CLA	C1C-C2C-C3C	-3.66	102.53	106.91
26	k	103	BCR	C33-C5-C6	-3.65	121.02	124.61
34	c	501	LMG	C7-O1-C1	-3.65	106.15	113.82
24	d	401	CLA	C1C-C2C-C3C	-3.64	102.55	106.91
24	d	401	CLA	CHC-C1C-C2C	-3.64	116.77	126.35
32	D	406	PL9	C42-C43-C44	-3.64	119.85	127.76
24	c	504	CLA	O2D-CGD-O1D	-3.62	116.31	123.79
24	b	619	CLA	C1C-C2C-C3C	-3.62	102.58	106.91
24	c	509	CLA	O1D-CGD-CBD	-3.62	119.44	124.62
24	b	608	CLA	O2A-CGA-O1A	-3.62	114.16	123.49
24	B	608	CLA	C1C-C2C-C3C	-3.61	102.58	106.91
24	c	514	CLA	C1C-C2C-C3C	-3.59	102.61	106.91
24	C	507	CLA	C1C-C2C-C3C	-3.59	102.61	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C3B-CAB-CBB	-3.57	119.00	126.32
24	c	515	CLA	C3B-CAB-CBB	-3.57	119.00	126.32
24	c	503	CLA	C1C-C2C-C3C	-3.57	102.64	106.91
26	d	405	BCR	C24-C23-C22	-3.56	120.79	126.22
24	B	615	CLA	O2D-CGD-O1D	-3.56	116.44	123.79
26	k	103	BCR	C38-C26-C25	-3.55	121.11	124.61
32	a	416	PL9	C27-C28-C29	-3.55	120.05	127.76
24	b	617	CLA	C4C-C3C-C2C	-3.54	101.20	106.94
26	A	410	BCR	C33-C5-C6	-3.54	121.13	124.61
24	B	606	CLA	C1C-C2C-C3C	-3.53	102.69	106.91
24	b	614	CLA	C1C-C2C-C3C	-3.53	102.69	106.91
32	a	416	PL9	C42-C43-C44	-3.52	120.11	127.76
24	A	406	CLA	C1C-C2C-C3C	-3.51	102.70	106.91
24	c	506	CLA	C1C-C2C-C3C	-3.51	102.70	106.91
25	d	403	PHO	C4C-C3C-C2C	-3.51	102.89	106.81
24	b	620	CLA	O2D-CGD-O1D	-3.51	116.54	123.79
24	b	608	CLA	O2D-CGD-O1D	-3.51	116.55	123.79
24	c	512	CLA	O1D-CGD-CBD	-3.50	119.60	124.62
24	c	511	CLA	O2D-CGD-O1D	-3.50	116.56	123.79
24	d	402	CLA	C1C-C2C-C3C	-3.49	102.74	106.91
25	A	407	PHO	C4C-C3C-C2C	-3.49	102.92	106.81
24	b	608	CLA	CAA-C2A-C3A	-3.49	103.19	113.22
24	B	615	CLA	C1C-C2C-C3C	-3.48	102.75	106.91
24	b	616	CLA	C1D-CHD-C4C	-3.47	117.35	122.60
24	b	607	CLA	C1D-CHD-C4C	-3.47	117.35	122.60
25	A	408	PHO	C4C-C3C-C2C	-3.47	102.94	106.81
24	B	610	CLA	C1D-CHD-C4C	-3.46	117.36	122.60
24	b	619	CLA	CHC-C1C-C2C	-3.46	117.25	126.35
24	b	618	CLA	C1C-C2C-C3C	-3.45	102.79	106.91
24	a	406	CLA	CHC-C1C-C2C	-3.44	117.30	126.35
24	B	609	CLA	C1C-C2C-C3C	-3.44	102.79	106.91
24	a	409	CLA	C1D-CHD-C4C	-3.43	117.41	122.60
24	B	616	CLA	C3B-CAB-CBB	-3.43	119.30	126.32
24	C	502	CLA	O2D-CGD-O1D	-3.43	116.71	123.79
26	d	405	BCR	C3-C4-C5	-3.42	108.44	113.87
27	a	411	SQD	C1-C2-C3	-3.42	103.23	109.97
24	C	506	CLA	C1D-CHD-C4C	-3.42	117.43	122.60
24	B	615	CLA	O2A-CGA-O1A	-3.42	114.67	123.49
24	c	513	CLA	C1D-CHD-C4C	-3.42	117.43	122.60
24	D	404	CLA	O2D-CGD-O1D	-3.42	116.74	123.79
24	D	401	CLA	CHC-C1C-C2C	-3.41	117.38	126.35
24	a	409	CLA	C3B-CAB-CBB	-3.40	119.36	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	O2D-CGD-O1D	-3.40	116.77	123.79
24	C	513	CLA	C1C-C2C-C3C	-3.40	102.84	106.91
24	B	603	CLA	CAA-C2A-C3A	-3.40	103.45	113.22
32	A	419	PL9	C42-C43-C44	-3.39	120.39	127.76
24	c	509	CLA	C1C-C2C-C3C	-3.39	102.85	106.91
24	b	608	CLA	C1C-C2C-C3C	-3.37	102.87	106.91
26	b	624	BCR	C38-C26-C25	-3.37	121.29	124.61
26	b	622	BCR	C7-C8-C9	-3.37	121.08	126.22
24	a	406	CLA	C1D-CHD-C4C	-3.36	117.52	122.60
24	b	621	CLA	O1D-CGD-CBD	-3.36	119.81	124.62
24	A	409	CLA	C1C-C2C-C3C	-3.35	102.90	106.91
24	C	511	CLA	C1D-CHD-C4C	-3.35	117.54	122.60
24	a	409	CLA	O2D-CGD-O1D	-3.34	116.89	123.79
24	C	505	CLA	O2D-CGD-O1D	-3.34	116.89	123.79
24	b	619	CLA	O2D-CGD-O1D	-3.34	116.90	123.79
24	B	613	CLA	C4C-C3C-C2C	-3.34	101.53	106.94
24	b	613	CLA	C1C-C2C-C3C	-3.33	102.92	106.91
24	B	606	CLA	C1D-CHD-C4C	-3.33	117.56	122.60
36	C	519	DGD	O3G-C3G-C2G	-3.33	103.07	110.99
24	b	621	CLA	CHC-C1C-C2C	-3.33	117.60	126.35
24	c	508	CLA	C1D-CHD-C4C	-3.32	117.58	122.60
24	B	617	CLA	O1D-CGD-CBD	-3.31	119.87	124.62
25	d	403	PHO	CHC-C1C-C2C	-3.31	118.11	125.61
24	b	607	CLA	CAA-C2A-C3A	-3.31	103.69	113.22
24	C	509	CLA	C1C-C2C-C3C	-3.31	102.95	106.91
24	A	405	CLA	CAA-C2A-C3A	-3.31	103.70	113.22
24	B	609	CLA	C1D-CHD-C4C	-3.31	117.60	122.60
24	B	604	CLA	C1C-C2C-C3C	-3.30	102.96	106.91
24	c	513	CLA	C1C-C2C-C3C	-3.30	102.97	106.91
24	B	617	CLA	CHC-C1C-C2C	-3.29	117.69	126.35
24	D	403	CLA	C1C-C2C-C3C	-3.29	102.97	106.91
24	c	510	CLA	C1C-C2C-C3C	-3.29	102.97	106.91
24	B	604	CLA	C1D-CHD-C4C	-3.28	117.63	122.60
24	C	508	CLA	C1D-CHD-C4C	-3.28	117.64	122.60
24	B	615	CLA	C3B-CAB-CBB	-3.28	119.61	126.32
24	a	409	CLA	CHC-C1C-C2C	-3.28	117.73	126.35
27	a	411	SQD	C45-O47-C7	-3.27	110.04	117.89
25	d	403	PHO	O2D-CGD-O1D	-3.27	117.04	123.79
24	c	508	CLA	CHC-C1C-C2C	-3.27	117.75	126.35
24	c	512	CLA	C1C-C2C-C3C	-3.27	103.00	106.91
24	B	612	CLA	O2D-CGD-O1D	-3.27	117.04	123.79
32	a	416	PL9	C7-C3-C2	-3.26	120.71	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	510	CLA	O2D-CGD-O1D	-3.26	117.06	123.79
24	C	513	CLA	C3B-CAB-CBB	-3.26	119.66	126.32
24	B	604	CLA	CAA-C2A-C3A	-3.26	103.86	113.22
24	A	406	CLA	CBC-CAC-C3C	-3.25	102.47	112.39
24	c	513	CLA	CHC-C1C-C2C	-3.25	117.80	126.35
24	C	509	CLA	CHC-C1C-C2C	-3.25	117.81	126.35
24	C	508	CLA	O1D-CGD-CBD	-3.24	119.97	124.62
24	C	506	CLA	O2D-CGD-O1D	-3.24	117.09	123.79
27	A	411	SQD	C1-C2-C3	-3.24	103.58	109.97
24	a	407	CLA	C1D-CHD-C4C	-3.24	117.70	122.60
24	b	607	CLA	O2D-CGD-O1D	-3.24	117.10	123.79
24	c	504	CLA	C1C-C2C-C3C	-3.23	103.04	106.91
24	C	513	CLA	O1D-CGD-CBD	-3.23	119.99	124.62
24	b	612	CLA	C1D-CHD-C4C	-3.23	117.72	122.60
24	a	406	CLA	O2A-CGA-O1A	-3.22	115.17	123.49
32	a	416	PL9	C7-C8-C9	-3.22	121.25	126.70
24	B	614	CLA	CHC-C1C-C2C	-3.21	117.90	126.35
24	C	509	CLA	O2A-CGA-O1A	-3.21	115.21	123.49
24	C	503	CLA	C1C-C2C-C3C	-3.21	103.07	106.91
24	b	612	CLA	C1C-C2C-C3C	-3.20	103.08	106.91
25	A	408	PHO	C4D-ND-C1D	-3.20	101.18	107.05
24	c	515	CLA	C1C-C2C-C3C	-3.20	103.08	106.91
24	b	611	CLA	C1D-CHD-C4C	-3.19	117.77	122.60
24	b	615	CLA	CAA-C2A-C3A	-3.19	104.05	113.22
26	D	405	BCR	C28-C27-C26	-3.19	108.81	113.87
24	B	607	CLA	C1C-C2C-C3C	-3.19	103.10	106.91
24	B	603	CLA	CHC-C1C-C2C	-3.18	117.98	126.35
25	A	407	PHO	O1D-CGD-CBD	-3.18	120.06	124.62
26	b	623	BCR	C38-C26-C25	-3.18	121.48	124.61
24	C	508	CLA	C1C-C2C-C3C	-3.18	103.11	106.91
24	c	511	CLA	C1C-C2C-C3C	-3.18	103.11	106.91
26	C	516	BCR	C24-C23-C22	-3.17	121.38	126.22
25	A	408	PHO	CHC-C1C-C2C	-3.17	118.44	125.61
24	B	610	CLA	C1C-C2C-C3C	-3.17	103.12	106.91
24	b	620	CLA	C1C-C2C-C3C	-3.17	103.12	106.91
24	b	606	CLA	C1C-C2C-C3C	-3.16	103.13	106.91
24	A	406	CLA	CAA-C2A-C3A	-3.16	104.14	113.22
37	D	408	LHG	O8-C23-O10	-3.16	115.34	123.49
24	C	511	CLA	C1C-C2C-C3C	-3.16	103.13	106.91
27	A	411	SQD	C45-O47-C7	-3.16	110.32	117.89
24	B	617	CLA	C4C-C3C-C2C	-3.15	101.84	106.94
24	b	607	CLA	C4C-C3C-C2C	-3.15	101.84	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	C1D-CHD-C4C	-3.15	117.84	122.60
32	A	419	PL9	C7-C3-C2	-3.15	120.81	123.42
24	C	507	CLA	CHC-C1C-C2C	-3.14	118.08	126.35
24	C	510	CLA	C1C-C2C-C3C	-3.14	103.15	106.91
24	a	409	CLA	C1C-C2C-C3C	-3.14	103.15	106.91
24	b	610	CLA	OBD-CAD-C3D	-3.14	121.96	128.35
24	C	506	CLA	C1C-C2C-C3C	-3.13	103.16	106.91
24	b	615	CLA	C1C-C2C-C3C	-3.13	103.16	106.91
24	a	407	CLA	CAA-C2A-C3A	-3.13	104.23	113.22
24	c	514	CLA	CBC-CAC-C3C	-3.12	102.86	112.39
24	C	502	CLA	C1C-C2C-C3C	-3.12	103.18	106.91
24	d	401	CLA	CMA-C3A-C2A	-3.12	100.55	114.35
24	a	406	CLA	CAA-C2A-C3A	-3.11	104.26	113.22
24	D	403	CLA	C4C-C3C-C2C	-3.11	101.89	106.94
25	A	408	PHO	CHD-C1D-C2D	-3.11	118.58	125.61
24	C	503	CLA	O2A-CGA-O1A	-3.11	115.47	123.49
24	B	612	CLA	C1D-CHD-C4C	-3.11	117.90	122.60
24	B	602	CLA	C1C-C2C-C3C	-3.10	103.20	106.91
24	C	504	CLA	C1C-C2C-C3C	-3.10	103.20	106.91
24	b	610	CLA	O2A-CGA-O1A	-3.10	115.49	123.49
24	B	611	CLA	C4C-C3C-C2C	-3.10	101.91	106.94
26	c	516	BCR	C31-C1-C6	-3.09	105.46	110.30
24	c	508	CLA	CAA-C2A-C3A	-3.09	104.34	113.22
24	c	510	CLA	C1D-CHD-C4C	-3.09	117.93	122.60
24	B	611	CLA	O2D-CGD-O1D	-3.09	117.42	123.79
24	b	618	CLA	CHC-C1C-C2C	-3.09	118.23	126.35
26	y	101	BCR	C28-C27-C26	-3.08	108.97	113.87
24	C	514	CLA	C3B-CAB-CBB	-3.08	120.01	126.32
24	c	504	CLA	CHC-C1C-C2C	-3.08	118.24	126.35
24	b	612	CLA	CAA-C2A-C3A	-3.08	104.37	113.22
24	b	620	CLA	CHC-C1C-C2C	-3.08	118.26	126.35
24	c	508	CLA	C1C-C2C-C3C	-3.07	103.23	106.91
24	B	602	CLA	O1D-CGD-CBD	-3.07	120.22	124.62
24	C	503	CLA	C3B-CAB-CBB	-3.07	120.03	126.32
24	B	603	CLA	C4C-C3C-C2C	-3.07	101.96	106.94
24	b	618	CLA	C1D-CHD-C4C	-3.07	117.96	122.60
32	A	419	PL9	C7-C8-C9	-3.07	121.50	126.70
24	b	610	CLA	C1D-CHD-C4C	-3.06	117.96	122.60
24	D	404	CLA	C1C-C2C-C3C	-3.06	103.24	106.91
26	H	101	BCR	C7-C8-C9	-3.06	121.55	126.22
24	B	617	CLA	C1D-CHD-C4C	-3.06	117.97	122.60
24	C	506	CLA	CHC-C1C-C2C	-3.05	118.32	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	406	PL9	C37-C38-C39	-3.05	121.13	127.76
24	b	611	CLA	O2D-CGD-O1D	-3.05	117.50	123.79
24	b	619	CLA	C3B-CAB-CBB	-3.05	120.08	126.32
24	d	404	CLA	C1C-C2C-C3C	-3.05	103.27	106.91
24	B	606	CLA	O2D-CGD-O1D	-3.04	117.50	123.79
24	C	514	CLA	C1D-CHD-C4C	-3.04	118.00	122.60
24	B	607	CLA	C3B-CAB-CBB	-3.04	120.10	126.32
24	B	603	CLA	C1D-CHD-C4C	-3.04	118.00	122.60
24	B	616	CLA	C4C-C3C-C2C	-3.03	102.03	106.94
24	B	616	CLA	CHC-C1C-C2C	-3.03	118.38	126.35
24	A	406	CLA	C1D-CHD-C4C	-3.03	118.02	122.60
24	C	513	CLA	C1D-CHD-C4C	-3.03	118.02	122.60
24	c	506	CLA	C3B-CAB-CBB	-3.02	120.13	126.32
24	a	407	CLA	C1C-C2C-C3C	-3.02	103.29	106.91
24	b	614	CLA	C1D-CHD-C4C	-3.02	118.03	122.60
24	b	615	CLA	C1D-CHD-C4C	-3.02	118.03	122.60
24	B	611	CLA	CAA-C2A-C3A	-3.02	104.53	113.22
24	b	618	CLA	C4C-C3C-C2C	-3.02	102.04	106.94
24	C	512	CLA	CHC-C1C-C2C	-3.02	118.41	126.35
24	C	512	CLA	C1C-C2C-C3C	-3.02	103.30	106.91
24	C	510	CLA	CHC-C1C-C2C	-3.02	118.42	126.35
24	C	509	CLA	O2D-CGD-O1D	-3.01	117.57	123.79
38	E	103	HEM	CBD-CAD-C3D	-3.01	104.79	113.55
38	E	103	HEM	CBA-CAA-C2A	-3.01	107.13	112.53
24	b	614	CLA	O2D-CGD-O1D	-3.01	117.57	123.79
24	b	616	CLA	CHC-C1C-C2C	-3.01	118.44	126.35
24	b	613	CLA	C3B-CAB-CBB	-3.01	120.17	126.32
24	c	503	CLA	CHC-C1C-C2C	-3.01	118.45	126.35
24	B	604	CLA	C4C-C3C-C2C	-3.00	102.07	106.94
24	c	507	CLA	C4C-C3C-C2C	-3.00	102.07	106.94
24	b	614	CLA	CHC-C1C-C2C	-3.00	118.46	126.35
24	b	612	CLA	C4C-C3C-C2C	-3.00	102.08	106.94
24	C	512	CLA	C1D-CHD-C4C	-3.00	118.07	122.60
24	a	409	CLA	C4C-C3C-C2C	-2.99	102.08	106.94
24	B	602	CLA	C1D-CHD-C4C	-2.99	118.07	122.60
24	b	612	CLA	CHC-C1C-C2C	-2.99	118.48	126.35
24	B	605	CLA	O2A-CGA-O1A	-2.99	115.78	123.49
24	b	616	CLA	C4C-C3C-C2C	-2.99	102.09	106.94
24	b	612	CLA	C4B-CHC-C1C	-2.99	122.84	129.26
24	B	605	CLA	C1C-NC-C4C	-2.98	102.65	106.27
24	B	609	CLA	CHC-C1C-C2C	-2.98	118.52	126.35
24	C	506	CLA	C4C-C3C-C2C	-2.98	102.11	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	612	CLA	C3B-CAB-CBB	-2.98	120.22	126.32
36	c	518	DGD	C2G-O2G-C1B	-2.98	110.75	117.89
24	A	406	CLA	CHC-C1C-C2C	-2.97	118.53	126.35
24	B	605	CLA	C1D-CHD-C4C	-2.97	118.11	122.60
24	c	511	CLA	CHC-C1C-C2C	-2.97	118.54	126.35
24	b	611	CLA	C3B-CAB-CBB	-2.97	120.25	126.32
24	A	409	CLA	C3B-CAB-CBB	-2.97	120.25	126.32
24	c	504	CLA	C3B-CAB-CBB	-2.97	120.25	126.32
26	C	516	BCR	C33-C5-C6	-2.96	121.70	124.61
24	d	404	CLA	CAA-C2A-C3A	-2.96	104.71	113.22
26	c	526	BCR	C38-C26-C25	-2.96	121.70	124.61
27	A	411	SQD	C1-O5-C5	-2.95	108.01	113.75
24	b	617	CLA	O2D-CGD-O1D	-2.95	117.69	123.79
24	B	610	CLA	CHC-C1C-C2C	-2.95	118.59	126.35
25	A	407	PHO	C4D-ND-C1D	-2.95	101.64	107.05
24	C	507	CLA	C1D-CHD-C4C	-2.95	118.14	122.60
24	b	611	CLA	C1C-C2C-C3C	-2.94	103.39	106.91
24	a	407	CLA	O2D-CGD-O1D	-2.94	117.72	123.79
24	b	621	CLA	C1C-C2C-C3C	-2.94	103.39	106.91
24	A	406	CLA	O2A-CGA-O1A	-2.94	115.90	123.49
24	C	507	CLA	CAA-C2A-C3A	-2.94	104.77	113.22
24	d	402	CLA	CHC-C1C-C2C	-2.94	118.63	126.35
24	B	612	CLA	C1C-C2C-C3C	-2.94	103.40	106.91
24	c	509	CLA	C4C-C3C-C2C	-2.93	102.18	106.94
24	b	612	CLA	C1C-NC-C4C	-2.93	102.70	106.27
26	K	101	BCR	C20-C21-C22	-2.93	122.97	127.20
24	C	504	CLA	CHC-C1C-C2C	-2.93	118.65	126.35
24	B	610	CLA	O2D-CGD-O1D	-2.93	117.74	123.79
24	c	509	CLA	CHC-C1C-C2C	-2.93	118.66	126.35
24	C	504	CLA	C4C-C3C-C2C	-2.93	102.19	106.94
24	B	611	CLA	CHC-C1C-C2C	-2.92	118.66	126.35
36	c	517	DGD	C2G-O2G-C1B	-2.92	110.88	117.89
24	B	603	CLA	O2D-CGD-O1D	-2.92	117.76	123.79
24	C	514	CLA	C1C-C2C-C3C	-2.92	103.42	106.91
24	b	616	CLA	C1C-C2C-C3C	-2.92	103.42	106.91
24	c	505	CLA	C1C-C2C-C3C	-2.92	103.42	106.91
34	Z	101	LMG	C7-O1-C1	-2.92	107.69	113.82
24	c	515	CLA	C1D-CHD-C4C	-2.92	118.19	122.60
24	b	621	CLA	C4C-C3C-C2C	-2.92	102.21	106.94
24	c	506	CLA	CHC-C1C-C2C	-2.92	118.68	126.35
26	c	526	BCR	C15-C14-C13	-2.92	122.98	127.20
24	B	617	CLA	O2D-CGD-O1D	-2.91	117.78	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	615	CLA	C2A-C1A-CHA	-2.91	118.53	123.89
24	b	621	CLA	C1D-CHD-C4C	-2.91	118.20	122.60
26	B	620	BCR	C28-C27-C26	-2.90	109.26	113.87
26	T	102	BCR	C28-C27-C26	-2.90	109.26	113.87
24	b	616	CLA	C3B-CAB-CBB	-2.90	120.38	126.32
24	b	615	CLA	C4C-C3C-C2C	-2.90	102.23	106.94
24	c	507	CLA	CHC-C1C-C2C	-2.90	118.72	126.35
24	B	616	CLA	C1C-C2C-C3C	-2.90	103.44	106.91
24	C	509	CLA	C1D-CHD-C4C	-2.90	118.22	122.60
26	B	620	BCR	C24-C23-C22	-2.90	121.80	126.22
24	A	405	CLA	CAA-C2A-C1A	-2.90	102.25	112.47
24	B	608	CLA	CAA-C2A-C3A	-2.90	104.89	113.22
24	A	405	CLA	C1C-NC-C4C	-2.89	102.75	106.27
24	B	612	CLA	CHC-C1C-C2C	-2.89	118.75	126.35
26	d	405	BCR	C28-C27-C26	-2.89	109.28	113.87
25	A	407	PHO	C1C-C2C-C3C	-2.89	103.04	106.50
24	c	506	CLA	C1D-CHD-C4C	-2.89	118.23	122.60
24	b	610	CLA	CHC-C1C-C2C	-2.89	118.75	126.35
24	c	515	CLA	CHC-C1C-C2C	-2.89	118.75	126.35
24	B	611	CLA	C1C-C2C-C3C	-2.89	103.45	106.91
37	L	101	LHG	C6-C5-C4	-2.89	105.32	112.07
24	d	402	CLA	O2A-CGA-O1A	-2.89	116.05	123.49
24	D	404	CLA	C4C-C3C-C2C	-2.88	102.26	106.94
24	D	401	CLA	O2A-CGA-O1A	-2.88	116.06	123.49
24	c	515	CLA	CAA-C2A-C3A	-2.88	104.94	113.22
24	B	613	CLA	O2D-CGD-O1D	-2.88	117.84	123.79
24	B	603	CLA	C1C-C2C-C3C	-2.88	103.47	106.91
25	a	408	PHO	C4D-ND-C1D	-2.88	101.77	107.05
24	b	616	CLA	C4B-CHC-C1C	-2.87	123.09	129.26
24	C	512	CLA	C4C-C3C-C2C	-2.87	102.28	106.94
24	B	616	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
24	b	617	CLA	C2A-C1A-CHA	-2.87	118.61	123.89
24	d	401	CLA	CAA-C2A-C3A	-2.86	104.99	113.22
26	A	410	BCR	C15-C14-C13	-2.86	123.07	127.20
24	A	405	CLA	C4C-C3C-C2C	-2.86	102.31	106.94
24	D	401	CLA	CBC-CAC-C3C	-2.85	103.68	112.39
24	C	503	CLA	C1D-CHD-C4C	-2.85	118.29	122.60
24	D	404	CLA	CHC-C1C-C2C	-2.85	118.86	126.35
24	c	507	CLA	C1C-C2C-C3C	-2.85	103.50	106.91
24	c	503	CLA	OBD-CAD-C3D	-2.85	122.55	128.35
24	c	507	CLA	C3B-CAB-CBB	-2.84	120.50	126.32
24	b	619	CLA	C4-C3-C2	-2.84	117.92	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	409	LHG	O8-C23-O10	-2.84	116.16	123.49
24	B	607	CLA	O2D-CGD-O1D	-2.84	117.93	123.79
24	B	612	CLA	C4C-C3C-C2C	-2.84	102.34	106.94
24	b	609	CLA	C1C-NC-C4C	-2.83	102.82	106.27
24	B	607	CLA	O1D-CGD-CBD	-2.83	120.56	124.62
24	c	514	CLA	O2D-CGD-O1D	-2.83	117.94	123.79
27	F	101	SQD	C1-C2-C3	-2.83	104.39	109.97
24	C	514	CLA	O2D-CGD-O1D	-2.83	117.95	123.79
24	C	505	CLA	CHC-C1C-C2C	-2.83	118.91	126.35
24	B	605	CLA	CHC-C1C-C2C	-2.83	118.92	126.35
24	C	507	CLA	O2D-CGD-O1D	-2.82	117.96	123.79
37	E	101	LHG	C5-O7-C7	-2.82	111.12	117.89
24	c	505	CLA	C4C-C3C-C2C	-2.82	102.37	106.94
24	B	614	CLA	C4B-CHC-C1C	-2.82	123.20	129.26
24	c	503	CLA	C1D-CHD-C4C	-2.82	118.33	122.60
32	d	406	PL9	C42-C43-C44	-2.82	121.63	127.76
24	B	604	CLA	O2A-CGA-O1A	-2.82	116.22	123.49
24	C	505	CLA	C1D-CHD-C4C	-2.82	118.34	122.60
32	D	406	PL9	C40-C39-C38	-2.82	117.97	123.50
27	b	601	SQD	C1-C2-C3	-2.81	104.43	109.97
24	B	606	CLA	CHC-C1C-C2C	-2.81	118.95	126.35
24	C	503	CLA	C4C-C3C-C2C	-2.81	102.38	106.94
26	a	410	BCR	C33-C5-C6	-2.81	121.84	124.61
24	C	510	CLA	C4C-C3C-C2C	-2.81	102.38	106.94
26	Y	101	BCR	C15-C14-C13	-2.81	123.14	127.20
32	A	419	PL9	C35-C34-C33	-2.81	117.98	123.50
24	c	514	CLA	O1D-CGD-CBD	-2.81	120.60	124.62
25	d	403	PHO	CHD-C1D-C2D	-2.81	119.26	125.61
24	B	602	CLA	C4C-C3C-C2C	-2.81	102.39	106.94
24	d	402	CLA	C2A-C1A-CHA	-2.81	118.72	123.89
26	c	516	BCR	C3-C4-C5	-2.81	109.42	113.87
24	b	606	CLA	CHC-C1C-C2C	-2.80	118.98	126.35
24	D	403	CLA	CHC-C1C-C2C	-2.80	118.98	126.35
24	d	401	CLA	C4B-CHC-C1C	-2.80	123.24	129.26
32	d	406	PL9	C7-C8-C9	-2.80	121.95	126.70
24	B	609	CLA	C4C-C3C-C2C	-2.80	102.40	106.94
24	c	514	CLA	CHC-C1C-C2C	-2.80	118.99	126.35
24	d	401	CLA	C2A-C1A-CHA	-2.80	118.73	123.89
24	C	514	CLA	C4C-C3C-C2C	-2.80	102.40	106.94
26	Y	101	BCR	C16-C17-C18	-2.80	123.15	127.20
24	b	615	CLA	CHC-C1C-C2C	-2.80	119.00	126.35
24	B	608	CLA	CHC-C1C-C2C	-2.80	119.00	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	512	CLA	C1D-CHD-C4C	-2.80	118.37	122.60
24	C	513	CLA	CHC-C1C-C2C	-2.79	119.00	126.35
24	A	409	CLA	C2A-C1A-CHA	-2.79	118.74	123.89
27	b	601	SQD	C44-O6-C1	-2.79	107.96	113.82
38	e	102	HEM	CBD-CAD-C3D	-2.79	105.44	113.55
24	c	507	CLA	C1D-CHD-C4C	-2.79	118.38	122.60
24	a	409	CLA	CAA-C2A-C3A	-2.79	105.20	113.22
24	A	405	CLA	C2A-C1A-CHA	-2.79	118.75	123.89
24	C	512	CLA	C3B-CAB-CBB	-2.78	120.62	126.32
24	C	502	CLA	C4C-C3C-C2C	-2.78	102.43	106.94
24	B	615	CLA	CHC-C1C-C2C	-2.77	119.05	126.35
24	b	620	CLA	C3B-CAB-CBB	-2.77	120.64	126.32
24	c	504	CLA	C4C-C3C-C2C	-2.77	102.44	106.94
24	c	510	CLA	C4C-C3C-C2C	-2.77	102.44	106.94
26	C	515	BCR	C16-C17-C18	-2.77	123.19	127.20
26	A	410	BCR	C38-C26-C25	-2.77	121.88	124.61
24	b	620	CLA	C4C-C3C-C2C	-2.77	102.45	106.94
24	C	514	CLA	CHC-C1C-C2C	-2.77	119.08	126.35
24	c	503	CLA	C3B-CAB-CBB	-2.76	120.66	126.32
24	C	506	CLA	C3B-CAB-CBB	-2.76	120.67	126.32
24	C	502	CLA	CHC-C1C-C2C	-2.76	119.09	126.35
24	b	611	CLA	C4C-C3C-C2C	-2.76	102.46	106.94
24	C	508	CLA	C4C-C3C-C2C	-2.76	102.47	106.94
24	C	503	CLA	CHC-C1C-C2C	-2.76	119.10	126.35
32	D	406	PL9	C37-C38-C39	-2.76	121.77	127.76
24	A	409	CLA	CAA-C2A-C3A	-2.76	105.29	113.22
24	d	404	CLA	C3B-CAB-CBB	-2.76	120.68	126.32
24	B	613	CLA	C1C-C2C-C3C	-2.76	103.61	106.91
27	A	411	SQD	C44-O6-C1	-2.76	108.03	113.82
24	C	509	CLA	C4C-C3C-C2C	-2.75	102.48	106.94
24	B	602	CLA	CHC-C1C-C2C	-2.75	119.12	126.35
24	B	605	CLA	O2D-CGD-O1D	-2.75	118.11	123.79
30	m	102	LMT	C1'-O5'-C5'	-2.75	108.41	113.75
24	b	608	CLA	CMA-C3A-C2A	-2.74	102.21	114.35
24	c	504	CLA	C1D-CHD-C4C	-2.74	118.45	122.60
26	b	622	BCR	C15-C14-C13	-2.74	123.24	127.20
26	B	619	BCR	C28-C27-C26	-2.73	109.53	113.87
24	a	407	CLA	OBD-CAD-C3D	-2.73	122.78	128.35
24	b	615	CLA	O1D-CGD-CBD	-2.73	120.70	124.62
24	b	616	CLA	O2D-CGD-O1D	-2.73	118.15	123.79
24	B	613	CLA	CHC-C1C-C2C	-2.73	119.17	126.35
26	h	101	BCR	C16-C17-C18	-2.73	123.25	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	408	PHO	CHC-C1C-C2C	-2.73	119.44	125.61
24	b	606	CLA	C4C-C3C-C2C	-2.73	102.52	106.94
24	b	607	CLA	CHC-C1C-C2C	-2.72	119.19	126.35
24	C	511	CLA	CHC-C1C-C2C	-2.72	119.19	126.35
24	c	512	CLA	CHC-C1C-C2C	-2.72	119.19	126.35
34	C	521	LMG	C8-O7-C10	-2.72	111.36	117.89
24	b	608	CLA	C2A-C1A-CHA	-2.72	118.88	123.89
24	a	406	CLA	CAA-C2A-C1A	-2.72	102.89	112.47
24	B	610	CLA	C4C-C3C-C2C	-2.72	102.53	106.94
24	D	403	CLA	C1C-NC-C4C	-2.72	102.97	106.27
24	A	405	CLA	CHC-C1C-C2C	-2.71	119.21	126.35
24	c	508	CLA	C4C-C3C-C2C	-2.71	102.54	106.94
26	K	101	BCR	C37-C22-C21	-2.71	118.90	122.90
24	b	617	CLA	OBD-CAD-C3D	-2.71	122.83	128.35
37	D	409	LHG	C5-O7-C7	-2.70	111.41	117.89
32	D	406	PL9	C15-C14-C13	-2.70	118.20	123.50
24	d	402	CLA	C4C-C3C-C2C	-2.69	102.57	106.94
24	d	404	CLA	C4C-C3C-C2C	-2.69	102.57	106.94
24	D	404	CLA	C1D-CHD-C4C	-2.69	118.53	122.60
30	I	102	LMT	C2'-C3'-C4'	-2.69	103.69	109.60
24	B	617	CLA	C4B-CHC-C1C	-2.69	123.48	129.26
24	c	503	CLA	O2A-CGA-O1A	-2.69	116.55	123.49
24	b	613	CLA	CHC-C1C-C2C	-2.69	119.28	126.35
24	B	612	CLA	C4B-CHC-C1C	-2.69	123.49	129.26
24	a	407	CLA	C3B-CAB-CBB	-2.68	120.83	126.32
24	a	407	CLA	CHC-C1C-C2C	-2.68	119.30	126.35
25	d	403	PHO	C4D-ND-C1D	-2.68	102.13	107.05
27	a	411	SQD	C44-O6-C1	-2.68	108.20	113.82
24	b	606	CLA	O2D-CGD-O1D	-2.68	118.27	123.79
26	K	101	BCR	C24-C23-C22	-2.68	122.14	126.22
24	b	609	CLA	CHC-C1C-C2C	-2.68	119.31	126.35
24	c	513	CLA	C3B-CAB-CBB	-2.67	120.85	126.32
24	c	509	CLA	O2A-CGA-O1A	-2.67	116.60	123.49
24	B	603	CLA	C3B-CAB-CBB	-2.67	120.86	126.32
24	c	503	CLA	C4C-C3C-C2C	-2.67	102.61	106.94
24	C	511	CLA	C4C-C3C-C2C	-2.67	102.61	106.94
24	B	616	CLA	C1D-CHD-C4C	-2.67	118.56	122.60
24	B	608	CLA	OBD-CAD-C3D	-2.66	122.92	128.35
32	D	406	PL9	C12-C13-C14	-2.66	121.97	127.76
26	h	101	BCR	C11-C10-C9	-2.66	123.35	127.20
24	B	617	CLA	C1C-C2C-C3C	-2.66	103.72	106.91
26	B	620	BCR	C3-C4-C5	-2.66	109.64	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	526	BCR	C7-C8-C9	-2.66	122.16	126.22
34	j	101	LMG	O8-C28-O10	-2.66	116.63	123.49
24	b	613	CLA	C4C-C3C-C2C	-2.66	102.63	106.94
24	c	511	CLA	C4C-C3C-C2C	-2.66	102.63	106.94
26	K	101	BCR	C7-C8-C9	-2.65	122.17	126.22
24	B	606	CLA	C4C-C3C-C2C	-2.65	102.64	106.94
24	B	608	CLA	C4B-CHC-C1C	-2.65	123.57	129.26
24	B	608	CLA	C2A-C1A-CHA	-2.65	119.01	123.89
24	c	515	CLA	C4C-C3C-C2C	-2.65	102.65	106.94
24	C	502	CLA	O2A-CGA-O1A	-2.64	116.67	123.49
24	B	604	CLA	C2A-C1A-CHA	-2.64	119.02	123.89
38	e	102	HEM	C1D-CHD-C4C	-2.64	121.40	125.82
26	c	516	BCR	C15-C14-C13	-2.64	123.38	127.20
24	b	613	CLA	O2D-CGD-O1D	-2.64	118.34	123.79
26	y	101	BCR	C16-C17-C18	-2.64	123.39	127.20
25	A	407	PHO	CHD-C1D-C2D	-2.64	119.64	125.61
24	A	409	CLA	C4C-C3C-C2C	-2.64	102.66	106.94
25	d	403	PHO	C4-C3-C2	-2.64	118.32	123.50
24	a	407	CLA	CBC-CAC-C3C	-2.64	104.34	112.39
25	d	403	PHO	C1C-C2C-C3C	-2.63	103.35	106.50
25	A	408	PHO	O2D-CGD-O1D	-2.63	118.35	123.79
24	c	510	CLA	CHC-C1C-C2C	-2.63	119.43	126.35
24	B	609	CLA	CAA-C2A-C3A	-2.63	105.65	113.22
32	d	406	PL9	C22-C23-C24	-2.63	122.04	127.76
24	b	616	CLA	C2A-C1A-CHA	-2.63	119.04	123.89
24	B	606	CLA	C2A-C1A-CHA	-2.63	119.05	123.89
24	b	619	CLA	C1D-CHD-C4C	-2.62	118.63	122.60
24	c	509	CLA	C1D-CHD-C4C	-2.62	118.63	122.60
26	a	410	BCR	C38-C26-C25	-2.62	122.03	124.61
24	D	404	CLA	O2A-CGA-O1A	-2.62	116.73	123.49
24	B	607	CLA	C4C-C3C-C2C	-2.62	102.69	106.94
24	C	502	CLA	CBC-CAC-C3C	-2.62	104.39	112.39
24	b	611	CLA	CHC-C1C-C2C	-2.62	119.47	126.35
36	C	517	DGD	O1G-C1A-O1A	-2.62	116.74	123.49
26	D	405	BCR	C15-C14-C13	-2.62	123.42	127.20
24	c	514	CLA	C1D-CHD-C4C	-2.61	118.64	122.60
26	B	618	BCR	C7-C8-C9	-2.61	122.23	126.22
36	c	517	DGD	O1G-C1A-O1A	-2.61	116.75	123.49
24	C	514	CLA	C2A-C1A-CHA	-2.61	119.08	123.89
24	b	610	CLA	C2A-C1A-CHA	-2.61	119.08	123.89
24	B	604	CLA	O2D-CGD-O1D	-2.61	118.40	123.79
24	a	407	CLA	C4C-C3C-C2C	-2.61	102.71	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	C4C-C3C-C2C	-2.61	102.71	106.94
24	d	401	CLA	C3B-CAB-CBB	-2.61	120.98	126.32
24	b	607	CLA	C1C-C2C-C3C	-2.61	103.79	106.91
24	C	505	CLA	CAA-C2A-C3A	-2.60	105.73	113.22
24	c	514	CLA	CBA-CAA-C2A	-2.60	106.39	113.73
24	b	618	CLA	C1C-NC-C4C	-2.60	103.11	106.27
24	B	616	CLA	C4B-CHC-C1C	-2.60	123.68	129.26
24	B	613	CLA	C2A-C1A-CHA	-2.60	119.10	123.89
24	d	402	CLA	C4A-NA-C1A	-2.60	102.99	106.36
24	C	508	CLA	OBD-CAD-C3D	-2.60	123.06	128.35
24	b	620	CLA	C1D-CHD-C4C	-2.59	118.67	122.60
24	d	401	CLA	C4C-C3C-C2C	-2.59	102.74	106.94
24	c	512	CLA	C4C-C3C-C2C	-2.59	102.74	106.94
24	b	606	CLA	C2A-C1A-CHA	-2.59	119.11	123.89
24	d	404	CLA	C1D-CHD-C4C	-2.59	118.68	122.60
24	d	404	CLA	CHC-C1C-C2C	-2.59	119.55	126.35
24	b	609	CLA	C4C-C3C-C2C	-2.59	102.75	106.94
24	b	612	CLA	O2A-CGA-O1A	-2.59	116.82	123.49
26	h	101	BCR	C10-C11-C12	-2.59	115.24	123.13
24	c	505	CLA	O2A-CGA-O1A	-2.59	116.82	123.49
24	B	611	CLA	OBD-CAD-C3D	-2.59	123.08	128.35
24	C	510	CLA	C4-C3-C2	-2.58	118.43	123.50
24	b	608	CLA	CHC-C1C-C2C	-2.58	119.56	126.35
24	C	510	CLA	C1D-CHD-C4C	-2.58	118.69	122.60
24	D	404	CLA	CAA-C2A-C3A	-2.58	105.80	113.22
24	B	605	CLA	C4C-C3C-C2C	-2.58	102.76	106.94
24	C	503	CLA	C2A-C1A-CHA	-2.57	119.14	123.89
24	b	617	CLA	CHC-C1C-C2C	-2.57	119.59	126.35
24	b	611	CLA	O2A-CGA-O1A	-2.57	116.87	123.49
24	B	614	CLA	C4C-C3C-C2C	-2.57	102.78	106.94
24	C	507	CLA	C4C-C3C-C2C	-2.57	102.78	106.94
27	A	411	SQD	O48-C23-O10	-2.56	116.87	123.49
26	T	102	BCR	C29-C28-C27	-2.56	105.07	111.53
25	d	403	PHO	C4D-CHA-C1A	-2.56	119.37	125.06
24	A	405	CLA	CMA-C3A-C2A	-2.56	103.04	114.35
24	B	606	CLA	C1C-NC-C4C	-2.55	103.17	106.27
32	A	419	PL9	C25-C24-C23	-2.55	118.49	123.50
30	m	103	LMT	C1-O1'-C1'	-2.55	109.48	113.94
24	b	619	CLA	C4B-CHC-C1C	-2.55	123.78	129.26
26	C	516	BCR	C3-C4-C5	-2.55	109.82	113.87
24	c	509	CLA	C3B-CAB-CBB	-2.55	121.11	126.32
24	C	509	CLA	CAA-C2A-C3A	-2.54	105.90	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	C1D-CHD-C4C	-2.54	118.75	122.60
24	b	616	CLA	C1C-NC-C4C	-2.54	103.17	106.27
24	B	607	CLA	CHC-C1C-C2C	-2.54	119.66	126.35
24	C	507	CLA	CBC-CAC-C3C	-2.54	104.63	112.39
24	C	509	CLA	C2A-C1A-CHA	-2.54	119.21	123.89
24	c	510	CLA	CAA-C2A-C3A	-2.54	105.91	113.22
37	d	408	LHG	O8-C23-O10	-2.54	116.94	123.49
24	A	405	CLA	C4A-NA-C1A	-2.53	103.08	106.36
24	c	512	CLA	CBC-CAC-C3C	-2.53	104.66	112.39
24	B	607	CLA	CAA-C2A-C3A	-2.53	105.94	113.22
24	b	618	CLA	C4B-CHC-C1C	-2.53	123.83	129.26
24	B	607	CLA	C1C-NC-C4C	-2.53	103.19	106.27
24	a	406	CLA	C4C-C3C-C2C	-2.53	102.84	106.94
24	A	409	CLA	O2A-CGA-O1A	-2.53	116.97	123.49
24	b	613	CLA	C2A-C1A-CHA	-2.53	119.23	123.89
24	b	619	CLA	CAA-C2A-C3A	-2.53	105.96	113.22
24	C	502	CLA	C1D-CHD-C4C	-2.52	118.79	122.60
26	A	410	BCR	C7-C8-C9	-2.52	122.38	126.22
32	D	406	PL9	C27-C28-C29	-2.52	122.29	127.76
24	c	509	CLA	O2D-CGD-O1D	-2.52	118.60	123.79
24	B	615	CLA	CBC-CAC-C3C	-2.51	104.72	112.39
24	b	609	CLA	C4B-CHC-C1C	-2.51	123.86	129.26
26	c	516	BCR	C33-C5-C6	-2.51	122.14	124.61
24	a	407	CLA	O2A-CGA-O1A	-2.51	117.01	123.49
27	b	601	SQD	O47-C7-O49	-2.51	116.93	123.67
24	D	403	CLA	O2D-CGD-O1D	-2.51	118.60	123.79
24	c	508	CLA	O2A-CGA-O1A	-2.51	117.01	123.49
24	b	619	CLA	O2A-CGA-O1A	-2.51	117.01	123.49
24	D	401	CLA	CMA-C3A-C2A	-2.51	103.24	114.35
24	c	506	CLA	C4C-C3C-C2C	-2.51	102.87	106.94
24	B	603	CLA	CAA-CBA-CGA	-2.51	105.97	113.32
24	d	402	CLA	C1C-NC-C4C	-2.50	103.22	106.27
24	B	608	CLA	O2D-CGD-O1D	-2.50	118.63	123.79
24	A	409	CLA	CHC-C1C-C2C	-2.50	119.78	126.35
24	c	509	CLA	C1C-NC-C4C	-2.50	103.23	106.27
38	v	202	HEM	C3B-CAB-CBB	-2.50	120.63	124.46
24	c	507	CLA	C1C-NC-C4C	-2.49	103.24	106.27
24	D	404	CLA	C3B-CAB-CBB	-2.49	121.22	126.32
24	c	508	CLA	CBC-CAC-C3C	-2.49	104.78	112.39
24	b	614	CLA	C4C-C3C-C2C	-2.49	102.90	106.94
27	l	101	SQD	C1-O5-C5	-2.49	108.91	113.75
34	c	521	LMG	C8-O7-C10	-2.49	111.92	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PHO	O2A-CGA-O1A	-2.49	117.07	123.49
32	d	406	PL9	C40-C39-C38	-2.48	118.63	123.50
24	D	401	CLA	C1D-CHD-C4C	-2.48	118.85	122.60
26	a	410	BCR	C15-C14-C13	-2.47	123.62	127.20
24	B	608	CLA	CBC-CAC-C3C	-2.47	104.84	112.39
26	c	526	BCR	C11-C10-C9	-2.47	123.63	127.20
24	b	619	CLA	C2A-C1A-CHA	-2.47	119.33	123.89
26	c	526	BCR	C24-C23-C22	-2.47	122.45	126.22
36	c	517	DGD	O3G-C3G-C2G	-2.47	105.11	110.99
24	B	615	CLA	C1D-CHD-C4C	-2.47	118.87	122.60
25	A	407	PHO	C4D-CHA-C1A	-2.47	119.58	125.06
24	b	616	CLA	OBD-CAD-C3D	-2.47	123.32	128.35
24	C	502	CLA	C3B-CAB-CBB	-2.46	121.28	126.32
24	C	508	CLA	CHC-C1C-C2C	-2.46	119.87	126.35
24	C	514	CLA	CAA-C2A-C3A	-2.46	106.14	113.22
30	a	417	LMT	C1-O1'-C1'	-2.46	109.64	113.94
24	b	618	CLA	C4-C3-C2	-2.46	118.67	123.50
24	b	611	CLA	CAA-C2A-C3A	-2.46	106.14	113.22
24	c	513	CLA	CBC-CAC-C3C	-2.46	104.89	112.39
24	a	406	CLA	C2A-C1A-CHA	-2.46	119.36	123.89
24	d	401	CLA	O2A-CGA-O1A	-2.46	117.15	123.49
24	c	505	CLA	CHC-C1C-C2C	-2.45	119.90	126.35
24	B	612	CLA	C2A-C1A-CHA	-2.45	119.37	123.89
24	b	619	CLA	C4C-C3C-C2C	-2.45	102.97	106.94
24	B	605	CLA	C4B-CHC-C1C	-2.45	124.00	129.26
25	A	408	PHO	C4-C3-C2	-2.45	118.70	123.50
24	b	621	CLA	O2A-CGA-O1A	-2.45	117.18	123.49
24	b	610	CLA	CBC-CAC-C3C	-2.44	104.93	112.39
32	D	406	PL9	C31-C32-C33	-2.44	105.29	111.69
25	A	407	PHO	CBA-CAA-C2A	-2.44	106.84	113.73
24	A	409	CLA	C4B-CHC-C1C	-2.44	124.01	129.26
24	D	403	CLA	CMA-C3A-C2A	-2.44	103.54	114.35
24	B	610	CLA	C2A-C1A-CHA	-2.44	119.39	123.89
24	B	615	CLA	C4C-C3C-C2C	-2.44	102.99	106.94
24	d	402	CLA	C4-C3-C2	-2.43	118.72	123.50
24	B	616	CLA	OBD-CAD-C3D	-2.43	123.39	128.35
26	c	526	BCR	C20-C21-C22	-2.43	123.69	127.20
24	A	405	CLA	C3B-CAB-CBB	-2.43	121.35	126.32
25	A	408	PHO	C4D-CHA-C1A	-2.43	119.66	125.06
24	B	604	CLA	CHC-C1C-C2C	-2.43	119.96	126.35
32	d	406	PL9	C31-C32-C33	-2.43	105.33	111.69
24	d	404	CLA	O2D-CGD-O1D	-2.43	118.78	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	403	CLA	C4B-CHC-C1C	-2.43	124.05	129.26
24	b	606	CLA	O1D-CGD-CBD	-2.42	121.15	124.62
24	c	509	CLA	C4B-CHC-C1C	-2.42	124.06	129.26
24	D	403	CLA	C3B-CAB-CBB	-2.42	121.36	126.32
26	t	101	BCR	C11-C10-C9	-2.42	123.70	127.20
26	D	405	BCR	C10-C11-C12	-2.42	115.75	123.13
24	c	505	CLA	O2D-CGD-O1D	-2.42	118.80	123.79
34	Z	101	LMG	C9-C8-C7	-2.41	106.42	112.07
24	c	506	CLA	O1D-CGD-CBD	-2.41	121.17	124.62
24	B	612	CLA	C4-C3-C2	-2.41	118.77	123.50
24	b	613	CLA	CAA-C2A-C3A	-2.41	106.29	113.22
26	B	620	BCR	C36-C18-C17	-2.41	119.35	122.90
24	A	405	CLA	C1D-CHD-C4C	-2.41	118.96	122.60
24	c	505	CLA	O1D-CGD-CBD	-2.41	121.17	124.62
24	C	508	CLA	CBC-CAC-C3C	-2.40	105.05	112.39
24	B	608	CLA	C1C-NC-C4C	-2.40	103.35	106.27
26	h	101	BCR	C7-C8-C9	-2.40	122.55	126.22
26	b	624	BCR	C3-C4-C5	-2.40	110.06	113.87
24	d	402	CLA	CMA-C3A-C2A	-2.40	103.73	114.35
38	E	103	HEM	C1D-CHD-C4C	-2.40	121.81	125.82
37	d	409	LHG	C5-O7-C7	-2.40	112.13	117.89
24	B	604	CLA	O1D-CGD-CBD	-2.40	121.18	124.62
34	B	621	LMG	C9-C8-C7	-2.40	106.47	112.07
24	B	616	CLA	CBC-CAC-C3C	-2.40	105.08	112.39
24	d	401	CLA	CBC-CAC-C3C	-2.40	105.08	112.39
24	b	617	CLA	C1C-C2C-C3C	-2.39	104.05	106.91
24	B	609	CLA	C3B-CAB-CBB	-2.39	121.43	126.32
24	B	606	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
27	a	411	SQD	O47-C7-O49	-2.39	117.26	123.67
24	b	608	CLA	C4C-C3C-C2C	-2.38	103.08	106.94
24	B	606	CLA	CAA-C2A-C3A	-2.38	106.36	113.22
26	K	101	BCR	C38-C26-C25	-2.38	122.27	124.61
26	h	101	BCR	C31-C1-C6	-2.38	106.57	110.30
32	D	406	PL9	C7-C8-C9	-2.38	122.66	126.70
24	B	607	CLA	C4B-CHC-C1C	-2.38	124.16	129.26
24	C	504	CLA	O2A-CGA-O1A	-2.38	117.36	123.49
24	b	613	CLA	C4B-CHC-C1C	-2.37	124.16	129.26
24	C	504	CLA	C1C-NC-C4C	-2.37	103.38	106.27
24	D	403	CLA	C2A-C1A-CHA	-2.37	119.51	123.89
26	C	516	BCR	C21-C20-C19	-2.37	115.90	123.13
24	D	404	CLA	C2A-C1A-CHA	-2.37	119.52	123.89
35	V	204	HTG	C1-C2-C3	-2.37	105.44	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	601	SQD	O48-C23-O10	-2.37	117.38	123.49
24	B	608	CLA	C4C-C3C-C2C	-2.37	103.10	106.94
24	b	607	CLA	C2A-C1A-CHA	-2.37	119.53	123.89
26	B	620	BCR	C7-C8-C9	-2.37	122.61	126.22
24	a	406	CLA	OBD-CAD-C3D	-2.37	123.53	128.35
24	B	605	CLA	O1D-CGD-CBD	-2.36	121.23	124.62
24	D	403	CLA	OBD-CAD-C3D	-2.36	123.53	128.35
24	C	509	CLA	C3B-CAB-CBB	-2.36	121.48	126.32
26	C	516	BCR	C38-C26-C25	-2.36	122.29	124.61
24	b	607	CLA	O2A-CGA-O1A	-2.36	117.40	123.49
24	b	621	CLA	C4B-CHC-C1C	-2.36	124.19	129.26
24	B	607	CLA	CBC-CAC-C3C	-2.36	105.19	112.39
24	b	610	CLA	C4C-C3C-C2C	-2.36	103.11	106.94
24	c	510	CLA	C2A-C1A-CHA	-2.36	119.54	123.89
24	A	406	CLA	CMA-C3A-C2A	-2.36	103.93	114.35
26	y	101	BCR	C10-C11-C12	-2.35	115.95	123.13
36	h	102	DGD	O4D-C4D-C3D	-2.35	105.04	110.34
32	d	406	PL9	C3-C2-C1	-2.35	121.53	122.97
24	A	406	CLA	C2A-C1A-CHA	-2.35	119.55	123.89
25	A	408	PHO	C1C-C2C-C3C	-2.35	103.69	106.50
26	Y	101	BCR	C40-C30-C25	-2.35	106.62	110.30
24	b	615	CLA	O2A-CGA-O1A	-2.34	117.44	123.49
34	J	101	LMG	C9-C8-C7	-2.34	106.59	112.07
24	b	613	CLA	CMA-C3A-C2A	-2.34	104.00	114.35
26	a	410	BCR	C34-C9-C10	-2.34	119.44	122.90
24	A	409	CLA	CMA-C3A-C2A	-2.34	104.00	114.35
26	B	620	BCR	C15-C14-C13	-2.34	123.82	127.20
24	B	608	CLA	O2A-CGA-O1A	-2.34	117.46	123.49
37	D	410	LHG	O8-C23-O10	-2.34	117.46	123.49
24	b	620	CLA	C4B-CHC-C1C	-2.34	124.24	129.26
24	C	504	CLA	C4B-CHC-C1C	-2.33	124.25	129.26
24	c	515	CLA	C2A-C1A-CHA	-2.33	119.59	123.89
36	h	102	DGD	O1G-C1A-O1A	-2.33	117.48	123.49
24	b	611	CLA	C4B-CHC-C1C	-2.33	124.26	129.26
38	V	203	HEM	C3B-C4B-NB	-2.33	107.17	111.63
24	b	617	CLA	O2A-CGA-O1A	-2.33	117.49	123.49
26	Y	101	BCR	C10-C11-C12	-2.33	116.04	123.13
32	D	406	PL9	C7-C3-C2	-2.33	121.49	123.42
26	T	102	BCR	C7-C6-C5	-2.33	116.05	121.37
24	C	511	CLA	C4-C3-C2	-2.32	118.94	123.50
24	B	614	CLA	C1C-NC-C4C	-2.32	103.44	106.27
24	C	505	CLA	C3B-CAB-CBB	-2.32	121.57	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	518	DGD	O2G-C1B-O1B	-2.32	117.44	123.67
24	A	409	CLA	C1D-CHD-C4C	-2.32	119.09	122.60
25	A	408	PHO	C3B-C2B-C1B	-2.32	101.31	106.33
32	D	406	PL9	C22-C23-C24	-2.32	122.73	127.76
24	a	406	CLA	CMA-C3A-C2A	-2.31	104.11	114.35
24	B	608	CLA	C4-C3-C2	-2.31	118.96	123.50
32	A	419	PL9	C16-C17-C18	-2.31	105.63	111.69
24	B	603	CLA	CBC-CAC-C3C	-2.31	105.33	112.39
25	a	408	PHO	CHD-C1D-C2D	-2.31	120.38	125.61
24	c	512	CLA	C4-C3-C2	-2.31	118.96	123.50
24	b	606	CLA	C3B-CAB-CBB	-2.31	121.59	126.32
24	c	506	CLA	OBD-CAD-C3D	-2.31	123.64	128.35
32	a	416	PL9	C35-C34-C33	-2.31	118.97	123.50
24	d	402	CLA	C4B-CHC-C1C	-2.31	124.30	129.26
24	b	613	CLA	C1D-CHD-C4C	-2.31	119.11	122.60
24	C	513	CLA	CBC-CAC-C3C	-2.31	105.34	112.39
24	B	606	CLA	C3B-CAB-CBB	-2.31	121.60	126.32
26	B	618	BCR	C11-C10-C9	-2.31	123.87	127.20
38	V	203	HEM	CBA-CAA-C2A	-2.31	108.40	112.53
24	D	401	CLA	OBD-CAD-C3D	-2.30	123.65	128.35
27	F	101	SQD	C1-O5-C5	-2.30	109.27	113.75
24	c	513	CLA	O2D-CGD-O1D	-2.30	119.04	123.79
32	D	406	PL9	C36-C37-C38	-2.30	105.67	111.69
24	C	506	CLA	C1C-NC-C4C	-2.30	103.47	106.27
24	B	604	CLA	C1C-NC-C4C	-2.30	103.47	106.27
24	C	510	CLA	C3B-CAB-CBB	-2.30	121.62	126.32
24	B	605	CLA	C2A-C1A-CHA	-2.30	119.66	123.89
24	B	602	CLA	CAA-C2A-C3A	-2.29	106.62	113.22
24	d	404	CLA	C2A-C1A-CHA	-2.29	119.66	123.89
24	d	404	CLA	CGD-CBD-CAD	-2.29	102.86	110.62
26	c	516	BCR	C28-C27-C26	-2.29	110.23	113.87
37	d	410	LHG	O8-C23-O10	-2.29	117.58	123.49
24	a	406	CLA	C1C-NC-C4C	-2.29	103.48	106.27
24	C	505	CLA	C4C-C3C-C2C	-2.29	103.23	106.94
24	c	513	CLA	C4C-C3C-C2C	-2.29	103.23	106.94
26	B	618	BCR	C34-C9-C10	-2.29	119.52	122.90
24	c	513	CLA	C4B-CHC-C1C	-2.29	124.35	129.26
24	b	616	CLA	O1D-CGD-CBD	-2.28	121.35	124.62
27	a	402	SQD	C45-O47-C7	-2.28	112.41	117.89
32	d	406	PL9	C12-C13-C14	-2.28	122.80	127.76
24	B	614	CLA	O2A-CGA-O1A	-2.28	117.61	123.49
24	D	401	CLA	O2D-CGD-O1D	-2.28	119.08	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	v	202	HEM	C3B-C4B-NB	-2.28	107.27	111.63
24	C	502	CLA	CAA-C2A-C3A	-2.28	106.67	113.22
24	b	619	CLA	CBC-CAC-C3C	-2.28	105.44	112.39
24	C	502	CLA	C2A-C1A-CHA	-2.27	119.70	123.89
24	b	609	CLA	O2A-CGA-O1A	-2.27	117.63	123.49
24	d	402	CLA	C1D-CHD-C4C	-2.27	119.16	122.60
26	A	410	BCR	C37-C22-C21	-2.27	119.55	122.90
24	b	612	CLA	O2D-CGD-O1D	-2.27	119.10	123.79
24	c	513	CLA	O2A-CGA-O1A	-2.26	117.65	123.49
35	V	204	HTG	O5-C1-C2	-2.26	107.11	110.19
24	c	503	CLA	C2A-C1A-CHA	-2.26	119.72	123.89
24	C	504	CLA	C2A-C1A-CHA	-2.26	119.72	123.89
24	b	613	CLA	O1D-CGD-CBD	-2.26	121.38	124.62
24	c	510	CLA	C1C-NC-C4C	-2.26	103.52	106.27
24	c	506	CLA	CAA-C2A-C3A	-2.26	106.72	113.22
36	H	102	DGD	O1G-C1A-O1A	-2.26	117.67	123.49
32	d	406	PL9	C11-C12-C13	-2.26	105.78	111.69
37	d	408	LHG	C5-O7-C7	-2.25	112.48	117.89
27	a	402	SQD	O48-C23-O10	-2.25	117.68	123.49
36	C	518	DGD	O1G-C1A-O1A	-2.25	117.68	123.49
34	J	101	LMG	O8-C28-O10	-2.25	117.68	123.49
24	c	513	CLA	C4-C3-C2	-2.25	119.08	123.50
24	c	508	CLA	CGD-CBD-CAD	-2.25	103.00	110.62
26	H	101	BCR	C37-C22-C21	-2.25	119.58	122.90
24	C	513	CLA	O2D-CGD-O1D	-2.24	119.16	123.79
24	A	406	CLA	O1D-CGD-CBD	-2.24	121.41	124.62
24	C	507	CLA	O2A-CGA-O1A	-2.24	117.70	123.49
37	D	409	LHG	O7-C7-O9	-2.24	117.65	123.67
24	c	505	CLA	C2A-C1A-CHA	-2.24	119.76	123.89
24	B	608	CLA	C1D-CHD-C4C	-2.24	119.22	122.60
24	c	511	CLA	O2A-CGA-O1A	-2.24	117.72	123.49
24	B	611	CLA	C3B-CAB-CBB	-2.24	121.74	126.32
24	c	506	CLA	O2A-CGA-O1A	-2.23	117.72	123.49
24	B	610	CLA	CBC-CAC-C3C	-2.23	105.58	112.39
24	B	612	CLA	C4A-NA-C1A	-2.23	103.47	106.36
24	B	611	CLA	C1C-NC-C4C	-2.23	103.56	106.27
24	B	615	CLA	C4B-CHC-C1C	-2.23	124.47	129.26
24	c	511	CLA	OBD-CAD-C3D	-2.23	123.81	128.35
24	b	608	CLA	OBD-CAD-C3D	-2.23	123.81	128.35
24	B	616	CLA	C4A-NA-C1A	-2.23	103.47	106.36
24	b	608	CLA	O1D-CGD-CBD	-2.23	121.43	124.62
24	B	602	CLA	O2D-CGD-O1D	-2.22	119.20	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	410	BCR	C40-C30-C25	-2.22	106.82	110.30
24	c	514	CLA	C2A-C1A-CHA	-2.22	119.79	123.89
24	C	512	CLA	O2D-CGD-O1D	-2.22	119.20	123.79
24	B	603	CLA	C4B-CHC-C1C	-2.22	124.49	129.26
26	B	620	BCR	C16-C17-C18	-2.22	123.99	127.20
24	c	505	CLA	C1C-NC-C4C	-2.22	103.57	106.27
24	C	508	CLA	O2A-CGA-O1A	-2.22	117.76	123.49
26	C	516	BCR	C11-C10-C9	-2.22	124.00	127.20
24	c	506	CLA	O2D-CGD-O1D	-2.22	119.21	123.79
26	t	101	BCR	C15-C16-C17	-2.22	118.49	123.39
24	c	507	CLA	O1D-CGD-CBD	-2.21	121.45	124.62
24	B	609	CLA	C4B-CHC-C1C	-2.21	124.50	129.26
24	d	401	CLA	O2D-CGD-O1D	-2.21	119.22	123.79
24	c	510	CLA	C3B-CAB-CBB	-2.21	121.79	126.32
24	b	607	CLA	O1D-CGD-CBD	-2.21	121.45	124.62
24	b	606	CLA	CAA-C2A-C3A	-2.21	106.86	113.22
24	b	620	CLA	O2A-CGA-O1A	-2.21	117.78	123.49
37	l	102	LHG	C6-C5-C4	-2.21	106.90	112.07
34	c	501	LMG	O7-C10-O9	-2.21	117.75	123.67
24	b	614	CLA	C1C-NC-C4C	-2.21	103.59	106.27
38	V	203	HEM	C1D-CHD-C4C	-2.20	122.14	125.82
24	B	609	CLA	O2D-CGD-O1D	-2.20	119.24	123.79
26	T	102	BCR	C21-C20-C19	-2.20	116.41	123.13
24	C	513	CLA	CBA-CAA-C2A	-2.20	107.52	113.73
34	C	520	LMG	O8-C28-O10	-2.20	117.81	123.49
26	b	623	BCR	C3-C4-C5	-2.20	110.37	113.87
32	A	419	PL9	C3-C2-C1	-2.20	121.63	122.97
26	a	410	BCR	C35-C13-C14	-2.20	119.65	122.90
26	y	101	BCR	C38-C26-C25	-2.20	122.45	124.61
32	A	419	PL9	C10-C9-C8	-2.20	119.19	123.50
26	B	620	BCR	C10-C11-C12	-2.20	116.44	123.13
25	d	403	PHO	C3B-C2B-C1B	-2.19	101.57	106.33
26	y	101	BCR	C21-C20-C19	-2.19	116.44	123.13
24	B	609	CLA	C1C-NC-C4C	-2.19	103.60	106.27
24	B	606	CLA	O2A-CGA-O1A	-2.19	117.83	123.49
26	t	101	BCR	C21-C20-C19	-2.19	116.45	123.13
32	a	416	PL9	C12-C13-C14	-2.19	123.00	127.76
24	B	607	CLA	C4A-NA-C1A	-2.19	103.52	106.36
27	F	101	SQD	C44-O6-C1	-2.19	109.22	113.82
24	D	403	CLA	C4A-NA-C1A	-2.19	103.53	106.36
26	b	624	BCR	C16-C17-C18	-2.18	124.04	127.20
24	c	503	CLA	CBC-CAC-C3C	-2.18	105.73	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	612	CLA	CBC-CAC-C3C	-2.18	105.73	112.39
24	B	611	CLA	C1D-CHD-C4C	-2.18	119.30	122.60
24	c	504	CLA	C2A-C1A-CHA	-2.18	119.87	123.89
26	Y	101	BCR	C21-C20-C19	-2.18	116.48	123.13
24	c	512	CLA	C2A-C1A-CHA	-2.18	119.87	123.89
32	A	419	PL9	C12-C13-C14	-2.18	123.03	127.76
24	A	409	CLA	O2D-CGD-O1D	-2.18	119.29	123.79
32	D	406	PL9	C3-C2-C1	-2.18	121.64	122.97
26	a	410	BCR	C37-C22-C21	-2.17	119.69	122.90
24	a	409	CLA	C2A-C1A-CHA	-2.17	119.88	123.89
24	D	401	CLA	C4B-CHC-C1C	-2.17	124.59	129.26
24	b	610	CLA	C5-C3-C2	-2.17	116.93	121.05
24	b	618	CLA	O2A-CGA-O1A	-2.17	117.89	123.49
24	b	613	CLA	O2A-CGA-O1A	-2.17	117.90	123.49
24	B	613	CLA	C1C-NC-C4C	-2.17	103.63	106.27
24	b	620	CLA	C4A-NA-C1A	-2.17	103.55	106.36
24	C	508	CLA	C1C-NC-C4C	-2.16	103.64	106.27
37	d	408	LHG	O7-C7-O9	-2.16	117.88	123.67
24	b	614	CLA	CBC-CAC-C3C	-2.16	105.81	112.39
24	b	608	CLA	C5-C3-C2	-2.16	116.96	121.05
24	C	503	CLA	C1C-NC-C4C	-2.15	103.65	106.27
24	c	514	CLA	C4C-C3C-C2C	-2.15	103.45	106.94
24	B	610	CLA	C4B-CHC-C1C	-2.15	124.64	129.26
24	C	510	CLA	C2A-C1A-CHA	-2.15	119.92	123.89
26	K	101	BCR	C31-C1-C6	-2.15	106.93	110.30
24	C	505	CLA	C2A-C1A-CHA	-2.15	119.92	123.89
24	c	504	CLA	C4B-CHC-C1C	-2.15	124.64	129.26
24	c	508	CLA	C3B-CAB-CBB	-2.15	121.92	126.32
24	C	507	CLA	C3B-CAB-CBB	-2.15	121.92	126.32
26	D	405	BCR	C37-C22-C21	-2.14	119.73	122.90
24	c	503	CLA	C4B-CHC-C1C	-2.14	124.66	129.26
24	b	614	CLA	CGD-CBD-CAD	-2.14	103.37	110.62
24	D	404	CLA	CMA-C3A-C2A	-2.14	104.89	114.35
24	B	616	CLA	C11-C10-C8	-2.14	108.40	115.49
26	C	516	BCR	C40-C30-C25	-2.14	106.95	110.30
36	C	518	DGD	O6D-C1D-O3G	-2.13	104.91	110.05
26	b	623	BCR	C37-C22-C21	-2.13	119.75	122.90
27	l	101	SQD	C45-O47-C7	-2.13	112.78	117.89
30	A	417	LMT	C1B-O1B-C4'	-2.13	112.44	118.01
24	c	511	CLA	C2A-C1A-CHA	-2.13	119.96	123.89
32	A	419	PL9	C45-C44-C43	-2.13	119.32	123.50
26	y	101	BCR	C40-C30-C25	-2.13	106.96	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	CBC-CAC-C3C	-2.13	105.89	112.39
24	B	603	CLA	C2A-C1A-CHA	-2.13	119.96	123.89
24	a	406	CLA	C3B-CAB-CBB	-2.13	121.96	126.32
24	c	511	CLA	C4-C3-C2	-2.13	119.32	123.50
24	B	616	CLA	C1C-NC-C4C	-2.13	103.68	106.27
24	b	612	CLA	C2A-C1A-CHA	-2.13	119.97	123.89
24	b	616	CLA	O2A-CGA-O1A	-2.13	118.00	123.49
32	d	406	PL9	O1-C4-C3	-2.12	118.08	120.71
24	c	505	CLA	C4A-NA-C1A	-2.12	103.61	106.36
24	C	513	CLA	C4B-CHC-C1C	-2.12	124.70	129.26
24	c	514	CLA	OBD-CAD-C3D	-2.12	124.02	128.35
24	B	605	CLA	OBD-CAD-C3D	-2.12	124.03	128.35
24	b	620	CLA	C11-C10-C8	-2.12	108.45	115.49
24	d	401	CLA	C1D-CHD-C4C	-2.12	119.39	122.60
25	a	408	PHO	O2D-CGD-O1D	-2.12	119.41	123.79
27	A	416	SQD	O48-C23-O10	-2.12	118.02	123.49
24	b	609	CLA	C3B-CAB-CBB	-2.12	121.98	126.32
24	a	406	CLA	O2D-CGD-O1D	-2.12	119.42	123.79
24	d	401	CLA	C1C-NC-C4C	-2.12	103.69	106.27
26	d	405	BCR	C40-C30-C25	-2.12	106.98	110.30
24	c	506	CLA	C4B-CHC-C1C	-2.12	124.71	129.26
26	k	103	BCR	C11-C10-C9	-2.12	124.14	127.20
24	C	502	CLA	C1C-NC-C4C	-2.12	103.69	106.27
26	t	101	BCR	C7-C6-C5	-2.12	116.53	121.37
24	C	503	CLA	OBD-CAD-C3D	-2.12	124.04	128.35
36	H	102	DGD	C3G-C2G-C1G	-2.11	107.12	112.07
24	B	614	CLA	C4-C3-C2	-2.11	119.35	123.50
24	B	603	CLA	O2A-CGA-O1A	-2.11	118.04	123.49
24	b	613	CLA	OBD-CAD-C3D	-2.11	124.04	128.35
24	b	615	CLA	C1C-NC-C4C	-2.11	103.70	106.27
37	L	101	LHG	O8-C23-O10	-2.11	118.04	123.49
26	t	101	BCR	C3-C4-C5	-2.11	110.52	113.87
24	B	611	CLA	CAA-CBA-CGA	-2.11	107.14	113.32
26	b	624	BCR	C10-C11-C12	-2.11	116.70	123.13
26	d	405	BCR	C16-C17-C18	-2.11	124.15	127.20
24	B	617	CLA	C4-C3-C2	-2.11	119.36	123.50
24	B	617	CLA	OBD-CAD-C3D	-2.11	124.05	128.35
24	C	505	CLA	CBC-CAC-C3C	-2.11	105.96	112.39
24	B	610	CLA	O2A-CGA-O1A	-2.11	118.06	123.49
25	a	408	PHO	C3B-C2B-C1B	-2.10	101.78	106.33
24	b	613	CLA	C11-C10-C8	-2.10	108.52	115.49
24	b	614	CLA	C2A-C1A-CHA	-2.10	120.02	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	402	CLA	CAA-C2A-C3A	-2.10	107.18	113.22
32	A	419	PL9	C17-C18-C19	-2.10	123.20	127.76
37	D	408	LHG	O7-C7-O9	-2.10	118.03	123.67
27	A	411	SQD	O47-C7-O49	-2.10	118.04	123.67
26	y	101	BCR	C24-C23-C22	-2.10	123.02	126.22
24	d	404	CLA	O2A-CGA-O1A	-2.10	118.08	123.49
24	b	614	CLA	C3B-CAB-CBB	-2.10	122.03	126.32
24	b	610	CLA	C3B-CAB-CBB	-2.10	122.03	126.32
26	K	101	BCR	C11-C10-C9	-2.10	124.17	127.20
38	v	202	HEM	CBA-CAA-C2A	-2.10	108.77	112.53
24	b	621	CLA	C1C-NC-C4C	-2.10	103.72	106.27
24	A	405	CLA	CAA-CBA-CGA	-2.09	107.19	113.32
27	f	101	SQD	O47-C7-O49	-2.09	118.05	123.67
24	b	611	CLA	C1C-NC-C4C	-2.09	103.72	106.27
26	b	622	BCR	C3-C4-C5	-2.09	110.55	113.87
30	m	102	LMT	C3'-C4'-C5'	-2.09	106.11	110.84
37	d	409	LHG	O8-C23-O10	-2.09	118.10	123.49
26	T	102	BCR	C19-C18-C17	-2.09	115.62	118.98
24	b	607	CLA	CMA-C3A-C2A	-2.09	105.12	114.35
24	A	406	CLA	O2D-CGD-O1D	-2.09	119.48	123.79
24	B	612	CLA	C1C-NC-C4C	-2.08	103.73	106.27
24	B	615	CLA	C4-C3-C2	-2.08	119.41	123.50
24	C	506	CLA	C2A-C1A-CHA	-2.08	120.05	123.89
24	C	514	CLA	C4-C3-C2	-2.08	119.42	123.50
38	E	103	HEM	C3C-CAC-CBC	-2.08	121.27	124.46
24	B	603	CLA	C4-C3-C2	-2.08	119.42	123.50
24	c	508	CLA	OBD-CAD-C3D	-2.07	124.12	128.35
24	b	619	CLA	C1C-NC-C4C	-2.07	103.75	106.27
24	c	504	CLA	O2A-CGA-O1A	-2.07	118.14	123.49
24	c	507	CLA	C4A-NA-C1A	-2.07	103.67	106.36
24	b	612	CLA	O1D-CGD-CBD	-2.07	121.65	124.62
32	d	406	PL9	C36-C37-C38	-2.07	106.27	111.69
24	c	510	CLA	O2A-CGA-O1A	-2.07	118.15	123.49
24	C	511	CLA	CAA-C2A-C3A	-2.07	107.27	113.22
24	A	406	CLA	C4C-C3C-C2C	-2.07	103.59	106.94
26	a	410	BCR	C3-C4-C5	-2.06	110.59	113.87
24	c	515	CLA	O2A-CGA-O1A	-2.06	118.16	123.49
24	b	610	CLA	C1C-NC-C4C	-2.06	103.76	106.27
26	a	410	BCR	C28-C27-C26	-2.06	110.59	113.87
38	v	202	HEM	C1D-CHD-C4C	-2.06	122.38	125.82
24	b	613	CLA	CBC-CAC-C3C	-2.06	106.10	112.39
24	C	508	CLA	C3B-CAB-CBB	-2.06	122.10	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	C4A-NA-C1A	-2.06	103.69	106.36
24	C	503	CLA	CBC-CAC-C3C	-2.06	106.10	112.39
26	y	101	BCR	C35-C13-C14	-2.06	119.86	122.90
26	C	516	BCR	C28-C27-C26	-2.06	110.60	113.87
24	B	607	CLA	C2A-C1A-CHA	-2.06	120.10	123.89
24	B	604	CLA	CAA-C2A-C1A	-2.05	105.22	112.47
24	B	602	CLA	C2A-C1A-CHA	-2.05	120.11	123.89
32	D	406	PL9	C45-C44-C43	-2.05	119.47	123.50
24	B	617	CLA	C1C-NC-C4C	-2.05	103.77	106.27
32	d	406	PL9	C27-C28-C29	-2.05	123.30	127.76
36	h	102	DGD	C3G-O3G-C1D	-2.05	109.51	113.82
26	H	101	BCR	C24-C23-C22	-2.05	123.09	126.22
26	B	618	BCR	C21-C20-C19	-2.05	116.88	123.13
34	B	621	LMG	C30-C29-C28	-2.05	105.54	113.59
36	h	102	DGD	O2G-C1B-O1B	-2.05	118.17	123.67
24	B	613	CLA	C1D-CHD-C4C	-2.05	119.50	122.60
26	c	526	BCR	C16-C17-C18	-2.04	124.24	127.20
24	C	510	CLA	C1C-NC-C4C	-2.04	103.79	106.27
24	D	401	CLA	O1D-CGD-CBD	-2.04	121.70	124.62
26	d	405	BCR	C29-C28-C27	-2.04	106.39	111.53
36	C	517	DGD	C3G-C2G-C1G	-2.04	107.30	112.07
24	C	509	CLA	O1D-CGD-CBD	-2.04	121.70	124.62
26	c	526	BCR	C31-C1-C6	-2.04	107.11	110.30
24	B	610	CLA	C4-C3-C2	-2.04	119.50	123.50
26	c	526	BCR	C21-C20-C19	-2.04	116.92	123.13
24	b	607	CLA	C4A-NA-C1A	-2.03	103.72	106.36
24	B	617	CLA	C2A-C1A-CHA	-2.03	120.14	123.89
24	C	510	CLA	C4B-CHC-C1C	-2.03	124.90	129.26
24	B	612	CLA	O2A-CGA-O1A	-2.03	118.25	123.49
32	a	416	PL9	C25-C24-C23	-2.03	119.51	123.50
24	b	614	CLA	C4-C3-C2	-2.03	119.52	123.50
26	b	622	BCR	C39-C30-C25	-2.03	107.12	110.30
26	b	624	BCR	C21-C20-C19	-2.03	116.95	123.13
34	c	521	LMG	O8-C28-O10	-2.02	118.27	123.49
24	b	617	CLA	C4B-CHC-C1C	-2.02	124.91	129.26
24	b	619	CLA	OBD-CAD-C3D	-2.02	124.22	128.35
24	C	506	CLA	O1D-CGD-CBD	-2.02	121.72	124.62
24	a	409	CLA	CMA-C3A-C2A	-2.02	105.40	114.35
26	K	101	BCR	C16-C17-C18	-2.02	124.28	127.20
36	c	519	DGD	O1G-C1A-O1A	-2.02	118.28	123.49
24	B	611	CLA	C2A-C1A-CHA	-2.02	120.17	123.89
24	D	403	CLA	O2A-CGA-O1A	-2.02	118.28	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	515	BCR	C15-C14-C13	-2.02	124.28	127.20
24	B	610	CLA	CGD-CBD-CAD	-2.02	103.78	110.62
24	C	514	CLA	OBD-CAD-C3D	-2.02	124.24	128.35
32	A	419	PL9	C30-C29-C28	-2.02	119.54	123.50
24	C	504	CLA	C3B-CAB-CBB	-2.02	122.19	126.32
24	d	404	CLA	C4A-NA-C1A	-2.02	103.75	106.36
24	c	506	CLA	C1C-NC-C4C	-2.01	103.82	106.27
24	B	603	CLA	C4A-NA-C1A	-2.01	103.75	106.36
26	c	516	BCR	C35-C13-C14	-2.01	119.93	122.90
26	D	405	BCR	C29-C28-C27	-2.01	106.46	111.53
24	b	611	CLA	C2A-C1A-CHA	-2.01	120.19	123.89
24	B	611	CLA	C4B-CHC-C1C	-2.01	124.95	129.26
24	c	515	CLA	C4B-CHC-C1C	-2.01	124.95	129.26
27	l	101	SQD	C1-C2-C3	-2.01	106.01	109.97
27	a	411	SQD	O48-C23-O10	-2.01	118.31	123.49
24	a	409	CLA	OBD-CAD-C3D	-2.01	124.26	128.35
26	h	101	BCR	C36-C18-C17	-2.00	119.94	122.90
24	c	514	CLA	C4B-CHC-C1C	-2.00	124.96	129.26
24	b	609	CLA	O2D-CGD-O1D	-2.00	119.66	123.79
24	a	407	CLA	CAA-CBA-CGA	2.00	119.18	113.32
24	b	617	CLA	CHB-C4A-NA	2.00	127.28	124.51
25	A	408	PHO	CBD-CHA-C1A	2.00	131.08	126.36
24	B	614	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	b	614	CLA	C6-C5-C3	2.01	116.89	112.48
24	B	603	CLA	O2A-CGA-CBA	2.01	118.02	111.90
24	b	615	CLA	CHB-C4A-NA	2.01	127.29	124.51
25	a	408	PHO	C2C-C1C-NC	2.01	112.75	109.73
36	d	407	DGD	O6D-C5D-C6D	2.01	110.72	106.61
25	a	408	PHO	CMC-C2C-C1C	2.01	128.34	125.06
35	c	523	HTG	C1-O5-C5	2.02	116.58	112.74
26	K	101	BCR	C33-C5-C4	2.02	117.25	113.43
24	C	509	CLA	C3D-CAD-CBD	2.02	110.45	107.60
24	c	504	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	b	613	CLA	C4-C3-C5	2.03	118.51	115.41
26	b	622	BCR	C24-C25-C26	2.03	126.03	121.37
24	a	409	CLA	CED-O2D-CGD	2.04	120.77	115.99
35	D	411	HTG	O5-C1-C2	2.04	112.96	110.19
24	b	610	CLA	CMB-C2B-C1B	2.04	131.74	128.36
30	I	102	LMT	C1B-C2B-C3B	2.04	114.00	109.97
24	B	615	CLA	CED-O2D-CGD	2.05	120.79	115.99
25	A	407	PHO	CHC-C1C-NC	2.05	128.49	124.66
35	C	523	HTG	O5-C1-C2	2.05	112.97	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	CED-O2D-CGD	2.05	120.80	115.99
24	b	621	CLA	CED-O2D-CGD	2.05	120.81	115.99
24	C	513	CLA	CHB-C4A-NA	2.05	127.35	124.51
24	c	508	CLA	CHB-C4A-NA	2.06	127.35	124.51
24	B	608	CLA	CMB-C2B-C3B	2.06	129.11	125.09
24	b	615	CLA	CMB-C2B-C3B	2.06	129.12	125.09
36	C	519	DGD	C1G-O1G-C1A	2.06	122.61	116.85
24	B	606	CLA	O2A-CGA-CBA	2.06	118.18	111.90
34	J	101	LMG	O8-C28-C29	2.06	118.18	111.90
24	B	602	CLA	CHB-C4A-NA	2.06	127.36	124.51
38	E	103	HEM	CHC-C4B-NB	2.07	129.50	124.52
24	A	409	CLA	CMB-C2B-C3B	2.07	129.14	125.09
24	c	510	CLA	CHB-C4A-NA	2.07	127.38	124.51
35	b	604	HTG	O5-C1-C2	2.07	113.00	110.19
36	C	519	DGD	O1G-C1A-C2A	2.07	118.22	111.90
24	C	503	CLA	C3D-CAD-CBD	2.07	110.53	107.60
24	B	609	CLA	CHB-C4A-NA	2.08	127.38	124.51
24	b	611	CLA	CHB-C4A-NA	2.08	127.38	124.51
35	b	627	HTG	C1-C2-C3	2.08	115.29	110.69
25	A	407	PHO	C4-C3-C5	2.08	118.58	115.41
34	C	501	LMG	O1-C1-C2	2.08	110.67	108.04
34	C	521	LMG	O6-C5-C6	2.08	111.61	106.36
24	c	512	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	D	401	CLA	C4-C3-C5	2.08	118.59	115.41
35	B	631	HTG	C1-O5-C5	2.09	116.72	112.74
24	b	607	CLA	CMB-C2B-C3B	2.09	129.18	125.09
26	B	620	BCR	C34-C9-C8	2.10	121.59	118.10
25	a	408	PHO	CMB-C2B-C1B	2.10	128.48	125.06
24	D	401	CLA	CAA-CBA-CGA	2.10	119.48	113.32
26	D	405	BCR	C29-C30-C25	2.10	113.70	110.36
30	D	402	LMT	C3B-C4B-C5B	2.11	113.87	110.20
24	b	612	CLA	O2A-CGA-CBA	2.11	118.32	111.90
24	C	513	CLA	CED-O2D-CGD	2.11	120.94	115.99
26	y	101	BCR	C1-C6-C7	2.11	121.73	115.82
35	B	622	HTG	O5-C1-C2	2.11	113.06	110.19
24	B	607	CLA	CMB-C2B-C3B	2.11	129.22	125.09
24	B	604	CLA	CED-O2D-CGD	2.12	120.95	115.99
24	b	614	CLA	CED-O2D-CGD	2.12	120.95	115.99
36	C	517	DGD	O6D-C5D-C6D	2.12	110.94	106.61
25	a	408	PHO	C4D-C3D-CAD	2.12	109.33	105.51
24	B	610	CLA	CMB-C2B-C1B	2.12	131.88	128.36
34	C	520	LMG	O6-C5-C6	2.13	111.74	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	CAA-CBA-CGA	2.13	119.56	113.32
24	b	619	CLA	CHB-C4A-NA	2.14	127.47	124.51
30	D	402	LMT	O5'-C5'-C4'	2.14	114.26	109.75
24	B	614	CLA	CMB-C2B-C3B	2.14	129.28	125.09
24	b	621	CLA	CMB-C2B-C3B	2.15	129.28	125.09
24	c	508	CLA	CMC-C2C-C1C	2.15	128.34	125.02
35	B	622	HTG	C1-O5-C5	2.15	116.83	112.74
26	c	516	BCR	C2-C1-C6	2.15	113.77	110.36
26	B	619	BCR	C2-C1-C6	2.15	113.77	110.36
24	b	615	CLA	C4-C3-C5	2.15	118.70	115.41
24	C	514	CLA	CHB-C4A-NA	2.16	127.49	124.51
36	d	407	DGD	C1E-O6E-C5E	2.16	117.93	113.75
24	B	617	CLA	C4-C3-C5	2.16	118.70	115.41
24	B	611	CLA	CMB-C2B-C3B	2.16	129.31	125.09
26	d	405	BCR	C38-C26-C27	2.16	117.52	113.43
30	m	102	LMT	O1'-C1'-C2'	2.16	110.77	108.04
24	B	603	CLA	CAC-C3C-C4C	2.16	127.97	124.83
24	c	510	CLA	CAC-C3C-C4C	2.16	127.97	124.83
24	b	607	CLA	CMC-C2C-C1C	2.16	128.37	125.02
24	B	604	CLA	C6-C5-C3	2.17	117.24	112.48
24	C	510	CLA	CMC-C2C-C1C	2.17	128.37	125.02
35	c	522	HTG	C1-O5-C5	2.17	116.87	112.74
24	B	613	CLA	O2A-CGA-CBA	2.17	118.52	111.90
26	T	102	BCR	C35-C13-C12	2.17	121.72	118.10
24	A	406	CLA	CED-O2D-CGD	2.17	121.09	115.99
24	B	616	CLA	O2A-CGA-CBA	2.18	118.53	111.90
24	b	606	CLA	CMB-C2B-C3B	2.18	129.35	125.09
24	b	606	CLA	CMC-C2C-C1C	2.18	128.39	125.02
24	c	512	CLA	CAC-C3C-C4C	2.19	128.00	124.83
25	d	403	PHO	C3C-C4C-NC	2.19	113.77	110.24
24	C	504	CLA	CMB-C2B-C3B	2.20	129.39	125.09
24	c	512	CLA	CMB-C2B-C3B	2.21	129.41	125.09
24	a	407	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	b	618	CLA	CMC-C2C-C1C	2.21	128.44	125.02
24	c	515	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	B	616	CLA	CED-O2D-CGD	2.22	121.21	115.99
26	K	101	BCR	C29-C30-C25	2.23	113.89	110.36
26	b	623	BCR	C29-C30-C25	2.23	113.89	110.36
24	c	514	CLA	CED-O2D-CGD	2.23	121.22	115.99
24	C	509	CLA	CMB-C2B-C3B	2.24	129.46	125.09
24	b	621	CLA	C4-C3-C5	2.24	118.82	115.41
36	D	407	DGD	O6D-C5D-C6D	2.24	111.18	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	419	PL9	C40-C39-C41	2.24	118.83	115.41
24	b	613	CLA	CMB-C2B-C3B	2.24	129.47	125.09
38	E	103	HEM	CMD-C2D-C3D	2.24	124.28	114.35
26	b	622	BCR	C29-C30-C25	2.25	113.92	110.36
24	C	509	CLA	C4-C3-C5	2.25	118.84	115.41
27	A	416	SQD	O5-C5-C4	2.25	113.91	109.68
24	B	602	CLA	CAC-C3C-C4C	2.25	128.10	124.83
24	D	404	CLA	CMC-C2C-C1C	2.25	128.50	125.02
26	c	526	BCR	C2-C1-C6	2.25	113.93	110.36
24	c	506	CLA	O2A-CGA-CBA	2.25	118.77	111.90
37	D	408	LHG	C6-O8-C23	2.26	123.16	116.85
26	T	102	BCR	C29-C30-C25	2.26	113.94	110.36
32	D	406	PL9	C10-C9-C11	2.26	118.86	115.41
24	C	511	CLA	O2A-CGA-CBA	2.26	118.79	111.90
27	A	416	SQD	O6-C1-C2	2.26	110.90	108.04
24	d	402	CLA	CMB-C2B-C3B	2.26	129.52	125.09
35	C	522	HTG	O5-C1-C2	2.26	113.26	110.19
24	B	610	CLA	C6-C5-C3	2.27	117.46	112.48
24	C	504	CLA	CMC-C2C-C1C	2.27	128.53	125.02
24	B	611	CLA	CMC-C2C-C1C	2.27	128.53	125.02
24	B	614	CLA	CMC-C2C-C1C	2.28	128.54	125.02
24	A	409	CLA	CHB-C4A-NA	2.28	127.66	124.51
32	D	406	PL9	C20-C19-C21	2.28	118.89	115.41
24	C	508	CLA	CMB-C2B-C3B	2.28	129.55	125.09
34	j	101	LMG	O8-C28-C29	2.28	118.86	111.90
24	d	402	CLA	CAC-C3C-C4C	2.29	128.15	124.83
26	h	101	BCR	C29-C30-C25	2.29	113.98	110.36
24	c	514	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	B	617	CLA	CMB-C2B-C3B	2.29	129.57	125.09
24	A	406	CLA	CAA-CBA-CGA	2.29	120.02	113.32
24	b	614	CLA	O2A-CGA-CBA	2.29	118.88	111.90
24	c	515	CLA	CMB-C2B-C3B	2.29	129.57	125.09
24	b	611	CLA	O2A-CGA-CBA	2.29	118.89	111.90
24	d	404	CLA	CMB-C2B-C3B	2.30	129.58	125.09
24	B	610	CLA	O2A-CGA-CBA	2.30	118.90	111.90
24	C	510	CLA	CMB-C2B-C3B	2.30	129.59	125.09
25	A	408	PHO	C2A-C1A-NA	2.30	115.03	112.08
36	D	407	DGD	O6E-C5E-C4E	2.30	114.01	109.68
24	C	513	CLA	CAC-C3C-C4C	2.31	128.18	124.83
24	b	614	CLA	CAC-C3C-C4C	2.31	128.18	124.83
24	D	401	CLA	O2A-CGA-CBA	2.31	118.94	111.90
24	b	618	CLA	CAC-C3C-C4C	2.31	128.19	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	401	LMT	C1'-O5'-C5'	2.32	118.24	113.75
24	C	506	CLA	O2A-CGA-CBA	2.32	118.97	111.90
26	d	405	BCR	C37-C22-C23	2.32	121.97	118.10
25	A	408	PHO	O2A-CGA-CBA	2.33	118.99	111.90
30	b	602	LMT	O5'-C1'-C2'	2.33	115.05	110.28
25	A	407	PHO	C3C-C4C-NC	2.33	114.00	110.24
24	c	511	CLA	CMB-C2B-C3B	2.33	129.65	125.09
24	B	615	CLA	CMB-C2B-C3B	2.33	129.65	125.09
24	c	503	CLA	CMC-C2C-C1C	2.33	128.63	125.02
36	h	102	DGD	O5D-C1E-C2E	2.33	110.99	108.04
24	c	504	CLA	CAC-C3C-C4C	2.33	128.22	124.83
36	C	519	DGD	O2G-C1B-C2B	2.34	116.60	111.53
24	B	605	CLA	CAC-C3C-C4C	2.34	128.22	124.83
24	C	510	CLA	O2A-CGA-CBA	2.34	119.03	111.90
25	d	403	PHO	CBD-CHA-C1A	2.35	131.90	126.36
24	B	608	CLA	CAC-C3C-C4C	2.35	128.25	124.83
26	D	405	BCR	C30-C25-C24	2.36	122.41	115.82
36	H	102	DGD	O1G-C1A-C2A	2.36	119.08	111.90
24	b	620	CLA	CMC-C2C-C1C	2.36	128.67	125.02
25	A	407	PHO	CBD-CHA-C1A	2.36	131.91	126.36
36	d	407	DGD	O6E-C5E-C4E	2.36	114.11	109.68
24	c	510	CLA	O2A-CGA-CBA	2.37	119.11	111.90
24	C	511	CLA	CMB-C2B-C3B	2.37	129.72	125.09
24	B	617	CLA	O2A-CGA-CBA	2.38	119.14	111.90
32	a	416	PL9	C45-C44-C46	2.38	119.04	115.41
27	a	402	SQD	O6-C1-C2	2.38	111.04	108.04
24	B	604	CLA	CAC-C3C-C4C	2.38	128.29	124.83
34	B	621	LMG	O8-C28-C29	2.38	119.16	111.90
24	b	616	CLA	O2A-CGA-CBA	2.39	119.17	111.90
36	C	517	DGD	O1G-C1A-C2A	2.39	119.19	111.90
26	D	405	BCR	C37-C22-C23	2.39	122.08	118.10
24	b	611	CLA	CMB-C2B-C3B	2.39	129.77	125.09
30	m	103	LMT	C1B-O5B-C5B	2.39	118.39	113.75
24	d	401	CLA	O2A-CGA-CBA	2.40	119.21	111.90
26	d	405	BCR	C29-C30-C25	2.40	114.16	110.36
24	B	604	CLA	CMB-C2B-C3B	2.40	129.79	125.09
30	a	401	LMT	O5'-C5'-C4'	2.41	114.83	109.75
32	d	406	PL9	C8-C7-C3	2.41	119.12	111.60
24	D	401	CLA	CHB-C4A-NA	2.41	127.84	124.51
38	v	202	HEM	CMD-C2D-C3D	2.41	125.01	114.35
24	C	512	CLA	CMC-C2C-C1C	2.42	128.76	125.02
36	d	407	DGD	O1G-C1A-C2A	2.42	119.28	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t	101	BCR	C2-C1-C6	2.43	114.21	110.36
24	C	506	CLA	CMC-C2C-C1C	2.43	128.78	125.02
30	m	103	LMT	O5B-C5B-C4B	2.43	114.25	109.68
24	c	508	CLA	CMB-C2B-C3B	2.44	129.85	125.09
26	t	101	BCR	C1-C6-C7	2.44	122.64	115.82
35	b	627	HTG	C1-O5-C5	2.44	117.39	112.74
24	C	504	CLA	CAC-C3C-C4C	2.44	128.37	124.83
26	b	624	BCR	C2-C1-C6	2.44	114.22	110.36
36	c	518	DGD	O1G-C1A-C2A	2.44	119.35	111.90
26	K	101	BCR	C2-C1-C6	2.44	114.23	110.36
32	a	416	PL9	C53-C6-C1	2.45	120.78	114.94
24	B	602	CLA	CMC-C2C-C1C	2.45	128.81	125.02
37	l	102	LHG	O8-C23-C24	2.45	119.36	111.90
24	b	612	CLA	CAA-CBA-CGA	2.45	120.49	113.32
24	A	406	CLA	O2A-CGA-CBA	2.45	119.37	111.90
32	d	406	PL9	C35-C34-C36	2.45	119.16	115.41
24	B	612	CLA	O2A-CGA-CBA	2.45	119.38	111.90
36	D	407	DGD	O5D-C1E-C2E	2.46	111.14	108.04
24	b	612	CLA	CAC-C3C-C4C	2.46	128.40	124.83
30	D	402	LMT	O1B-C4'-C3'	2.46	113.52	107.17
24	D	401	CLA	CMC-C2C-C1C	2.46	128.83	125.02
24	d	401	CLA	CAA-CBA-CGA	2.47	120.53	113.32
24	D	404	CLA	O2A-CGA-CBA	2.47	119.41	111.90
32	d	406	PL9	C53-C6-C1	2.47	120.83	114.94
24	C	507	CLA	CMC-C2C-C1C	2.47	128.84	125.02
24	C	508	CLA	C3B-C4B-NB	2.47	112.40	109.21
24	b	608	CLA	CMB-C2B-C3B	2.47	129.92	125.09
24	c	508	CLA	C4-C3-C5	2.47	119.18	115.41
24	C	503	CLA	CAC-C3C-C4C	2.48	128.42	124.83
24	c	511	CLA	CMC-C2C-C1C	2.48	128.85	125.02
24	B	610	CLA	C4-C3-C5	2.48	119.19	115.41
24	c	513	CLA	CMB-C2B-C3B	2.48	129.94	125.09
24	C	502	CLA	O2A-CGA-CBA	2.48	119.46	111.90
24	c	508	CLA	CED-O2D-CGD	2.49	121.82	115.99
24	b	617	CLA	CAC-C3C-C4C	2.49	128.44	124.83
24	d	404	CLA	O2A-CGA-CBA	2.49	119.49	111.90
24	C	510	CLA	CAC-C3C-C4C	2.49	128.45	124.83
34	z	101	LMG	O1-C1-C2	2.50	111.19	108.04
26	T	102	BCR	C1-C6-C7	2.50	122.81	115.82
24	c	503	CLA	C4-C3-C5	2.50	119.23	115.41
24	B	609	CLA	CMC-C2C-C1C	2.50	128.89	125.02
35	b	628	HTG	C1-O5-C5	2.50	117.51	112.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	CAC-C3C-C4C	2.50	128.46	124.83
24	D	401	CLA	CMB-C2B-C3B	2.50	129.98	125.09
24	c	508	CLA	O2A-CGA-CBA	2.50	119.53	111.90
32	A	419	PL9	C53-C6-C1	2.51	120.93	114.94
24	d	402	CLA	CMC-C2C-C1C	2.51	128.90	125.02
27	a	411	SQD	O7-S-C6	2.51	109.06	106.94
24	B	607	CLA	CAC-C3C-C4C	2.51	128.47	124.83
25	d	403	PHO	O2A-CGA-CBA	2.51	119.55	111.90
30	A	417	LMT	C1'-O5'-C5'	2.51	118.62	113.75
24	b	609	CLA	C4-C3-C5	2.51	119.25	115.41
24	C	508	CLA	O2A-CGA-CBA	2.51	119.56	111.90
24	b	616	CLA	C4-C3-C5	2.52	119.25	115.41
24	c	515	CLA	C4-C3-C5	2.52	119.26	115.41
24	B	606	CLA	CAC-C3C-C4C	2.52	128.49	124.83
24	c	513	CLA	O2A-CGA-CBA	2.53	119.60	111.90
24	a	409	CLA	O2A-CGA-CBA	2.53	119.61	111.90
24	C	514	CLA	O2A-CGA-CBA	2.53	119.61	111.90
34	C	501	LMG	O8-C28-C29	2.53	119.61	111.90
24	A	406	CLA	CMC-C2C-C1C	2.53	128.94	125.02
24	C	503	CLA	C4-C3-C5	2.53	119.28	115.41
32	D	406	PL9	C53-C6-C1	2.54	121.00	114.94
24	c	506	CLA	C6-C5-C3	2.54	118.05	112.48
26	H	101	BCR	C29-C30-C25	2.54	114.38	110.36
24	b	615	CLA	CMC-C2C-C1C	2.54	128.95	125.02
24	C	508	CLA	CAC-C3C-C4C	2.55	128.53	124.83
37	d	409	LHG	O8-C23-C24	2.55	119.68	111.90
24	C	511	CLA	CAC-C3C-C4C	2.55	128.53	124.83
34	c	520	LMG	O8-C28-C29	2.55	119.68	111.90
24	C	504	CLA	O2A-CGA-CBA	2.56	119.70	111.90
24	b	607	CLA	O2A-CGA-CBA	2.56	119.70	111.90
24	B	613	CLA	C4-C3-C5	2.56	119.32	115.41
24	B	616	CLA	C4-C3-C5	2.56	119.32	115.41
26	Y	101	BCR	C37-C22-C23	2.56	122.36	118.10
24	A	405	CLA	O2A-CGA-CBA	2.57	119.72	111.90
24	d	401	CLA	CAC-C3C-C4C	2.57	128.56	124.83
25	A	408	PHO	CMC-C2C-C1C	2.57	129.25	125.06
24	B	613	CLA	CMB-C2B-C3B	2.57	130.12	125.09
34	c	501	LMG	O8-C28-C29	2.58	119.75	111.90
24	C	506	CLA	C4-C3-C5	2.58	119.35	115.41
24	c	503	CLA	CAC-C3C-C4C	2.58	128.58	124.83
24	c	507	CLA	CMC-C2C-C1C	2.59	129.02	125.02
24	c	512	CLA	O2A-CGA-CBA	2.59	119.79	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PHO	C3C-C4C-NC	2.59	114.43	110.24
38	E	103	HEM	C2D-C3D-C4D	2.60	105.90	101.50
37	D	409	LHG	O8-C23-C24	2.60	119.81	111.90
24	A	409	CLA	O2A-CGA-CBA	2.60	119.82	111.90
24	b	615	CLA	CAC-C3C-C4C	2.60	128.61	124.83
25	A	407	PHO	C4D-C3D-CAD	2.60	110.19	105.51
24	a	409	CLA	CHB-C4A-NA	2.61	128.12	124.51
38	e	102	HEM	CAD-CBD-CGD	2.61	123.65	113.02
24	a	407	CLA	C4-C3-C5	2.62	119.41	115.41
34	z	101	LMG	O6-C5-C4	2.62	114.60	109.68
25	A	408	PHO	C2C-C1C-NC	2.62	113.66	109.73
30	b	602	LMT	O5'-C5'-C4'	2.63	115.29	109.75
36	D	407	DGD	O1G-C1A-C2A	2.63	119.90	111.90
24	b	610	CLA	O2A-CGA-CBA	2.63	119.92	111.90
24	c	511	CLA	C4-C3-C5	2.63	119.43	115.41
24	c	514	CLA	C4-C3-C5	2.64	119.44	115.41
25	A	407	PHO	C2B-C1B-NB	2.65	113.70	109.73
24	c	503	CLA	O2A-CGA-CBA	2.65	119.97	111.90
34	Z	101	LMG	C4-C3-C2	2.65	115.74	110.79
32	A	419	PL9	C8-C7-C3	2.65	119.89	111.60
24	b	611	CLA	C4-C3-C5	2.66	119.46	115.41
34	z	101	LMG	C3-C4-C5	2.66	114.83	110.20
24	b	614	CLA	C4-C3-C5	2.66	119.47	115.41
26	b	624	BCR	C37-C22-C23	2.66	122.53	118.10
35	B	624	HTG	C1-C2-C3	2.66	116.58	110.69
37	E	101	LHG	O8-C23-C24	2.66	120.02	111.90
24	b	613	CLA	CAC-C3C-C4C	2.67	128.70	124.83
27	F	101	SQD	O48-C23-C24	2.67	120.04	111.90
24	C	507	CLA	O2A-CGA-CBA	2.67	120.04	111.90
24	B	608	CLA	O2A-CGA-CBA	2.68	120.06	111.90
24	D	404	CLA	CAC-C3C-C4C	2.68	128.72	124.83
36	c	517	DGD	O1G-C1A-C2A	2.68	120.06	111.90
24	D	403	CLA	CAC-C3C-C4C	2.68	128.72	124.83
24	b	608	CLA	CAC-C3C-C4C	2.68	128.73	124.83
24	c	510	CLA	CMC-C2C-C1C	2.68	129.17	125.02
34	C	521	LMG	O8-C28-C29	2.69	120.08	111.90
24	C	513	CLA	O2A-CGA-CBA	2.69	120.09	111.90
24	A	406	CLA	CAC-C3C-C4C	2.69	128.74	124.83
24	c	511	CLA	O2A-CGA-CBA	2.69	120.10	111.90
34	c	521	LMG	O8-C28-C29	2.69	120.10	111.90
24	B	605	CLA	O2A-CGA-CBA	2.70	120.12	111.90
24	C	503	CLA	CMC-C2C-C1C	2.70	129.20	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	CMB-C2B-C3B	2.70	130.37	125.09
32	a	416	PL9	C35-C34-C36	2.71	119.55	115.41
26	B	620	BCR	C2-C1-C6	2.71	114.65	110.36
24	b	616	CLA	CAC-C3C-C4C	2.71	128.76	124.83
25	a	408	PHO	C3C-C4C-NC	2.71	114.62	110.24
24	c	515	CLA	O2A-CGA-CBA	2.71	120.16	111.90
24	c	514	CLA	CMC-C2C-C1C	2.71	129.22	125.02
34	b	625	LMG	O7-C10-C11	2.72	117.44	111.53
24	C	505	CLA	C4-C3-C5	2.72	119.56	115.41
24	B	602	CLA	C4-C3-C5	2.72	119.57	115.41
27	l	101	SQD	O48-C23-C24	2.72	120.20	111.90
24	a	407	CLA	CAC-C3C-C4C	2.73	128.79	124.83
24	a	407	CLA	CMC-C2C-C1C	2.73	129.25	125.02
24	C	513	CLA	CMC-C2C-C1C	2.74	129.26	125.02
25	d	403	PHO	C2C-C1C-NC	2.74	113.83	109.73
38	e	102	HEM	CMD-C2D-C3D	2.74	126.47	114.35
24	A	406	CLA	CMB-C2B-C3B	2.74	130.45	125.09
24	b	609	CLA	O2A-CGA-CBA	2.74	120.26	111.90
24	b	618	CLA	O2A-CGA-CBA	2.74	120.26	111.90
24	B	614	CLA	O2A-CGA-CBA	2.75	120.28	111.90
24	a	409	CLA	CAC-C3C-C4C	2.75	128.82	124.83
24	c	504	CLA	O2A-CGA-CBA	2.76	120.30	111.90
26	T	102	BCR	C2-C1-C6	2.76	114.73	110.36
24	c	505	CLA	O2A-CGA-CBA	2.76	120.31	111.90
24	d	404	CLA	CAC-C3C-C4C	2.76	128.84	124.83
24	b	613	CLA	CMC-C2C-C1C	2.76	129.29	125.02
38	V	203	HEM	CMD-C2D-C3D	2.76	126.57	114.35
32	A	419	PL9	C30-C29-C31	2.77	119.63	115.41
36	h	102	DGD	O1G-C1A-C2A	2.77	120.33	111.90
27	A	411	SQD	O48-C23-C24	2.77	120.34	111.90
24	b	609	CLA	CAC-C3C-C4C	2.77	128.86	124.83
24	b	619	CLA	C4-C3-C5	2.78	119.65	115.41
24	b	616	CLA	CMC-C2C-C1C	2.78	129.32	125.02
32	D	406	PL9	C15-C14-C16	2.78	119.66	115.41
24	B	604	CLA	O2A-CGA-CBA	2.79	120.40	111.90
27	a	411	SQD	O48-C23-C24	2.79	120.40	111.90
32	d	406	PL9	C20-C19-C21	2.79	119.67	115.41
36	C	518	DGD	O1G-C1A-C2A	2.79	120.41	111.90
38	e	102	HEM	C2D-C3D-C4D	2.80	106.24	101.50
24	B	614	CLA	CAC-C3C-C4C	2.80	128.90	124.83
24	B	603	CLA	CMB-C2B-C3B	2.80	130.57	125.09
24	C	509	CLA	CAC-C3C-C4C	2.80	128.90	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	CMC-C2C-C1C	2.80	129.36	125.02
24	B	609	CLA	O2A-CGA-CBA	2.81	120.46	111.90
24	D	404	CLA	C4-C3-C5	2.81	119.70	115.41
27	f	101	SQD	O48-C23-C24	2.81	120.47	111.90
27	A	416	SQD	C3-C4-C5	2.81	115.10	110.20
24	B	611	CLA	C3B-C4B-NB	2.82	112.86	109.21
32	a	416	PL9	C40-C39-C41	2.82	119.72	115.41
24	c	509	CLA	CAC-C3C-C4C	2.82	128.93	124.83
24	b	607	CLA	CAC-C3C-C4C	2.82	128.93	124.83
37	D	410	LHG	O8-C23-C24	2.82	120.51	111.90
30	A	417	LMT	O5'-C5'-C4'	2.83	115.72	109.75
25	d	403	PHO	CAC-C3C-C4C	2.83	128.46	125.16
24	C	507	CLA	CAC-C3C-C4C	2.83	128.94	124.83
25	A	407	PHO	CAC-C3C-C4C	2.83	128.47	125.16
24	c	515	CLA	CAC-C3C-C4C	2.83	128.94	124.83
24	B	602	CLA	CMB-C2B-C3B	2.83	130.63	125.09
24	b	619	CLA	CMC-C2C-C1C	2.84	129.41	125.02
24	C	513	CLA	CMB-C2B-C3B	2.84	130.65	125.09
24	c	506	CLA	CAC-C3C-C4C	2.84	128.96	124.83
24	B	606	CLA	C4-C3-C5	2.85	119.75	115.41
24	B	602	CLA	O2A-CGA-CBA	2.85	120.58	111.90
24	b	619	CLA	O2A-CGA-CBA	2.85	120.58	111.90
32	D	406	PL9	C25-C24-C26	2.85	119.76	115.41
27	F	101	SQD	C3-C4-C5	2.85	115.17	110.20
37	d	408	LHG	O8-C23-C24	2.85	120.59	111.90
24	c	510	CLA	C4-C3-C5	2.85	119.77	115.41
24	C	503	CLA	C3B-C4B-NB	2.86	112.91	109.21
34	z	101	LMG	O8-C28-C29	2.87	120.63	111.90
24	B	612	CLA	C4-C3-C5	2.87	119.79	115.41
27	f	101	SQD	O5-C5-C4	2.87	115.07	109.68
32	A	419	PL9	C35-C34-C36	2.87	119.79	115.41
24	A	405	CLA	CMC-C2C-C1C	2.87	129.47	125.02
25	a	408	PHO	CAC-C3C-C4C	2.88	128.52	125.16
24	C	510	CLA	C4-C3-C5	2.88	119.80	115.41
32	d	406	PL9	C15-C14-C16	2.88	119.81	115.41
24	C	509	CLA	O2A-CGA-CBA	2.88	120.68	111.90
24	a	407	CLA	C3B-C4B-NB	2.88	112.93	109.21
24	C	512	CLA	CAC-C3C-C4C	2.88	129.02	124.83
24	C	503	CLA	O2A-CGA-CBA	2.88	120.69	111.90
24	B	612	CLA	CMC-C2C-C1C	2.89	129.49	125.02
24	b	606	CLA	O2A-CGA-CBA	2.89	120.70	111.90
36	c	519	DGD	O2G-C1B-C2B	2.89	117.81	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	CMC-C2C-C1C	2.89	129.49	125.02
32	A	419	PL9	C45-C44-C46	2.89	119.82	115.41
24	A	409	CLA	C3B-C4B-NB	2.89	112.95	109.21
24	B	612	CLA	CAC-C3C-C4C	2.90	129.03	124.83
26	B	619	BCR	C29-C30-C25	2.91	114.96	110.36
37	d	410	LHG	O8-C23-C24	2.91	120.75	111.90
24	a	407	CLA	O2A-CGA-CBA	2.91	120.76	111.90
37	L	101	LHG	O8-C23-C24	2.91	120.77	111.90
24	c	515	CLA	CMC-C2C-C1C	2.92	129.54	125.02
24	c	513	CLA	CAC-C3C-C4C	2.92	129.07	124.83
24	b	606	CLA	C3B-C4B-NB	2.92	112.99	109.21
24	B	611	CLA	C4-C3-C5	2.93	119.88	115.41
32	a	416	PL9	C25-C24-C26	2.93	119.88	115.41
24	c	510	CLA	CMB-C2B-C3B	2.93	130.82	125.09
38	v	202	HEM	C2D-C3D-C4D	2.94	106.48	101.50
24	b	618	CLA	C4-C3-C5	2.94	119.90	115.41
34	c	501	LMG	O1-C1-C2	2.94	111.75	108.04
24	c	509	CLA	CMC-C2C-C1C	2.94	129.57	125.02
24	c	514	CLA	O2A-CGA-CBA	2.95	120.88	111.90
24	c	505	CLA	CAC-C3C-C4C	2.96	129.12	124.83
24	b	617	CLA	O2A-CGA-CBA	2.96	120.91	111.90
36	d	407	DGD	O5D-C1E-C2E	2.96	111.78	108.04
24	c	505	CLA	C3B-C4B-NB	2.96	113.04	109.21
24	b	615	CLA	O2A-CGA-CBA	2.97	120.94	111.90
27	A	416	SQD	O9-S-C6	2.97	109.44	106.94
24	b	611	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	c	514	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	c	513	CLA	CMC-C2C-C1C	2.97	129.62	125.02
35	C	523	HTG	O5-C5-C4	2.97	115.26	109.68
24	D	401	CLA	CAC-C3C-C4C	2.97	129.15	124.83
24	b	612	CLA	C4-C3-C5	2.98	119.95	115.41
24	C	513	CLA	C4-C3-C5	2.98	119.96	115.41
24	c	509	CLA	C4-C3-C5	2.98	119.96	115.41
24	B	605	CLA	C4-C3-C5	2.98	119.97	115.41
24	b	620	CLA	CAC-C3C-C4C	2.99	129.17	124.83
24	b	609	CLA	C3B-C4B-NB	2.99	113.08	109.21
25	a	408	PHO	C2B-C1B-NB	3.00	114.22	109.73
24	C	504	CLA	C4-C3-C5	3.00	119.99	115.41
25	A	407	PHO	C2C-C1C-NC	3.00	114.22	109.73
38	E	103	HEM	CAD-CBD-CGD	3.00	125.25	113.02
24	c	509	CLA	O2A-CGA-CBA	3.00	121.05	111.90
24	D	403	CLA	CMC-C2C-C1C	3.01	129.68	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	I	102	LMT	C1'-O5'-C5'	3.01	119.59	113.75
24	A	409	CLA	CMC-C2C-C1C	3.01	129.68	125.02
36	c	519	DGD	O1G-C1A-C2A	3.01	121.09	111.90
37	d	408	LHG	O7-C7-C8	3.03	118.11	111.53
24	C	511	CLA	CMC-C2C-C1C	3.03	129.71	125.02
24	B	614	CLA	O2D-CGD-CBD	3.03	115.46	111.30
24	B	614	CLA	CED-O2D-CGD	3.04	123.13	115.99
37	D	408	LHG	O8-C23-C24	3.06	121.23	111.90
24	A	406	CLA	C4-C3-C5	3.06	120.08	115.41
24	c	506	CLA	CMC-C2C-C1C	3.06	129.76	125.02
24	B	611	CLA	O2A-CGA-CBA	3.06	121.24	111.90
34	b	625	LMG	O8-C28-C29	3.07	121.26	111.90
36	H	102	DGD	O2G-C1B-C2B	3.07	118.21	111.53
25	d	403	PHO	C2B-C1B-NB	3.08	114.34	109.73
24	A	405	CLA	CAC-C3C-C4C	3.09	129.31	124.83
24	B	604	CLA	C4-C3-C5	3.09	120.13	115.41
24	C	511	CLA	C4-C3-C5	3.09	120.13	115.41
24	C	508	CLA	C4-C3-C5	3.10	120.14	115.41
24	C	506	CLA	CAC-C3C-C4C	3.10	129.33	124.83
24	B	602	CLA	C3B-C4B-NB	3.10	113.22	109.21
24	B	615	CLA	CAC-C3C-C4C	3.11	129.34	124.83
30	I	102	LMT	C1B-O5B-C5B	3.11	119.79	113.75
24	C	502	CLA	CMC-C2C-C1C	3.11	129.84	125.02
24	B	607	CLA	C4-C3-C5	3.12	120.17	115.41
24	A	405	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	b	611	CLA	CAC-C3C-C4C	3.12	129.36	124.83
24	C	514	CLA	C4-C3-C5	3.12	120.17	115.41
24	c	509	CLA	C3B-C4B-NB	3.12	113.25	109.21
24	B	614	CLA	C4-C3-C5	3.12	120.18	115.41
24	b	613	CLA	C3B-C4B-NB	3.12	113.25	109.21
24	c	512	CLA	CMC-C2C-C1C	3.12	129.85	125.02
24	B	615	CLA	O2A-CGA-CBA	3.13	121.44	111.90
24	d	404	CLA	C4-C3-C5	3.13	120.19	115.41
24	b	606	CLA	C4-C3-C5	3.14	120.20	115.41
30	m	103	LMT	O1'-C1'-C2'	3.14	112.01	108.04
34	Z	101	LMG	O6-C1-C2	3.15	116.74	110.28
24	B	606	CLA	C3B-C4B-NB	3.15	113.28	109.21
24	c	508	CLA	CAC-C3C-C4C	3.16	129.41	124.83
24	C	507	CLA	C4-C3-C5	3.16	120.24	115.41
38	V	203	HEM	C2D-C3D-C4D	3.16	106.86	101.50
24	B	617	CLA	CAC-C3C-C4C	3.16	129.42	124.83
27	f	101	SQD	O9-S-C6	3.17	109.61	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	510	CLA	C3B-C4B-NB	3.17	113.31	109.21
24	D	403	CLA	O2A-CGA-CBA	3.18	121.58	111.90
24	c	507	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	B	608	CLA	C3B-C4B-NB	3.18	113.32	109.21
34	j	101	LMG	O7-C10-C11	3.18	118.44	111.53
24	B	610	CLA	C3B-C4B-NB	3.18	113.33	109.21
24	b	612	CLA	CMC-C2C-C1C	3.19	129.95	125.02
24	d	402	CLA	C4-C3-C5	3.19	120.28	115.41
32	A	419	PL9	C25-C24-C26	3.19	120.28	115.41
32	d	406	PL9	C40-C39-C41	3.20	120.29	115.41
37	e	101	LHG	O8-C23-C24	3.20	121.64	111.90
24	b	607	CLA	C4-C3-C5	3.20	120.30	115.41
24	b	610	CLA	C3B-C4B-NB	3.20	113.35	109.21
24	b	608	CLA	CMC-C2C-C1C	3.20	129.98	125.02
27	a	411	SQD	O9-S-C6	3.21	109.65	106.94
24	b	616	CLA	C3B-C4B-NB	3.21	113.36	109.21
24	B	604	CLA	CMC-C2C-C1C	3.22	130.00	125.02
24	B	608	CLA	C4-C3-C5	3.22	120.32	115.41
32	d	406	PL9	C10-C9-C11	3.22	120.32	115.41
27	b	601	SQD	O48-C23-C24	3.22	121.71	111.90
27	b	601	SQD	O9-S-C6	3.22	109.66	106.94
24	b	610	CLA	CMC-C2C-C1C	3.22	130.00	125.02
24	b	613	CLA	O2A-CGA-CBA	3.22	121.72	111.90
24	b	615	CLA	C3B-C4B-NB	3.22	113.38	109.21
24	b	619	CLA	CAC-C3C-C4C	3.23	129.53	124.83
24	B	607	CLA	C3B-C4B-NB	3.24	113.40	109.21
27	A	416	SQD	O48-C23-C24	3.24	121.78	111.90
24	B	611	CLA	CAC-C3C-C4C	3.25	129.55	124.83
24	c	512	CLA	C4-C3-C5	3.25	120.38	115.41
24	c	511	CLA	CAC-C3C-C4C	3.26	129.56	124.83
24	b	621	CLA	CAC-C3C-C4C	3.26	129.57	124.83
25	A	408	PHO	C2B-C1B-NB	3.27	114.63	109.73
24	C	514	CLA	CMC-C2C-C1C	3.28	130.10	125.02
24	b	617	CLA	C3B-C4B-NB	3.29	113.46	109.21
24	B	616	CLA	C3B-C4B-NB	3.29	113.47	109.21
24	b	608	CLA	O2A-CGA-CBA	3.29	121.94	111.90
24	B	615	CLA	CMC-C2C-C1C	3.29	130.12	125.02
36	D	407	DGD	C1E-O6E-C5E	3.30	120.15	113.75
24	A	405	CLA	CMB-C2B-C3B	3.30	131.54	125.09
24	C	514	CLA	C3B-C4B-NB	3.30	113.48	109.21
24	a	409	CLA	C4-C3-C5	3.31	120.45	115.41
24	a	406	CLA	O2A-CGA-CBA	3.31	121.98	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	CAC-C3C-C4C	3.32	129.65	124.83
24	b	607	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	C	506	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	b	610	CLA	C4-C3-C5	3.32	120.48	115.41
24	B	612	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	a	406	CLA	O2D-CGD-CBD	3.33	115.87	111.30
24	c	504	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	c	503	CLA	C3B-C4B-NB	3.34	113.52	109.21
32	A	419	PL9	C20-C19-C21	3.34	120.51	115.41
36	h	102	DGD	O2G-C1B-C2B	3.35	118.81	111.53
24	C	512	CLA	C4-C3-C5	3.36	120.53	115.41
27	a	402	SQD	O48-C23-C24	3.36	122.13	111.90
24	B	606	CLA	CMC-C2C-C1C	3.37	130.23	125.02
24	C	513	CLA	C3B-C4B-NB	3.37	113.56	109.21
24	c	505	CLA	CMC-C2C-C1C	3.37	130.23	125.02
24	D	403	CLA	CED-O2D-CGD	3.38	123.91	115.99
36	D	407	DGD	C3D-C4D-C5D	3.38	116.09	110.20
35	b	628	HTG	O5-C1-C2	3.38	114.78	110.19
24	C	502	CLA	C3B-C4B-NB	3.38	113.58	109.21
37	D	408	LHG	O7-C7-C8	3.39	118.90	111.53
32	a	416	PL9	C10-C9-C11	3.41	120.61	115.41
34	c	520	LMG	O7-C10-C11	3.41	118.95	111.53
24	B	605	CLA	C3B-C4B-NB	3.41	113.62	109.21
37	L	101	LHG	O7-C7-C8	3.41	118.95	111.53
24	c	515	CLA	C3B-C4B-NB	3.41	113.62	109.21
32	a	416	PL9	C30-C29-C31	3.42	120.63	115.41
27	l	101	SQD	O9-S-C6	3.42	109.83	106.94
24	B	615	CLA	C3B-C4B-NB	3.43	113.64	109.21
37	D	410	LHG	O7-C7-C8	3.43	118.98	111.53
24	B	603	CLA	C3B-C4B-NB	3.43	113.65	109.21
24	b	621	CLA	O2A-CGA-CBA	3.43	122.36	111.90
24	D	404	CLA	C3B-C4B-NB	3.43	113.65	109.21
35	D	411	HTG	C1'-S1-C1	3.43	105.03	100.30
24	a	406	CLA	CAC-C3C-C4C	3.44	129.83	124.83
37	l	102	LHG	O7-C7-C8	3.45	119.02	111.53
32	a	416	PL9	C20-C19-C21	3.45	120.67	115.41
24	C	504	CLA	C3B-C4B-NB	3.46	113.68	109.21
24	d	404	CLA	CMC-C2C-C1C	3.46	130.38	125.02
24	C	508	CLA	CMC-C2C-C1C	3.47	130.40	125.02
24	B	608	CLA	CMC-C2C-C1C	3.47	130.40	125.02
24	d	404	CLA	C3B-C4B-NB	3.48	113.71	109.21
24	b	614	CLA	C3B-C4B-NB	3.49	113.72	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	608	CLA	C3B-C4B-NB	3.50	113.73	109.21
25	d	403	PHO	C4-C3-C5	3.50	120.76	115.41
30	I	102	LMT	O1B-C4'-C3'	3.50	116.21	107.17
27	a	402	SQD	O9-S-C6	3.51	109.90	106.94
32	A	419	PL9	C15-C14-C16	3.51	120.77	115.41
37	d	410	LHG	O7-C7-C8	3.51	119.17	111.53
27	f	101	SQD	C1-O5-C5	3.51	120.57	113.75
32	A	419	PL9	C10-C9-C11	3.52	120.78	115.41
34	z	101	LMG	O7-C10-C11	3.52	119.19	111.53
24	c	506	CLA	C3B-C4B-NB	3.54	113.79	109.21
36	D	407	DGD	C4D-C3D-C2D	3.55	117.42	110.79
24	c	513	CLA	C4-C3-C5	3.56	120.84	115.41
24	B	604	CLA	C3B-C4B-NB	3.56	113.82	109.21
34	B	621	LMG	O7-C10-C11	3.58	119.32	111.53
24	C	505	CLA	CAC-C3C-C4C	3.59	130.04	124.83
27	A	416	SQD	O47-C7-C8	3.61	119.37	111.53
24	C	510	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	B	609	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	c	505	CLA	C4-C3-C5	3.62	120.94	115.41
25	A	408	PHO	C4-C3-C5	3.62	120.94	115.41
34	C	520	LMG	O7-C10-C11	3.63	119.42	111.53
34	J	101	LMG	O7-C10-C11	3.65	119.47	111.53
24	B	603	CLA	C4-C3-C5	3.66	121.00	115.41
24	b	617	CLA	C4-C3-C5	3.66	121.00	115.41
24	b	608	CLA	C4-C3-C5	3.67	121.01	115.41
37	e	101	LHG	O7-C7-C8	3.67	119.50	111.53
36	c	517	DGD	O2G-C1B-C2B	3.67	119.51	111.53
24	C	505	CLA	CMC-C2C-C1C	3.69	130.73	125.02
24	b	620	CLA	C3B-C4B-NB	3.69	113.98	109.21
24	b	609	CLA	CMC-C2C-C1C	3.70	130.75	125.02
36	D	407	DGD	C1D-C2D-C3D	3.71	117.28	109.97
24	d	402	CLA	O2A-CGA-CBA	3.72	123.22	111.90
24	C	511	CLA	C3B-C4B-NB	3.73	114.03	109.21
24	a	406	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	D	403	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	C	509	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	b	611	CLA	CMC-C2C-C1C	3.75	130.83	125.02
24	B	614	CLA	C3B-C4B-NB	3.75	114.06	109.21
37	D	409	LHG	O7-C7-C8	3.76	119.69	111.53
24	b	612	CLA	C3B-C4B-NB	3.76	114.08	109.21
24	c	513	CLA	C3B-C4B-NB	3.78	114.09	109.21
24	c	506	CLA	C4-C3-C5	3.78	121.17	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	411	SQD	O9-S-C6	3.78	110.12	106.94
25	A	408	PHO	CAC-C3C-C4C	3.78	129.57	125.16
37	d	409	LHG	O7-C7-C8	3.78	119.74	111.53
24	C	512	CLA	C3B-C4B-NB	3.78	114.10	109.21
24	b	619	CLA	C3B-C4B-NB	3.79	114.11	109.21
24	b	620	CLA	C4-C3-C5	3.79	121.20	115.41
24	A	409	CLA	C4-C3-C5	3.80	121.21	115.41
24	C	507	CLA	C3B-C4B-NB	3.80	114.13	109.21
24	d	402	CLA	C3B-C4B-NB	3.80	114.13	109.21
24	A	406	CLA	C3B-C4B-NB	3.80	114.13	109.21
38	v	202	HEM	CMC-C2C-C3C	3.82	126.06	116.53
24	c	507	CLA	CAC-C3C-C4C	3.82	130.38	124.83
36	C	518	DGD	O2G-C1B-C2B	3.85	119.89	111.53
34	Z	101	LMG	O7-C10-C11	3.86	119.92	111.53
37	E	101	LHG	O7-C7-C8	3.88	119.95	111.53
24	B	615	CLA	C4-C3-C5	3.88	121.33	115.41
24	c	508	CLA	C3B-C4B-NB	3.90	114.25	109.21
24	B	607	CLA	CMC-C2C-C1C	3.91	131.06	125.02
34	c	501	LMG	O7-C10-C11	3.91	120.02	111.53
24	C	505	CLA	C3B-C4B-NB	3.92	114.27	109.21
36	c	518	DGD	O2G-C1B-C2B	3.92	120.04	111.53
24	B	605	CLA	CMC-C2C-C1C	3.92	131.08	125.02
27	b	601	SQD	C3-C4-C5	3.94	117.06	110.20
32	D	406	PL9	C40-C39-C41	3.94	121.42	115.41
24	C	514	CLA	CAC-C3C-C4C	3.94	130.55	124.83
27	F	101	SQD	O47-C7-C8	3.95	120.11	111.53
24	B	613	CLA	CAC-C3C-C4C	3.95	130.57	124.83
35	O	303	HTG	C1'-S1-C1	3.97	105.77	100.30
27	F	101	SQD	O9-S-C6	3.97	110.29	106.94
24	c	511	CLA	C3B-C4B-NB	3.99	114.37	109.21
34	Z	101	LMG	C1-C2-C3	4.01	117.87	109.97
24	B	613	CLA	C3B-C4B-NB	4.01	114.39	109.21
34	C	520	LMG	O8-C28-C29	4.02	124.15	111.90
24	c	512	CLA	C3B-C4B-NB	4.03	114.42	109.21
24	D	401	CLA	C3B-C4B-NB	4.03	114.42	109.21
24	b	618	CLA	C3B-C4B-NB	4.05	114.45	109.21
38	V	203	HEM	CMC-C2C-C3C	4.07	126.70	116.53
27	a	402	SQD	O47-C7-C8	4.10	120.43	111.53
24	A	405	CLA	O2D-CGD-CBD	4.11	116.93	111.30
38	e	102	HEM	CAD-C3D-C4D	4.11	126.96	112.47
24	a	409	CLA	C3B-C4B-NB	4.13	114.55	109.21
32	a	416	PL9	C15-C14-C16	4.15	121.75	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	V	203	HEM	CAD-C3D-C4D	4.16	127.12	112.47
38	v	202	HEM	CMB-C2B-C3B	4.16	126.91	116.53
24	b	618	CLA	O2D-CGD-CBD	4.20	117.06	111.30
38	E	103	HEM	CAD-C3D-C4D	4.25	127.46	112.47
36	C	517	DGD	O2G-C1B-C2B	4.27	120.81	111.53
27	A	411	SQD	O47-C7-C8	4.34	120.95	111.53
38	v	202	HEM	CAD-C3D-C2D	4.34	125.69	113.22
36	d	407	DGD	O2G-C1B-C2B	4.34	120.97	111.53
38	e	102	HEM	CMB-C2B-C3B	4.35	127.38	116.53
38	v	202	HEM	CAD-C3D-C4D	4.36	127.83	112.47
24	d	404	CLA	O2D-CGD-CBD	4.37	117.30	111.30
35	B	624	HTG	O5-C1-C2	4.39	116.15	110.19
27	l	101	SQD	O47-C7-C8	4.41	121.10	111.53
24	B	617	CLA	C3B-C4B-NB	4.41	114.91	109.21
38	V	203	HEM	CAD-C3D-C2D	4.45	126.00	113.22
30	b	602	LMT	C1'-O5'-C5'	4.51	122.50	113.75
27	F	101	SQD	O7-S-C6	4.53	110.76	106.94
34	C	501	LMG	O7-C10-C11	4.54	121.39	111.53
35	C	523	HTG	C1-O5-C5	4.59	121.49	112.74
24	A	409	CLA	O2D-CGD-CBD	4.61	117.62	111.30
34	C	521	LMG	O7-C10-C11	4.61	121.56	111.53
34	c	521	LMG	O7-C10-C11	4.63	121.60	111.53
38	E	103	HEM	CMB-C2B-C3B	4.63	128.10	116.53
38	E	103	HEM	CAD-C3D-C2D	4.65	126.60	113.22
38	e	102	HEM	CMC-C2C-C3C	4.66	128.17	116.53
24	d	401	CLA	C3B-C4B-NB	4.66	115.24	109.21
38	E	103	HEM	CMC-C2C-C3C	4.67	128.19	116.53
24	B	616	CLA	O2D-CGD-CBD	4.71	117.76	111.30
38	e	102	HEM	CAD-C3D-C2D	4.71	126.76	113.22
27	f	101	SQD	O7-S-C6	4.72	110.92	106.94
24	b	621	CLA	C3B-C4B-NB	4.73	115.33	109.21
27	a	411	SQD	O47-C7-C8	4.76	121.87	111.53
24	c	508	CLA	O2D-CGD-CBD	4.77	117.85	111.30
36	D	407	DGD	O2G-C1B-C2B	4.82	122.00	111.53
27	f	101	SQD	O47-C7-C8	4.83	122.03	111.53
35	V	204	HTG	C1'-S1-C1	4.85	106.98	100.30
38	V	203	HEM	CMB-C2B-C3B	4.87	128.69	116.53
27	b	601	SQD	O47-C7-C8	4.88	122.13	111.53
24	C	504	CLA	O2D-CGD-CBD	4.93	118.06	111.30
27	l	101	SQD	O7-S-C6	4.94	111.11	106.94
24	D	403	CLA	O2D-CGD-CBD	4.95	118.09	111.30
35	b	627	HTG	C1'-S1-C1	4.95	107.12	100.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	l	101	SQD	O6-C1-C2	4.98	114.33	108.04
25	A	408	PHO	CMD-C2D-C1D	5.02	133.24	125.06
35	b	604	HTG	C1'-S1-C1	5.03	107.23	100.30
24	C	512	CLA	O2D-CGD-CBD	5.03	118.20	111.30
25	d	403	PHO	C2D-C1D-ND	5.05	117.31	109.73
35	B	623	HTG	C1'-S1-C1	5.10	107.33	100.30
24	B	609	CLA	O2D-CGD-CBD	5.11	118.32	111.30
24	c	515	CLA	O2D-CGD-CBD	5.18	118.41	111.30
25	A	407	PHO	C2D-C1D-ND	5.20	117.52	109.73
24	c	513	CLA	O2D-CGD-CBD	5.23	118.47	111.30
24	d	401	CLA	O2D-CGD-CBD	5.41	118.72	111.30
24	C	514	CLA	O2D-CGD-CBD	5.41	118.72	111.30
24	B	608	CLA	O2D-CGD-CBD	5.46	118.79	111.30
25	a	408	PHO	C2D-C1D-ND	5.54	118.04	109.73
24	b	617	CLA	C2C-C1C-NC	5.61	114.42	110.24
24	b	610	CLA	O2D-CGD-CBD	5.64	119.04	111.30
24	A	406	CLA	O2D-CGD-CBD	5.69	119.11	111.30
24	b	615	CLA	O2D-CGD-CBD	5.73	119.16	111.30
24	D	401	CLA	O2D-CGD-CBD	5.76	119.20	111.30
24	b	612	CLA	O2D-CGD-CBD	5.77	119.22	111.30
27	b	601	SQD	O7-S-C6	5.78	111.81	106.94
25	A	408	PHO	O2D-CGD-CBD	5.80	119.25	111.30
25	A	408	PHO	C2D-C1D-ND	5.81	118.45	109.73
24	C	507	CLA	O2D-CGD-CBD	5.82	119.28	111.30
24	B	612	CLA	O2D-CGD-CBD	5.83	119.30	111.30
27	F	101	SQD	O6-C1-C2	5.83	115.41	108.04
24	a	407	CLA	O2D-CGD-CBD	5.84	119.31	111.30
25	d	403	PHO	CMD-C2D-C1D	5.86	134.60	125.06
35	B	622	HTG	C1'-S1-C1	5.86	108.38	100.30
25	A	407	PHO	O2D-CGD-CBD	5.87	119.36	111.30
24	b	611	CLA	C2C-C1C-NC	5.88	114.62	110.24
24	D	404	CLA	C2C-C1C-NC	5.92	114.65	110.24
24	B	610	CLA	O2D-CGD-CBD	5.92	119.42	111.30
24	b	606	CLA	C2C-C1C-NC	5.98	114.69	110.24
24	a	407	CLA	C2C-C1C-NC	6.00	114.71	110.24
24	b	620	CLA	O2D-CGD-CBD	6.03	119.57	111.30
24	b	607	CLA	C2C-C1C-NC	6.05	114.74	110.24
24	c	506	CLA	O2D-CGD-CBD	6.06	119.61	111.30
24	c	514	CLA	C2C-C1C-NC	6.07	114.76	110.24
24	C	508	CLA	O2D-CGD-CBD	6.07	119.63	111.30
24	d	404	CLA	C2C-C1C-NC	6.09	114.78	110.24
27	a	411	SQD	O6-C1-C2	6.09	115.73	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	C2C-C1C-NC	6.09	114.78	110.24
24	A	409	CLA	C2C-C1C-NC	6.11	114.79	110.24
24	a	409	CLA	O2D-CGD-CBD	6.15	119.73	111.30
24	c	505	CLA	C2C-C1C-NC	6.16	114.83	110.24
24	B	603	CLA	O2D-CGD-CBD	6.16	119.75	111.30
24	b	608	CLA	C2C-C1C-NC	6.17	114.84	110.24
35	C	523	HTG	C1'-S1-C1	6.19	108.84	100.30
24	c	512	CLA	C2C-C1C-NC	6.23	114.88	110.24
24	B	602	CLA	C2C-C1C-NC	6.23	114.88	110.24
25	a	408	PHO	CMD-C2D-C1D	6.26	135.25	125.06
24	b	614	CLA	O2D-CGD-CBD	6.31	119.96	111.30
24	c	512	CLA	O2D-CGD-CBD	6.35	120.01	111.30
24	c	505	CLA	O2D-CGD-CBD	6.36	120.03	111.30
24	B	612	CLA	C2C-C1C-NC	6.36	114.98	110.24
24	c	510	CLA	C2C-C1C-NC	6.38	114.99	110.24
24	C	514	CLA	C2C-C1C-NC	6.38	115.00	110.24
24	B	615	CLA	C2C-C1C-NC	6.40	115.01	110.24
24	b	617	CLA	O2D-CGD-CBD	6.40	120.08	111.30
35	C	522	HTG	C1'-S1-C1	6.42	109.15	100.30
24	A	406	CLA	C2C-C1C-NC	6.42	115.03	110.24
24	C	508	CLA	C2C-C1C-NC	6.43	115.03	110.24
35	B	630	HTG	C1'-S1-C1	6.43	109.17	100.30
24	B	613	CLA	O2D-CGD-CBD	6.46	120.16	111.30
24	C	503	CLA	O2D-CGD-CBD	6.46	120.17	111.30
24	B	611	CLA	O2D-CGD-CBD	6.48	120.19	111.30
24	B	603	CLA	C2C-C1C-NC	6.49	115.07	110.24
25	A	407	PHO	CMD-C2D-C1D	6.50	135.63	125.06
24	B	607	CLA	C2C-C1C-NC	6.51	115.09	110.24
24	c	515	CLA	C2C-C1C-NC	6.51	115.09	110.24
24	C	511	CLA	C2C-C1C-NC	6.52	115.10	110.24
35	b	603	HTG	C1'-S1-C1	6.53	109.30	100.30
24	b	613	CLA	O2D-CGD-CBD	6.55	120.28	111.30
24	C	512	CLA	C2C-C1C-NC	6.56	115.13	110.24
24	b	615	CLA	C2C-C1C-NC	6.58	115.14	110.24
24	B	617	CLA	C2C-C1C-NC	6.59	115.15	110.24
24	c	504	CLA	C2C-C1C-NC	6.60	115.16	110.24
24	B	613	CLA	C2C-C1C-NC	6.62	115.17	110.24
24	B	604	CLA	O2D-CGD-CBD	6.62	120.39	111.30
24	b	621	CLA	O2D-CGD-CBD	6.66	120.43	111.30
24	C	502	CLA	C2C-C1C-NC	6.66	115.20	110.24
24	C	513	CLA	C2C-C1C-NC	6.67	115.21	110.24
24	C	511	CLA	O2D-CGD-CBD	6.67	120.45	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	616	CLA	C2C-C1C-NC	6.68	115.21	110.24
24	b	613	CLA	C2C-C1C-NC	6.68	115.22	110.24
24	b	616	CLA	O2D-CGD-CBD	6.70	120.50	111.30
24	B	605	CLA	O2D-CGD-CBD	6.71	120.50	111.30
24	B	616	CLA	C2C-C1C-NC	6.71	115.24	110.24
24	C	503	CLA	C2C-C1C-NC	6.73	115.25	110.24
24	b	620	CLA	C2C-C1C-NC	6.73	115.25	110.24
24	c	506	CLA	C2C-C1C-NC	6.74	115.26	110.24
24	B	604	CLA	C2C-C1C-NC	6.75	115.27	110.24
24	d	402	CLA	O2D-CGD-CBD	6.76	120.57	111.30
24	c	511	CLA	C2C-C1C-NC	6.76	115.28	110.24
24	B	611	CLA	C2C-C1C-NC	6.77	115.28	110.24
24	B	602	CLA	O2D-CGD-CBD	6.77	120.58	111.30
24	b	606	CLA	O2D-CGD-CBD	6.77	120.58	111.30
24	b	610	CLA	C2C-C1C-NC	6.77	115.28	110.24
35	c	523	HTG	C1'-S1-C1	6.80	109.67	100.30
27	b	601	SQD	O6-C1-C2	6.81	116.64	108.04
24	D	404	CLA	O2D-CGD-CBD	6.82	120.65	111.30
24	c	513	CLA	C2C-C1C-NC	6.84	115.33	110.24
25	d	403	PHO	O2D-CGD-CBD	6.84	120.69	111.30
24	B	615	CLA	O2D-CGD-CBD	6.85	120.69	111.30
24	C	510	CLA	C2C-C1C-NC	6.85	115.34	110.24
24	b	611	CLA	O2D-CGD-CBD	6.86	120.71	111.30
24	c	508	CLA	C2C-C1C-NC	6.87	115.36	110.24
24	C	509	CLA	O2D-CGD-CBD	6.87	120.73	111.30
24	c	510	CLA	O2D-CGD-CBD	6.89	120.75	111.30
24	C	504	CLA	C2C-C1C-NC	6.91	115.39	110.24
24	C	502	CLA	O2D-CGD-CBD	6.93	120.81	111.30
24	c	504	CLA	O2D-CGD-CBD	6.94	120.83	111.30
24	C	513	CLA	O2D-CGD-CBD	6.96	120.86	111.30
35	B	631	HTG	C1'-S1-C1	6.99	109.93	100.30
24	c	507	CLA	C2C-C1C-NC	7.00	115.46	110.24
24	a	409	CLA	C2C-C1C-NC	7.01	115.46	110.24
24	C	505	CLA	C2C-C1C-NC	7.03	115.48	110.24
24	b	619	CLA	O2D-CGD-CBD	7.04	120.96	111.30
24	b	612	CLA	C2C-C1C-NC	7.06	115.50	110.24
27	A	411	SQD	O6-C1-C2	7.07	116.97	108.04
24	B	608	CLA	C2C-C1C-NC	7.09	115.52	110.24
24	C	509	CLA	C2C-C1C-NC	7.11	115.54	110.24
24	B	609	CLA	C2C-C1C-NC	7.15	115.56	110.24
24	c	503	CLA	C2C-C1C-NC	7.15	115.56	110.24
24	c	509	CLA	C2C-C1C-NC	7.15	115.57	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	O2D-CGD-CBD	7.17	121.14	111.30
24	C	507	CLA	C2C-C1C-NC	7.20	115.60	110.24
24	C	506	CLA	C2C-C1C-NC	7.21	115.61	110.24
24	b	621	CLA	C2C-C1C-NC	7.22	115.61	110.24
24	B	606	CLA	O2D-CGD-CBD	7.28	121.29	111.30
24	b	614	CLA	C2C-C1C-NC	7.28	115.66	110.24
24	c	503	CLA	O2D-CGD-CBD	7.30	121.31	111.30
25	a	408	PHO	O2D-CGD-CBD	7.31	121.33	111.30
24	C	505	CLA	O2D-CGD-CBD	7.32	121.34	111.30
24	B	606	CLA	C2C-C1C-NC	7.37	115.73	110.24
24	b	607	CLA	O2D-CGD-CBD	7.40	121.45	111.30
24	b	619	CLA	C2C-C1C-NC	7.40	115.75	110.24
24	c	514	CLA	O2D-CGD-CBD	7.40	121.45	111.30
24	d	402	CLA	C2C-C1C-NC	7.40	115.75	110.24
24	B	607	CLA	O2D-CGD-CBD	7.41	121.47	111.30
24	c	511	CLA	O2D-CGD-CBD	7.43	121.49	111.30
24	D	403	CLA	C2C-C1C-NC	7.43	115.77	110.24
24	b	618	CLA	C2C-C1C-NC	7.43	115.78	110.24
24	b	609	CLA	C2C-C1C-NC	7.44	115.78	110.24
24	b	609	CLA	O2D-CGD-CBD	7.45	121.52	111.30
24	B	605	CLA	C2C-C1C-NC	7.61	115.91	110.24
24	D	401	CLA	C2C-C1C-NC	7.62	115.92	110.24
24	d	401	CLA	C2C-C1C-NC	7.62	115.92	110.24
24	c	507	CLA	O2D-CGD-CBD	7.62	121.76	111.30
35	c	522	HTG	C1'-S1-C1	7.74	110.97	100.30
24	c	509	CLA	O2D-CGD-CBD	7.75	121.94	111.30
24	B	614	CLA	C2C-C1C-NC	7.75	116.02	110.24
24	b	608	CLA	O2D-CGD-CBD	7.79	121.99	111.30
35	B	624	HTG	C1'-S1-C1	7.88	111.17	100.30
24	a	406	CLA	C2C-C1C-NC	7.96	116.17	110.24
24	A	405	CLA	C2C-C1C-NC	8.03	116.22	110.24
24	C	510	CLA	O2D-CGD-CBD	8.05	122.34	111.30
24	B	617	CLA	O2D-CGD-CBD	8.05	122.35	111.30
35	d	411	HTG	C1'-S1-C1	8.10	111.46	100.30
35	b	628	HTG	C1'-S1-C1	8.63	112.19	100.30

All (180) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA

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Mol	Chain	Res	Type	Atom
24	B	612	CLA	NC
24	D	403	CLA	ND
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA
24	c	514	CLA	NC
24	c	514	CLA	ND
24	c	514	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	C	504	CLA	NC
24	C	504	CLA	NA
24	b	608	CLA	NC
24	b	608	CLA	ND
24	d	404	CLA	NC
24	d	404	CLA	ND
24	d	404	CLA	NA
24	b	620	CLA	NA
24	b	620	CLA	NC
24	b	620	CLA	ND
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	C	506	CLA	ND
24	a	409	CLA	NC
24	a	409	CLA	ND
24	a	409	CLA	NA
24	b	614	CLA	NC
24	b	614	CLA	ND
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	609	CLA	NC
24	B	609	CLA	NA
24	b	621	CLA	NA

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Mol	Chain	Res	Type	Atom
24	b	621	CLA	NC
24	b	621	CLA	ND
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	D	404	CLA	NC
24	D	404	CLA	ND
24	D	404	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	C	503	CLA	NC
24	C	503	CLA	NA
24	c	504	CLA	NC
24	c	504	CLA	ND
24	c	504	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	606	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	A	409	CLA	NC
24	A	409	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	NA
24	b	618	CLA	NC
24	b	618	CLA	ND
24	b	618	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	C	514	CLA	NC
24	C	514	CLA	NA
24	a	407	CLA	NC

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Mol	Chain	Res	Type	Atom
24	a	407	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	ND
24	c	512	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	D	401	CLA	NC
24	D	401	CLA	ND
24	D	401	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	c	507	CLA	ND
24	d	401	CLA	NC
24	d	401	CLA	ND
24	d	401	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	ND
24	c	508	CLA	NA
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	NA
24	a	406	CLA	NC
24	a	406	CLA	ND
24	a	406	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	b	615	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	615	CLA	ND
24	b	615	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	B	617	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	d	402	CLA	ND
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	c	515	CLA	NC
24	c	515	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	ND
24	c	505	CLA	NA
24	A	405	CLA	NC
24	A	405	CLA	ND
24	A	405	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	NA
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	511	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	c	503	CLA	NC
24	c	503	CLA	ND
24	c	503	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	619	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	b	601	SQD	C45-O47-C7-C8
36	D	407	DGD	C2G-O2G-C1B-C2B
34	Z	101	LMG	C8-O7-C10-C11
27	f	101	SQD	C45-O47-C7-O49
27	f	101	SQD	C45-O47-C7-C8

There are no ring outliers.

86 monomers are involved in 236 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	405	CLA	4	0
24	A	406	CLA	6	0
25	A	408	PHO	2	0
24	A	409	CLA	3	0
26	A	410	BCR	3	0
27	A	411	SQD	6	0
28	A	412	GOL	2	0
28	A	413	GOL	2	0
27	A	416	SQD	2	0
32	A	419	PL9	4	0
24	B	602	CLA	1	0
24	B	604	CLA	3	0
24	B	605	CLA	1	0
24	B	606	CLA	6	0
24	B	607	CLA	2	0
24	B	608	CLA	2	0
24	B	609	CLA	2	0
24	B	610	CLA	7	0
24	B	611	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	612	CLA	1	0
24	B	613	CLA	5	0
24	B	614	CLA	5	0
24	B	615	CLA	4	0
24	B	616	CLA	1	0
24	B	617	CLA	10	0
26	B	618	BCR	2	0
26	B	619	BCR	1	0
26	B	620	BCR	3	0
34	B	621	LMG	2	0
35	B	623	HTG	1	0
28	B	628	GOL	1	0
28	B	633	GOL	1	0
30	B	634	LMT	1	0
28	B	635	GOL	2	0
34	C	501	LMG	5	0
24	C	502	CLA	4	0
24	C	503	CLA	7	0
24	C	504	CLA	4	0
24	C	505	CLA	4	0
24	C	506	CLA	1	0
24	C	507	CLA	7	0
24	C	508	CLA	6	0
24	C	509	CLA	6	0
24	C	510	CLA	4	0
24	C	511	CLA	6	0
24	C	512	CLA	4	0
24	C	513	CLA	6	0
24	C	514	CLA	9	0
26	C	515	BCR	3	0
26	C	516	BCR	4	0
36	C	517	DGD	4	0
36	C	518	DGD	3	0
36	C	519	DGD	3	0
34	C	520	LMG	4	0
34	C	521	LMG	2	0
35	C	522	HTG	1	0
35	C	523	HTG	2	0
28	C	524	GOL	1	0
28	C	525	GOL	2	0
24	D	401	CLA	6	0
30	D	402	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	403	CLA	1	0
24	D	404	CLA	4	0
26	D	405	BCR	4	0
36	D	407	DGD	6	0
37	D	408	LHG	2	0
37	D	410	LHG	10	0
35	D	411	HTG	3	0
37	E	101	LHG	6	0
27	F	101	SQD	5	0
26	H	101	BCR	6	0
36	H	102	DGD	2	0
30	I	102	LMT	2	0
34	J	101	LMG	3	0
26	K	101	BCR	2	0
37	L	101	LHG	1	0
30	M	101	LMT	1	0
30	M	102	LMT	2	0
28	T	101	GOL	1	0
26	T	102	BCR	5	0
35	V	204	HTG	1	0
28	V	205	GOL	2	0
28	V	207	GOL	1	0
28	V	208	GOL	1	0
26	Y	101	BCR	2	0
34	Z	101	LMG	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	0.72	47 (14%) 4 6	16, 23, 42, 79	0
1	a	334/344 (97%)	0.88	68 (20%) 1 1	17, 25, 48, 82	0
2	B	504/505 (99%)	0.31	44 (8%) 13 20	18, 27, 52, 90	0
2	b	504/505 (99%)	0.51	53 (10%) 8 13	19, 29, 60, 108	0
3	C	451/455 (99%)	0.28	28 (6%) 24 34	20, 32, 49, 89	0
3	c	455/455 (100%)	0.48	40 (8%) 12 20	23, 35, 50, 87	0
4	D	342/342 (100%)	0.93	67 (19%) 1 2	15, 24, 40, 114	0
4	d	341/342 (99%)	0.64	41 (12%) 6 10	18, 26, 42, 90	0
5	E	81/84 (96%)	1.27	19 (23%) 1 1	27, 40, 68, 97	0
5	e	81/84 (96%)	1.14	16 (19%) 1 2	32, 45, 77, 97	0
6	F	34/44 (77%)	0.39	6 (17%) 2 3	26, 35, 56, 64	0
6	f	32/44 (72%)	0.46	4 (12%) 5 9	31, 37, 84, 99	0
7	H	65/65 (100%)	0.39	3 (4%) 36 47	24, 34, 52, 97	0
7	h	65/65 (100%)	0.61	6 (9%) 11 18	28, 37, 58, 113	0
8	I	37/38 (97%)	0.86	5 (13%) 4 7	30, 34, 91, 101	0
8	i	37/38 (97%)	0.78	5 (13%) 4 7	29, 34, 79, 102	0
9	J	38/39 (97%)	0.79	8 (21%) 1 1	26, 38, 85, 109	0
9	j	38/39 (97%)	0.29	4 (10%) 8 13	30, 41, 84, 85	0
10	K	37/37 (100%)	0.20	0 100 100	31, 38, 55, 64	0
10	k	37/37 (100%)	0.91	8 (21%) 1 1	33, 42, 56, 66	0
11	L	37/37 (100%)	1.23	11 (29%) 1 0	16, 20, 66, 91	0
11	l	37/37 (100%)	1.10	7 (18%) 2 2	17, 21, 61, 91	0
12	M	33/36 (91%)	0.95	7 (21%) 1 1	18, 23, 44, 100	0
12	m	33/36 (91%)	0.82	6 (18%) 2 2	19, 23, 44, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.42	23 (9%) 10 17	16, 34, 65, 113	0
13	o	243/244 (99%)	0.93	53 (21%) 1 1	18, 35, 75, 122	0
14	T	29/31 (93%)	1.03	4 (13%) 4 7	17, 23, 48, 85	0
14	t	29/31 (93%)	0.59	2 (6%) 20 30	17, 23, 49, 85	0
15	U	97/104 (93%)	0.30	6 (6%) 24 34	22, 33, 53, 85	0
15	u	97/104 (93%)	-0.07	0 100 100	25, 34, 51, 85	0
16	V	137/137 (100%)	0.01	0 100 100	23, 33, 54, 70	0
16	v	137/137 (100%)	0.53	14 (10%) 9 14	26, 38, 57, 72	0
17	Y	29/30 (96%)	2.12	9 (31%) 1 0	38, 50, 91, 107	0
17	y	29/30 (96%)	2.00	9 (31%) 1 0	41, 54, 91, 107	0
18	X	39/40 (97%)	0.82	8 (20%) 1 1	32, 42, 80, 92	0
18	x	39/40 (97%)	1.65	11 (28%) 1 0	35, 45, 93, 96	0
19	Z	62/62 (100%)	1.35	19 (30%) 1 0	40, 52, 87, 98	0
19	z	62/62 (100%)	3.06	37 (59%) 0 0	44, 53, 87, 98	0
20	R	34/34 (100%)	9.53	34 (100%) 0 0	69, 93, 111, 118	0
All	All	5293/5382 (98%)	0.70	732 (13%) 4 7	15, 31, 63, 122	0

All (732) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	18.7
20	R	6	LEU	14.4
20	R	14	LEU	13.7
20	R	31	VAL	13.3
20	R	20	VAL	12.4
20	R	19	ALA	11.7
17	Y	18	VAL	11.5
20	R	16	ALA	11.5
20	R	25	PRO	11.1
20	R	5	VAL	11.0
19	z	3	ILE	10.7
20	R	27	ALA	10.5
20	R	23	ILE	10.4
20	R	32	GLN	10.4
20	R	15	ALA	10.0
19	z	62	VAL	10.0
17	Y	19	ILE	9.8

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Mol	Chain	Res	Type	RSRZ
18	x	38	GLN	9.8
20	R	13	LEU	9.7
8	i	37	LEU	9.7
20	R	34	LEU	9.7
19	z	5	PHE	9.6
17	y	19	ILE	9.6
20	R	24	LEU	9.4
20	R	21	ARG	9.4
20	R	26	TYR	9.0
20	R	10	LEU	9.0
7	h	65	LEU	9.0
20	R	9	LEU	8.9
17	y	18	VAL	8.6
20	R	7	VAL	8.4
4	D	11	GLU	8.4
20	R	22	ASN	8.4
20	R	29	LYS	8.3
20	R	12	VAL	8.3
1	A	11	ALA	8.1
20	R	17	GLY	8.0
18	x	2	THR	8.0
20	R	28	VAL	8.0
8	I	38	GLU	8.0
2	b	495	PHE	7.8
8	I	37	LEU	7.8
19	z	4	LEU	7.8
20	R	3	TRP	7.7
18	x	37	VAL	7.6
19	z	60	PHE	7.6
7	H	65	LEU	7.5
20	R	30	GLN	7.4
20	R	35	LEU	7.4
20	R	11	PRO	7.4
17	Y	22	LEU	7.2
19	Z	62	VAL	7.2
2	B	85	GLY	7.0
1	a	11	ALA	6.9
2	b	491	VAL	6.6
19	z	42	LEU	6.6
19	z	61	VAL	6.5
20	R	33	LYS	6.4
2	b	486	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
19	Z	3	ILE	6.4
17	y	20	ALA	6.4
18	x	34	ILE	6.3
13	o	246	ALA	6.3
13	O	60	ARG	6.3
2	b	499	VAL	6.2
5	e	5	THR	6.2
19	z	7	LEU	6.2
2	b	504	THR	6.1
2	b	293	ALA	6.0
10	k	18	PHE	6.0
13	o	36	GLN	6.0
17	Y	20	ALA	5.8
6	f	14	PRO	5.8
2	b	496	TYR	5.8
6	f	15	ILE	5.7
1	A	13	LEU	5.6
2	B	494	GLY	5.6
5	E	84	LYS	5.5
2	B	495	PHE	5.5
2	b	487	SER	5.5
19	Z	31	GLN	5.5
13	o	35	SER	5.4
18	x	40	SER	5.4
5	E	17	VAL	5.4
6	F	16	PHE	5.3
5	e	6	GLY	5.3
2	b	493	TRP	5.3
9	J	2	SER	5.3
19	z	41	PHE	5.3
17	y	22	LEU	5.2
4	D	12	ARG	5.2
19	z	33	TRP	5.2
7	H	66	GLY	5.2
5	e	4	THR	5.1
2	b	295	GLY	5.1
19	Z	36	SER	5.1
19	z	39	LEU	5.1
2	b	494	GLY	5.1
8	I	36	ASP	5.1
16	v	17	LYS	5.0
11	l	1	MET	5.0

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Mol	Chain	Res	Type	RSRZ
2	b	505	ARG	5.0
5	E	21	VAL	5.0
3	c	146	PHE	5.0
3	c	143	TYR	5.0
7	H	64	ALA	5.0
2	b	85	GLY	4.9
19	Z	7	LEU	4.9
13	o	25	THR	4.9
20	R	2	ASP	4.9
20	R	8	VAL	4.9
18	x	39	ARG	4.9
7	h	66	GLY	4.8
18	X	40	SER	4.8
6	f	16	PHE	4.8
19	z	2	THR	4.8
5	e	25	ILE	4.7
13	o	59	LYS	4.7
5	E	6	GLY	4.7
2	B	297	THR	4.7
13	o	23	ASP	4.7
4	D	201	VAL	4.7
13	o	133	VAL	4.7
13	o	56	PRO	4.7
2	b	502	VAL	4.7
19	Z	33	TRP	4.7
13	o	34	SER	4.6
19	Z	35	ARG	4.6
10	k	12	PRO	4.6
9	J	3	GLU	4.6
4	d	182	LEU	4.6
2	b	86	ILE	4.6
6	F	15	ILE	4.6
19	z	9	LEU	4.5
3	c	147	PHE	4.5
13	o	61	GLN	4.5
8	i	34	ARG	4.5
2	b	497	GLN	4.5
4	D	156	VAL	4.5
2	b	294	SER	4.5
2	B	486	LEU	4.5
4	d	179	PHE	4.4
13	o	87	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
2	b	84	THR	4.4
1	a	290	ILE	4.4
20	R	4	ARG	4.4
8	i	38	GLU	4.3
13	o	27	ARG	4.3
17	Y	25	ILE	4.3
17	Y	21	GLN	4.3
1	a	193	LEU	4.3
18	X	37	VAL	4.3
13	O	58	ASN	4.3
13	O	25	THR	4.2
2	b	485	GLU	4.2
13	o	4	THR	4.2
18	X	2	THR	4.2
13	o	32	ILE	4.2
13	o	26	ALA	4.2
19	z	35	ARG	4.2
13	o	58	ASN	4.2
19	z	1	MET	4.2
1	A	200	LEU	4.1
19	z	59	PHE	4.1
2	b	126	PRO	4.1
8	i	36	ASP	4.1
4	D	279	LEU	4.1
1	a	288	LEU	4.1
19	z	53	VAL	4.1
1	A	288	LEU	4.1
1	a	184	ILE	4.1
1	a	280	VAL	4.0
2	B	86[A]	ILE	4.0
1	a	197	PHE	4.0
4	D	153	PHE	4.0
13	o	38	TYR	4.0
3	C	432	VAL	4.0
4	D	191	TRP	3.9
2	B	84	THR	3.9
2	b	490	GLN	3.9
14	t	29	ILE	3.9
12	M	33	GLN	3.9
15	U	79	LEU	3.9
1	a	297	LEU	3.9
4	D	289	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
19	Z	4	LEU	3.9
13	O	27	ARG	3.9
4	D	205	LEU	3.9
13	o	37	THR	3.9
19	Z	32	ASP	3.8
1	a	285	PHE	3.8
13	o	208	THR	3.8
19	z	32	ASP	3.8
1	A	285	PHE	3.8
3	C	257	PHE	3.8
14	T	30	THR	3.8
1	a	200	LEU	3.8
13	o	60	ARG	3.8
15	U	8	GLU	3.8
12	m	34	LYS	3.7
1	a	192	ILE	3.7
17	y	41	VAL	3.7
3	c	134	ILE	3.7
2	b	127	ARG	3.7
4	d	12	ARG	3.7
3	c	21	ILE	3.7
4	D	238	THR	3.7
4	D	150	ILE	3.7
19	z	25	VAL	3.7
4	D	280	TRP	3.7
2	b	297	THR	3.7
13	O	62	GLU	3.7
14	T	9	ILE	3.6
2	b	290	ALA	3.6
13	o	33	ASP	3.6
2	B	489	GLU	3.6
13	O	56	PRO	3.6
4	D	152	VAL	3.6
11	L	2	GLU	3.6
4	D	196	PHE	3.6
4	d	196	PHE	3.6
5	E	4	THR	3.6
13	O	59	LYS	3.6
2	b	500	GLY	3.6
4	D	286	VAL	3.6
17	y	25	ILE	3.6
19	z	58	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	197	PHE	3.5
11	L	31	PHE	3.5
1	A	202	VAL	3.5
3	c	432	VAL	3.5
4	D	149	PRO	3.5
2	b	129	GLY	3.5
17	y	21	GLN	3.5
18	X	38	GLN	3.5
1	A	287	ALA	3.5
2	b	484	PRO	3.5
18	X	31	ILE	3.5
2	b	296	ALA	3.5
13	o	89	SER	3.5
19	z	30	PRO	3.5
2	B	298	LEU	3.5
2	b	292	LEU	3.5
4	D	293	LEU	3.5
3	c	145	SER	3.4
19	Z	60	PHE	3.4
2	B	461	LEU	3.4
4	D	276	VAL	3.4
1	a	163	ILE	3.4
3	C	262	ARG	3.4
9	J	6	ARG	3.4
19	z	6	GLN	3.4
3	C	253	LEU	3.4
1	a	161	TYR	3.4
11	l	2	GLU	3.4
5	e	84	LYS	3.4
4	d	14	TRP	3.4
13	o	132	ASN	3.4
1	a	202	VAL	3.4
19	Z	61	VAL	3.4
3	c	257	PHE	3.4
16	v	107	LEU	3.4
5	e	59	GLU	3.4
4	D	204	VAL	3.4
13	o	62	GLU	3.3
3	c	259	TRP	3.3
1	a	157	VAL	3.3
1	A	290	ILE	3.3
9	J	5	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
13	o	211	ILE	3.3
16	v	19	ILE	3.3
1	A	230	THR	3.3
2	B	457	VAL	3.3
19	z	40	ILE	3.3
10	k	14	ALA	3.3
2	b	488	PRO	3.3
11	l	3	PRO	3.3
4	D	160	TYR	3.3
1	A	186	PHE	3.2
6	F	14	PRO	3.2
16	v	110	LYS	3.2
19	Z	39	LEU	3.2
19	Z	42	LEU	3.2
19	z	31	GLN	3.2
18	x	36	LYS	3.2
4	D	175	VAL	3.2
5	e	21	VAL	3.2
13	O	28	GLY	3.2
3	C	436	PHE	3.2
2	B	496	TYR	3.2
13	o	91	GLY	3.2
17	Y	43	ARG	3.2
6	F	18	VAL	3.2
1	A	278	TRP	3.2
12	M	16[A]	LEU	3.2
4	D	148	ALA	3.2
19	Z	1	MET	3.2
1	A	193	LEU	3.2
2	b	298	LEU	3.2
11	L	29	LEU	3.2
13	O	93	LEU	3.2
2	b	501	ASP	3.1
13	o	24	ASP	3.1
13	o	126	VAL	3.1
3	C	260	ALA	3.1
14	T	13	ILE	3.1
3	C	143	TYR	3.1
4	d	283	ALA	3.1
19	Z	34	ASP	3.1
10	k	17	ILE	3.1
2	B	499	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
4	d	148	ALA	3.1
3	c	20	SER	3.1
1	A	321	ILE	3.1
4	d	325	ILE	3.1
3	C	431	PHE	3.1
4	d	184	PHE	3.1
2	B	293	ALA	3.1
4	d	201	VAL	3.1
13	o	135	SER	3.1
2	b	125	ASP	3.1
4	D	182	LEU	3.1
4	d	205	LEU	3.1
2	B	504	THR	3.1
5	E	5	THR	3.1
11	L	1	MET	3.1
3	c	411	ALA	3.1
4	D	275	PRO	3.1
4	d	175	VAL	3.1
9	J	24	VAL	3.1
13	O	61	GLN	3.1
2	B	487	SER	3.0
3	C	145[A]	SER	3.0
15	U	70	ARG	3.0
1	a	182	PHE	3.0
19	z	29	SER	3.0
4	d	178	ILE	3.0
18	X	34	ILE	3.0
1	A	12	ASN	3.0
4	d	185	PHE	3.0
5	E	19	TYR	3.0
3	c	144	SER	3.0
5	E	22	ILE	3.0
4	D	278	GLY	3.0
11	l	31	PHE	3.0
19	z	38	GLN	3.0
8	I	34	ARG	3.0
18	x	30	ALA	3.0
1	a	186	PHE	3.0
4	d	156	VAL	3.0
16	v	26	TYR	3.0
4	D	202	ALA	3.0
1	a	235	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	b	489	GLU	2.9
1	a	286	ALA	2.9
13	O	26	ALA	2.9
1	a	284	TRP	2.9
2	B	460	LEU	2.9
3	c	142	GLU	2.9
4	D	193	LEU	2.9
9	J	7	ILE	2.9
1	A	196	PRO	2.9
2	b	492	GLU	2.9
8	I	35	LYS	2.9
1	A	77	ILE	2.9
2	B	488	PRO	2.9
2	b	503	THR	2.9
1	a	205	VAL	2.9
2	B	502	VAL	2.9
19	z	49	ALA	2.9
4	D	200	GLY	2.9
13	o	131	PRO	2.9
13	o	134	THR	2.9
1	A	297	LEU	2.9
1	a	326	LEU	2.9
4	D	122	LEU	2.9
13	o	22	LEU	2.9
1	A	192	ILE	2.9
13	o	130	GLN	2.9
1	A	283	VAL	2.9
4	d	187	GLY	2.9
18	x	3	ILE	2.9
7	h	22	ALA	2.9
2	B	295	GLY	2.9
4	D	146	PHE	2.8
4	d	183	LEU	2.8
5	E	83	LEU	2.8
11	l	25	LEU	2.8
1	A	176	ILE	2.8
4	D	325	ILE	2.8
13	o	209	GLY	2.8
4	D	119	ALA	2.8
4	d	280	TRP	2.8
1	a	293	MET	2.8
1	a	295	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	b	291	SER	2.8
4	D	183	LEU	2.8
19	z	57	LEU	2.8
2	b	123	PHE	2.8
3	c	425	TRP	2.8
1	a	299	GLY	2.8
11	l	27	LEU	2.8
9	j	6	ARG	2.8
17	Y	30	ILE	2.8
10	k	13	GLU	2.8
3	c	410	VAL	2.8
19	z	56	VAL	2.8
2	B	462	PHE	2.8
2	B	464	PHE	2.8
13	O	65	PHE	2.8
3	c	426	LEU	2.8
11	L	23	LEU	2.8
13	o	63	ALA	2.8
1	a	194	MET	2.8
2	B	503	THR	2.8
3	c	428	THR	2.8
1	A	205	VAL	2.8
3	C	407	VAL	2.8
1	a	282	GLY	2.8
5	E	20	TRP	2.8
4	D	290	ALA	2.7
1	A	210	LEU	2.7
3	c	404	LEU	2.7
4	D	154	VAL	2.7
16	v	106	ASN	2.7
3	C	23	ALA	2.7
13	o	140	THR	2.7
3	C	259	TRP	2.7
3	c	140	LEU	2.7
12	M	34	LYS	2.7
5	e	61	ARG	2.7
1	A	203	ALA	2.7
4	D	192	THR	2.7
5	e	79	PHE	2.7
17	y	23	THR	2.7
4	D	199	MET	2.7
4	D	116	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
4	d	209	LEU	2.7
11	L	30	LEU	2.7
2	b	483	ASP	2.7
1	a	281	VAL	2.7
2	b	457	VAL	2.7
13	o	30	TYR	2.7
19	Z	2	THR	2.7
1	a	180	PHE	2.7
3	C	404	LEU	2.7
4	d	279	LEU	2.7
13	o	139	SER	2.7
4	D	284	ILE	2.7
13	o	64	GLU	2.7
3	C	255	THR	2.7
13	o	21	THR	2.7
1	a	287	ALA	2.7
2	B	459	ALA	2.7
19	z	10	ALA	2.7
16	v	16	GLY	2.7
1	A	184	ILE	2.6
3	c	155	ASN	2.6
13	o	243	ILE	2.6
4	D	281	MET	2.6
1	a	195	HIS	2.6
3	c	433	LEU	2.6
1	a	330	VAL	2.6
4	d	152	VAL	2.6
13	O	136	ILE	2.6
1	a	324	ALA	2.6
4	D	283	ALA	2.6
2	B	165	GLY	2.6
3	C	181	PHE	2.6
3	c	163	PHE	2.6
4	d	188	PHE	2.6
4	D	277	THR	2.6
9	j	2	SER	2.6
1	A	185	VAL	2.6
2	B	296	ALA	2.6
1	a	321	ILE	2.6
4	D	287	VAL	2.6
13	O	133	VAL	2.6
9	J	4	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
13	o	142	PHE	2.6
1	a	279	PRO	2.6
2	b	413	ASP	2.6
4	D	274	VAL	2.6
19	z	18	VAL	2.6
19	z	14	ILE	2.6
7	h	6	TRP	2.6
16	v	108	THR	2.6
1	A	182	PHE	2.6
1	A	300	PHE	2.6
3	c	431	PHE	2.6
4	d	193	LEU	2.6
4	d	289	LEU	2.6
4	d	321	LEU	2.6
19	Z	30	PRO	2.6
2	B	456	ALA	2.6
5	E	72	ALA	2.6
4	D	159	ILE	2.6
3	c	429	SER	2.6
5	E	73	LYS	2.5
5	E	81	GLU	2.5
13	o	245	PRO	2.5
1	A	201	GLY	2.5
1	A	180	PHE	2.5
4	D	181	PHE	2.5
12	m	13	LEU	2.5
16	v	95	LEU	2.5
13	o	66	VAL	2.5
1	A	160	ILE	2.5
14	t	30	THR	2.5
2	B	479	PHE	2.5
12	M	14	PHE	2.5
13	o	57	LYS	2.5
13	O	88	ASN	2.5
1	a	185	VAL	2.5
4	d	159	ILE	2.5
4	d	284	ILE	2.5
13	o	136	ILE	2.5
4	d	281	MET	2.5
2	b	302	TRP	2.5
4	D	185	PHE	2.5
12	m	14	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	281	VAL	2.5
1	a	203	ALA	2.5
7	h	64	ALA	2.5
3	C	425	TRP	2.5
3	C	435	PHE	2.5
4	D	184	PHE	2.5
4	D	203	GLY	2.5
4	d	329	MET	2.5
1	a	191	ASN	2.5
18	X	39	ARG	2.5
2	B	408	GLY	2.5
4	d	74	LEU	2.5
5	e	26	THR	2.5
1	A	284	TRP	2.4
1	a	278	TRP	2.4
2	B	453	PHE	2.4
3	c	201	ASN	2.4
8	i	35	LYS	2.4
18	x	8	LYS	2.4
3	c	166	ILE	2.4
12	m	33	GLN	2.4
4	D	170	ALA	2.4
1	A	282	GLY	2.4
13	O	137	THR	2.4
3	c	253	LEU	2.4
10	k	21	LEU	2.4
1	a	190	HIS	2.4
2	B	463	PHE	2.4
1	A	16	ARG	2.4
3	c	200	THR	2.4
7	h	23	PRO	2.4
19	Z	38	GLN	2.4
5	e	36	LEU	2.4
13	o	199	LEU	2.4
2	B	127	ARG	2.4
2	b	124	ARG	2.4
17	Y	26	ALA	2.4
3	C	428	THR	2.4
13	O	138	THR	2.4
2	B	402	TYR	2.4
2	B	324	LEU	2.4
1	a	283	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
5	e	17	VAL	2.4
1	A	188	ALA	2.4
1	a	188	ALA	2.4
3	c	434	ALA	2.4
3	c	207	ARG	2.4
4	d	328	TRP	2.4
16	v	86	GLN	2.4
1	a	341	LEU	2.4
3	c	401	LEU	2.4
16	v	15	GLU	2.4
1	A	324	ALA	2.4
13	O	24	ASP	2.4
1	a	300	PHE	2.4
2	b	363	PHE	2.4
13	o	239	PHE	2.4
15	U	73	GLN	2.3
1	A	198	HIS	2.3
2	b	460	LEU	2.3
4	D	158	LEU	2.3
4	D	291	LEU	2.3
13	O	87	VAL	2.3
2	B	325	PHE	2.3
13	o	95	PHE	2.3
2	B	505	ARG	2.3
3	C	261	ARG	2.3
19	z	47	TRP	2.3
6	F	13	TYR	2.3
2	B	497	GLN	2.3
5	E	46	VAL	2.3
13	o	141	ASP	2.3
1	A	211	PHE	2.3
1	a	160	ILE	2.3
11	L	24[A]	ILE	2.3
10	k	10	LYS	2.3
13	O	30	TYR	2.3
1	a	13	LEU	2.3
3	C	433	LEU	2.3
11	L	27	LEU	2.3
19	z	54	VAL	2.3
1	a	206	PHE	2.3
11	L	35	PHE	2.3
1	a	176	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
18	x	35	ASP	2.3
3	C	453	ALA	2.3
13	o	202	ALA	2.3
4	D	197	HIS	2.3
4	D	76	VAL	2.3
4	d	204	VAL	2.3
4	D	195	PRO	2.3
1	A	206	PHE	2.3
16	v	18	THR	2.3
1	a	172	MET	2.3
1	A	249	VAL	2.2
12	M	17	VAL	2.2
2	B	500	GLY	2.2
4	D	174	GLY	2.2
1	a	298	ASN	2.2
4	D	198	MET	2.2
4	d	202	ALA	2.2
1	a	210	LEU	2.2
1	a	291	SER	2.2
13	o	194	LYS	2.2
6	F	17	THR	2.2
9	J	28	PHE	2.2
14	T	8	PHE	2.2
18	X	3	ILE	2.2
2	B	291	SER	2.2
2	B	490	GLN	2.2
15	U	59	GLU	2.2
3	C	426	LEU	2.2
3	c	184	GLY	2.2
12	M	15	VAL	2.2
1	a	224	ILE	2.2
3	C	256	PRO	2.2
11	L	3	PRO	2.2
3	c	193	GLY	2.2
16	v	12	LEU	2.2
1	a	229	GLU	2.2
1	a	292	THR	2.2
3	c	141	GLU	2.2
1	A	286	ALA	2.2
1	a	156	ALA	2.2
2	b	304	ALA	2.2
4	D	151	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	152	LYS	2.2
1	a	78	ILE	2.2
19	z	34	ASP	2.2
4	d	296	TYR	2.2
1	a	228	THR	2.2
2	b	120	LEU	2.2
3	C	401	LEU	2.2
10	k	11	LEU	2.2
2	b	301	ALA	2.1
1	a	243	GLU	2.1
4	D	13	GLY	2.1
3	c	112	PHE	2.1
3	c	436	PHE	2.1
5	E	79	PHE	2.1
5	e	37	PHE	2.1
17	y	43	ARG	2.1
2	b	402	TYR	2.1
6	f	17	THR	2.1
4	D	321	LEU	2.1
3	C	155	ASN	2.1
3	c	183	GLY	2.1
4	d	212	ALA	2.1
13	O	63	ALA	2.1
2	B	302	TRP	2.1
3	C	284	PHE	2.1
1	A	78	ILE	2.1
1	A	153	SER	2.1
4	D	282	SER	2.1
12	m	9	ILE	2.1
5	E	42	LEU	2.1
11	L	25	LEU	2.1
15	U	62	LEU	2.1
2	b	82	GLY	2.1
4	d	195	PRO	2.1
4	d	237	PRO	2.1
3	c	262	ARG	2.1
12	m	15	VAL	2.1
5	E	59	GLU	2.1
4	D	188	PHE	2.1
4	d	181	PHE	2.1
4	d	191	TRP	2.1
9	j	4	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
19	z	12	LEU	2.1
3	C	434	ALA	2.1
2	B	349	LYS	2.1
9	j	5	GLY	2.1
4	D	273	PHE	2.1
13	o	65	PHE	2.1
4	D	114	ILE	2.1
1	a	12	ASN	2.1
1	a	151	LEU	2.1
2	b	223	GLN	2.1
4	d	291	LEU	2.1
2	b	498	LYS	2.1
13	O	57	LYS	2.1
5	e	81	GLU	2.1
1	A	327	GLY	2.1
1	a	162	PRO	2.1
5	E	82	GLN	2.1
5	E	77	GLU	2.0
1	a	155	PHE	2.0
2	B	242	ILE	2.0
2	B	301	ALA	2.0
4	d	299	ILE	2.0
11	l	24[A]	ILE	2.0
4	D	295	SER	2.0
1	a	289	GLY	2.0
4	D	285	GLY	2.0
12	M	11	THR	2.0
16	v	113	VAL	2.0
1	A	194	MET	2.0
1	A	293	MET	2.0
1	a	15	GLU	2.0
1	a	196	PRO	2.0
5	e	74	GLN	2.0
1	a	294	ALA	2.0
2	b	361	ALA	2.0
1	a	158	PHE	2.0
3	c	435	PHE	2.0
13	O	142	PHE	2.0
19	Z	41	PHE	2.0
5	e	7	GLU	2.0
3	c	412	THR	2.0
4	D	194	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
19	z	20	VAL	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
12	FME	M	1	10/11	0.96	0.14	-	23,34,56,61	0
14	FME	T	1	10/11	0.96	0.14	-	21,27,45,56	0
12	FME	m	1	10/11	0.93	0.15	-	25,31,61,62	0
9	FME	j	1	10/11	0.76	0.34	-	53,71,94,136	0
14	FME	t	1	10/11	0.95	0.11	-	13,22,33,65	0
8	FME	i	1	10/11	0.97	0.15	-	23,34,37,42	0
8	FME	I	1	10/11	0.97	0.11	-	22,34,37,40	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
29	UNL	k	102	10/-	0.58	0.61	26.13	54,83,94,102	0
28	GOL	b	633	6/6	0.95	0.29	15.05	32,54,63,71	0
29	UNL	j	103	10/-	0.61	0.32	12.31	44,61,67,73	0
29	UNL	k	101	32/-	0.70	0.38	10.71	42,75,105,108	0
30	LMT	B	634	25/35	0.78	0.27	9.82	32,63,105,111	0
28	GOL	c	525	6/6	0.90	0.24	9.13	43,46,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	GOL	t	102	6/6	0.77	0.34	8.12	29,60,65,69	0
27	SQD	a	402	54/54	0.76	0.23	7.65	34,61,79,100	0
30	LMT	f	102	35/35	0.60	0.36	7.63	56,83,109,113	0
28	GOL	C	524	6/6	0.88	0.21	7.38	39,45,57,60	0
36	DGD	d	407	62/66	0.59	0.44	7.05	41,88,117,122	0
28	GOL	V	205	6/6	0.79	0.40	6.97	37,54,59,72	0
28	GOL	b	632	6/6	0.81	0.29	6.03	40,46,68,69	0
32	PL9	a	416	55/55	0.75	0.27	5.87	50,76,94,95	0
30	LMT	E	102	35/35	0.61	0.34	5.82	43,81,105,107	0
28	GOL	v	203	6/6	0.75	0.29	5.78	50,69,71,78	0
35	HTG	V	204	19/19	0.88	0.26	5.70	40,65,99,175	0
29	UNL	X	101	10/-	0.85	0.15	5.37	29,37,41,42	0
35	HTG	b	627	19/19	0.89	0.23	5.36	27,44,80,80	0
30	LMT	M	101	35/35	0.66	0.28	5.35	35,60,79,85	0
29	UNL	J	103	10/-	0.71	0.43	5.30	38,53,73,75	0
29	UNL	I	101	40/-	0.76	0.29	5.11	27,63,114,119	0
30	LMT	b	602	25/35	0.79	0.30	5.10	22,63,102,106	0
28	GOL	F	103	6/6	0.91	0.18	4.95	52,59,65,68	0
28	GOL	c	527	6/6	0.89	0.21	4.95	36,57,61,63	0
28	GOL	B	629	6/6	0.94	0.24	4.90	24,40,61,78	0
32	PL9	A	419	55/55	0.68	0.29	4.81	38,66,87,92	0
28	GOL	B	628	6/6	0.88	0.23	4.66	35,46,67,70	0
28	GOL	B	627	6/6	0.85	0.22	4.59	31,35,43,44	0
30	LMT	m	103	35/35	0.65	0.27	4.55	30,60,86,90	0
28	GOL	a	413	6/6	0.79	0.23	4.18	38,67,69,71	0
26	BCR	B	619	40/40	0.90	0.16	3.93	17,25,44,46	0
30	LMT	a	417	35/35	0.76	0.42	3.77	52,76,90,94	0
30	LMT	a	401	35/35	0.82	0.19	3.67	28,61,79,86	0
29	UNL	i	101	40/-	0.73	0.24	3.62	36,64,96,108	0
29	UNL	D	413	40/-	0.81	0.20	3.54	33,55,105,108	0
24	CLA	b	606	65/65	0.92	0.18	3.51	30,46,82,98	0
34	LMG	J	101	51/55	0.92	0.22	3.49	20,37,78,86	0
34	LMG	Z	101	37/55	0.62	0.32	3.46	32,81,104,105	0
28	GOL	A	414	6/6	0.78	0.19	3.45	40,60,69,70	0
28	GOL	V	208	6/6	0.86	0.27	3.35	41,56,62,63	0
34	LMG	j	101	51/55	0.90	0.19	3.33	26,39,70,82	0
28	GOL	A	413	6/6	0.86	0.19	3.31	35,38,41,42	0
35	HTG	C	523	19/19	0.75	0.29	3.28	46,75,97,109	0
26	BCR	d	405	40/40	0.87	0.16	3.27	29,35,63,64	0
34	LMG	z	101	39/55	0.72	0.39	3.25	47,74,94,101	0
35	HTG	c	523	19/19	0.83	0.31	3.08	60,84,93,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	GOL	f	104	6/6	0.92	0.22	3.07	45,51,59,61	0
28	GOL	a	412	6/6	0.91	0.16	2.97	22,37,41,45	0
35	HTG	D	411	16/19	0.69	0.25	2.86	38,100,111,113	0
23	BCT	a	418	4/4	0.95	0.17	2.84	30,33,42,44	0
27	SQD	l	101	54/54	0.68	0.25	2.77	31,67,98,101	0
34	LMG	C	501	51/55	0.84	0.19	2.62	37,54,74,82	0
28	GOL	B	625	6/6	0.92	0.14	2.61	28,43,48,55	0
27	SQD	A	416	54/54	0.80	0.18	2.59	28,52,75,76	0
30	LMT	A	417	33/35	0.85	0.19	2.55	27,65,78,85	0
29	UNL	d	413	36/-	0.80	0.19	2.52	35,58,94,99	0
29	UNL	C	526	34/-	0.65	0.34	2.51	46,71,82,84	0
24	CLA	B	617	65/65	0.95	0.17	2.51	19,28,88,91	0
26	BCR	b	623	40/40	0.91	0.21	2.48	15,27,40,46	0
34	LMG	b	625	51/55	0.87	0.28	2.42	24,39,59,71	0
24	CLA	B	602	65/65	0.92	0.16	2.40	24,39,82,104	0
35	HTG	B	631	19/19	0.76	0.21	2.39	25,84,104,120	0
28	GOL	V	207	6/6	0.95	0.21	2.32	35,38,41,44	0
39	MG	j	102	1/1	0.98	0.16	2.30	34,34,34,34	0
28	GOL	B	626	6/6	0.89	0.21	2.24	32,37,40,59	0
29	UNL	d	412	17/-	0.84	0.16	2.23	31,48,79,85	0
30	LMT	I	102	35/35	0.75	0.34	2.09	59,81,95,100	0
28	GOL	V	206	6/6	0.87	0.21	2.09	21,38,44,48	0
36	DGD	D	407	62/66	0.51	0.49	2.09	44,89,114,119	0
27	SQD	b	601	54/54	0.72	0.23	1.96	36,58,91,95	0
35	HTG	B	630	19/19	0.86	0.18	1.84	30,54,78,81	0
37	LHG	L	101	49/49	0.93	0.23	1.81	15,29,47,58	0
34	LMG	c	501	51/55	0.80	0.21	1.72	39,60,77,85	0
37	LHG	d	408	49/49	0.90	0.23	1.67	26,34,46,50	0
29	UNL	x	101	10/-	0.76	0.17	1.63	35,44,57,58	0
27	SQD	a	411	54/54	0.90	0.23	1.62	32,56,75,78	0
29	UNL	D	412	17/-	0.91	0.16	1.59	24,45,74,78	0
37	LHG	D	408	49/49	0.90	0.25	1.50	16,31,43,54	0
34	LMG	B	621	51/55	0.83	0.25	1.46	20,35,52,64	0
28	GOL	b	629	6/6	0.93	0.13	1.42	32,40,48,57	0
32	PL9	d	406	55/55	0.90	0.21	1.41	16,23,35,47	0
28	GOL	T	101	6/6	0.89	0.18	1.38	35,60,64,65	0
28	GOL	v	204	6/6	0.84	0.20	1.36	47,64,70,92	0
37	LHG	l	102	49/49	0.90	0.19	1.33	19,30,48,57	0
37	LHG	E	101	42/49	0.69	0.25	1.33	38,73,93,103	0
24	CLA	c	515	65/65	0.86	0.27	1.33	37,51,79,88	0
35	HTG	B	623	19/19	0.84	0.16	1.33	29,42,64,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	BCR	B	618	40/40	0.93	0.16	1.31	15,23,33,41	0
28	GOL	B	633	6/6	0.92	0.10	1.31	27,36,40,41	0
25	PHO	A	408	64/64	0.95	0.26	1.30	16,22,30,32	0
32	PL9	D	406	55/55	0.91	0.24	1.28	14,23,36,43	0
24	CLA	A	409	65/65	0.95	0.12	1.28	18,27,83,92	0
30	LMT	b	626	25/35	0.69	0.30	1.23	33,67,110,115	0
27	SQD	f	101	43/54	0.82	0.30	1.23	55,82,109,117	0
25	PHO	d	403	64/64	0.94	0.21	1.21	20,25,34,38	0
24	CLA	B	611	65/65	0.95	0.12	1.21	19,26,36,39	0
34	LMG	C	521	51/55	0.79	0.23	1.21	31,74,90,96	0
28	GOL	b	630	6/6	0.92	0.16	1.15	37,48,50,52	0
27	SQD	A	411	54/54	0.90	0.21	1.14	26,51,71,78	0
34	LMG	C	520	51/55	0.77	0.28	1.13	26,61,82,87	0
24	CLA	c	510	65/65	0.93	0.16	1.13	24,31,70,87	0
24	CLA	A	405	65/65	0.94	0.26	1.12	15,18,26,50	0
24	CLA	b	612	65/65	0.93	0.21	1.12	14,23,30,36	0
24	CLA	D	403	65/65	0.96	0.28	1.10	14,19,36,42	0
24	CLA	A	406	65/65	0.95	0.26	1.09	15,19,84,88	0
36	DGD	C	519	62/66	0.93	0.23	1.08	20,30,58,63	0
35	HTG	d	411	16/19	0.67	0.27	1.05	54,73,84,87	0
24	CLA	C	509	65/65	0.91	0.16	1.01	21,29,78,80	0
24	CLA	d	402	65/65	0.96	0.24	1.00	18,22,38,46	0
26	BCR	D	405	40/40	0.91	0.14	1.00	22,31,61,77	0
37	LHG	D	409	49/49	0.94	0.18	1.00	17,27,48,60	0
26	BCR	b	622	40/40	0.91	0.17	0.98	16,26,33,36	0
24	CLA	a	407	65/65	0.94	0.26	0.98	19,25,72,79	0
37	LHG	d	409	49/49	0.93	0.14	0.97	17,26,39,55	0
36	DGD	h	102	62/66	0.87	0.17	0.97	23,35,52,69	0
26	BCR	Y	101	40/40	0.90	0.12	0.96	28,35,49,50	0
34	LMG	c	521	51/55	0.76	0.28	0.92	35,79,91,98	0
36	DGD	C	518	62/66	0.92	0.23	0.90	22,32,76,92	0
35	HTG	b	628	19/19	0.60	0.31	0.90	48,90,106,124	0
35	HTG	B	622	19/19	0.92	0.11	0.90	26,30,44,56	0
24	CLA	D	401	65/65	0.96	0.24	0.89	13,18,30,32	0
24	CLA	c	512	65/65	0.93	0.17	0.84	26,32,44,59	0
24	CLA	b	609	65/65	0.95	0.15	0.84	16,25,56,66	0
24	CLA	C	514	65/65	0.91	0.16	0.83	32,42,69,72	0
36	DGD	c	519	62/66	0.92	0.20	0.83	26,34,65,72	0
37	LHG	D	410	49/49	0.94	0.18	0.81	20,33,91,95	0
24	CLA	b	618	65/65	0.94	0.18	0.81	15,23,48,56	0
24	CLA	B	615	65/65	0.92	0.14	0.78	15,24,67,78	0
35	HTG	b	603	19/19	0.89	0.14	0.77	34,44,64,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
38	HEM	e	102	43/43	0.94	0.18	0.77	38,48,65,84	0
24	CLA	c	505	65/65	0.89	0.13	0.75	29,35,46,60	0
28	GOL	v	201	6/6	0.93	0.13	0.75	31,40,49,50	0
34	LMG	c	520	51/55	0.85	0.22	0.74	33,63,86,88	0
36	DGD	c	517	62/66	0.93	0.17	0.74	23,32,68,76	0
36	DGD	H	102	62/66	0.86	0.19	0.72	20,29,42,58	0
24	CLA	a	409	65/65	0.94	0.13	0.70	20,27,83,88	0
26	BCR	K	101	40/40	0.93	0.12	0.68	27,33,42,47	0
24	CLA	C	505	65/65	0.92	0.21	0.66	22,29,59,77	0
37	LHG	d	410	49/49	0.94	0.18	0.65	23,35,85,104	0
37	LHG	e	101	42/49	0.74	0.23	0.64	49,87,117,128	0
26	BCR	t	101	40/40	0.92	0.12	0.63	15,24,45,49	0
24	CLA	B	610	65/65	0.91	0.12	0.60	19,26,36,40	0
30	LMT	m	102	35/35	0.70	0.23	0.60	16,51,73,79	0
24	CLA	d	401	65/65	0.96	0.21	0.60	16,19,26,42	0
27	SQD	F	101	43/54	0.88	0.30	0.56	39,70,96,105	0
24	CLA	b	619	65/65	0.93	0.14	0.55	15,25,72,77	0
26	BCR	T	102	40/40	0.91	0.16	0.55	14,28,36,42	0
24	CLA	d	404	65/65	0.94	0.12	0.52	27,34,74,81	0
25	PHO	A	407	64/64	0.94	0.18	0.50	15,18,23,28	0
28	GOL	A	412	6/6	0.92	0.10	0.48	29,31,34,37	0
36	DGD	C	517	62/66	0.94	0.14	0.48	22,33,75,83	0
24	CLA	a	406	65/65	0.96	0.24	0.47	17,20,35,51	0
24	CLA	B	612	65/65	0.91	0.17	0.47	15,21,37,41	0
21	FE2	a	403	1/1	0.99	0.11	0.46	30,30,30,30	0
26	BCR	k	103	40/40	0.86	0.17	0.46	32,40,48,52	0
30	LMT	M	102	35/35	0.78	0.20	0.44	22,50,66,76	0
26	BCR	C	515	40/40	0.92	0.12	0.43	31,42,49,53	0
24	CLA	b	616	65/65	0.93	0.13	0.41	18,26,38,52	0
24	CLA	B	607	65/65	0.93	0.11	0.41	18,26,51,75	0
25	PHO	a	408	64/64	0.95	0.18	0.40	16,21,29,37	0
24	CLA	b	611	65/65	0.94	0.10	0.40	19,31,58,74	0
24	CLA	b	614	65/65	0.89	0.12	0.37	24,31,41,50	0
24	CLA	C	507	65/65	0.92	0.16	0.36	28,42,81,88	0
24	CLA	B	604	65/65	0.91	0.12	0.35	18,25,32,40	0
30	LMT	D	402	35/35	0.68	0.25	0.34	32,75,96,97	0
24	CLA	b	610	65/65	0.95	0.11	0.33	18,24,37,42	0
28	GOL	V	201	6/6	0.92	0.11	0.31	27,29,40,41	0
24	CLA	B	614	65/65	0.94	0.17	0.30	14,22,45,52	0
28	GOL	v	205	6/6	0.93	0.17	0.28	25,39,52,58	0
36	DGD	c	518	62/66	0.90	0.19	0.28	24,35,79,94	0
24	CLA	b	621	65/65	0.92	0.15	0.27	21,35,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	BCR	c	516	40/40	0.91	0.12	0.26	29,36,47,57	0
24	CLA	b	608	65/65	0.94	0.11	0.24	22,29,38,42	0
24	CLA	B	608	65/65	0.92	0.18	0.24	13,20,31,35	0
24	CLA	B	616	65/65	0.95	0.11	0.22	19,28,48,60	0
24	CLA	c	514	65/65	0.90	0.18	0.22	34,43,67,76	0
24	CLA	c	507	65/65	0.91	0.12	0.22	22,31,52,62	0
26	BCR	H	101	40/40	0.88	0.13	0.19	21,32,48,52	0
24	CLA	C	504	65/65	0.92	0.12	0.17	24,33,42,48	0
24	CLA	b	617	65/65	0.94	0.11	0.17	18,26,36,50	0
24	CLA	C	510	65/65	0.95	0.11	0.16	25,32,51,57	0
24	CLA	c	506	65/65	0.90	0.17	0.15	26,33,51,61	0
24	CLA	C	511	65/65	0.93	0.15	0.15	23,29,41,62	0
24	CLA	c	503	65/65	0.93	0.11	0.13	29,34,45,54	0
24	CLA	b	607	65/65	0.92	0.12	0.10	23,30,38,41	0
28	GOL	b	631	6/6	0.91	0.11	0.09	39,46,48,60	0
24	CLA	B	605	65/65	0.94	0.14	0.08	15,22,51,63	0
26	BCR	y	101	40/40	0.92	0.12	0.06	31,40,53,60	0
26	BCR	b	624	40/40	0.92	0.10	0.05	20,32,46,52	0
21	FE2	A	401	1/1	0.99	0.10	0.01	27,27,27,27	0
26	BCR	B	620	40/40	0.95	0.10	0.01	22,29,42,47	0
24	CLA	b	620	65/65	0.91	0.11	-0.00	22,31,51,74	0
24	CLA	C	502	65/65	0.93	0.11	-0.03	25,32,47,58	0
24	CLA	c	513	65/65	0.91	0.12	-0.04	30,39,50,54	0
24	CLA	B	609	65/65	0.95	0.14	-0.04	17,22,32,36	0
24	CLA	b	615	65/65	0.94	0.11	-0.04	21,28,39,46	0
24	CLA	B	613	65/65	0.95	0.11	-0.05	15,23,32,35	0
24	CLA	B	606	65/65	0.95	0.09	-0.06	16,22,34,38	0
24	CLA	c	504	65/65	0.94	0.14	-0.06	26,32,45,55	0
24	CLA	C	513	65/65	0.93	0.12	-0.08	29,42,67,74	0
38	HEM	v	202	43/43	0.97	0.10	-0.10	29,33,40,48	0
24	CLA	C	512	65/65	0.93	0.11	-0.10	26,32,41,48	0
24	CLA	B	603	65/65	0.91	0.12	-0.12	18,25,32,38	0
24	CLA	b	613	65/65	0.94	0.11	-0.12	22,29,38,42	0
26	BCR	c	526	40/40	0.90	0.16	-0.13	39,48,59,63	0
24	CLA	C	506	65/65	0.95	0.10	-0.14	21,29,45,53	0
26	BCR	A	410	40/40	0.95	0.10	-0.16	16,26,33,35	0
24	CLA	D	404	65/65	0.95	0.12	-0.17	21,28,73,84	0
28	GOL	c	524	6/6	0.98	0.15	-0.17	25,28,30,34	0
23	BCT	A	404	4/4	0.96	0.10	-0.20	27,30,39,40	0
26	BCR	h	101	40/40	0.87	0.12	-0.23	27,35,46,49	0
35	HTG	O	303	19/19	0.94	0.09	-0.28	24,32,47,48	0
28	GOL	C	525	6/6	0.95	0.13	-0.31	20,24,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	BCR	a	410	40/40	0.94	0.09	-0.34	16,24,31,33	0
24	CLA	c	509	65/65	0.92	0.12	-0.36	27,34,49,58	0
24	CLA	C	508	65/65	0.93	0.11	-0.36	25,35,48,57	0
38	HEM	E	103	43/43	0.96	0.17	-0.45	27,38,50,56	0
24	CLA	c	508	65/65	0.93	0.12	-0.47	30,41,65,70	0
26	BCR	C	516	40/40	0.94	0.09	-0.56	25,34,43,46	0
24	CLA	c	511	65/65	0.96	0.10	-0.57	29,36,49,55	0
24	CLA	C	503	65/65	0.94	0.12	-0.59	22,28,40,51	0
22	CL	a	405	1/1	0.99	0.12	-0.92	26,26,26,26	0
38	HEM	V	203	43/43	0.97	0.08	-1.09	23,26,31,36	0
31	OEX	A	418	10/10	0.99	0.09	-1.53	16,23,28,32	0
31	OEX	a	415	10/10	0.99	0.11	-1.57	20,24,35,37	0
22	CL	a	404	1/1	1.00	0.10	-2.07	20,20,20,20	0
22	CL	A	403	1/1	0.98	0.07	-2.18	23,23,23,23	0
22	CL	A	402	1/1	0.99	0.10	-2.49	19,19,19,19	0
33	CA	O	301	1/1	0.97	0.05	-2.99	56,56,56,56	0
33	CA	o	301	1/1	0.94	0.07	-3.37	62,62,62,62	0
33	CA	c	502	1/1	0.96	0.04	-3.41	44,44,44,44	0
39	MG	J	102	1/1	0.97	0.04	-3.51	28,28,28,28	0
29	UNL	M	103	10/-	0.85	0.18	-	34,42,59,64	0
33	CA	b	605	1/1	0.67	0.14	-	95,95,95,95	0
22	CL	V	202	1/1	0.95	0.05	-	63,63,63,63	0
22	CL	u	201	1/1	0.95	0.05	-	63,63,63,63	0
29	UNL	B	632	33/-	0.74	0.24	-	32,70,105,113	0
29	UNL	A	415	28/-	0.62	0.31	-	55,65,84,90	0
29	UNL	b	634	33/-	0.65	0.26	-	42,71,112,116	0
28	GOL	T	103	6/6	0.69	0.31	-	63,76,80,81	0
35	HTG	C	522	19/19	0.91	0.18	-	53,65,89,95	0
35	HTG	B	624	19/19	0.71	0.35	-	38,95,102,121	0
28	GOL	O	302	6/6	0.68	0.18	-	52,61,64,70	0
33	CA	f	103	1/1	0.89	0.12	-	72,72,72,72	0
35	HTG	c	522	19/19	0.86	0.17	-	63,69,80,85	0
35	HTG	b	604	19/19	0.62	0.19	-	50,80,106,112	0
33	CA	B	601	1/1	0.77	0.09	-	79,79,79,79	0
33	CA	F	102	1/1	0.88	0.14	-	72,72,72,72	0
29	UNL	m	101	10/-	0.86	0.25	-	37,51,60,62	0
29	UNL	a	414	30/-	0.63	0.28	-	45,65,86,89	0
28	GOL	B	635	6/6	0.22	0.43	-	82,91,97,98	0

6.5 Other polymers (i)

There are no such residues in this entry.