Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:42 PM GMT

PDB ID	:	4TNH
Title	:	RT XFEL structure of Photosystem II in the dark state at 4.9 A resolution
Authors	:	Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on	:	2014-06-04
Resolution	:	4.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

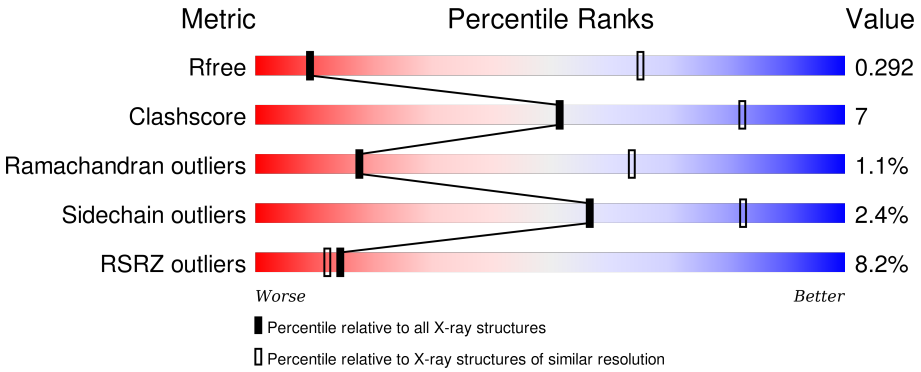
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1118 (6.10-3.60)
Clashscore	102246	1018 (6.10-3.66)
Ramachandran outliers	100387	1157 (6.10-3.60)
Sidechain outliers	100360	1135 (6.10-3.60)
RSRZ outliers	91569	1121 (6.10-3.60)

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	9%, 69%, 27%
1	a	344	13%, 95%
2	B	510	8%, 76%, 19%
2	b	510	9%, 94%

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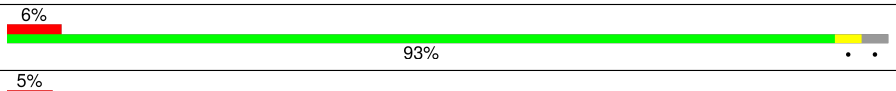
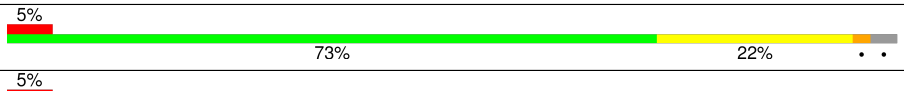
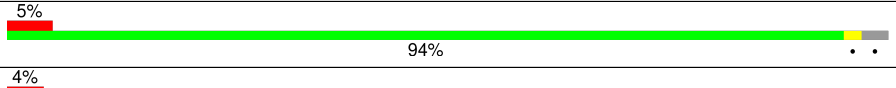
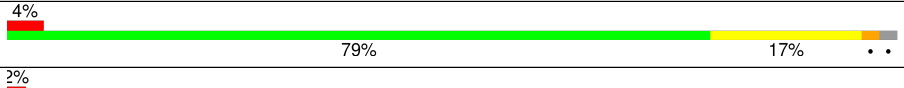
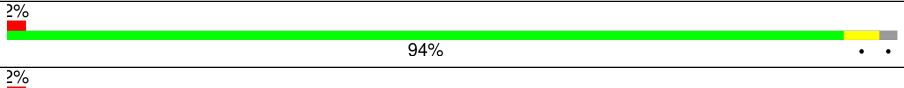
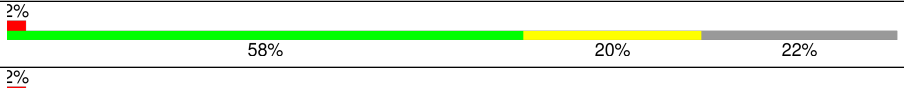
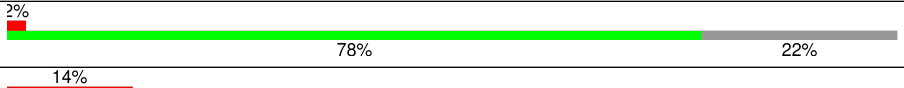
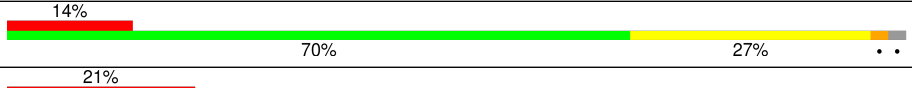
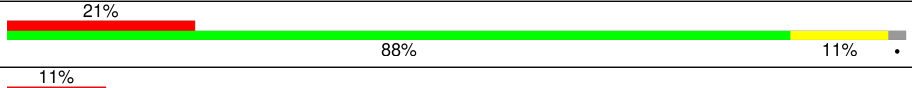
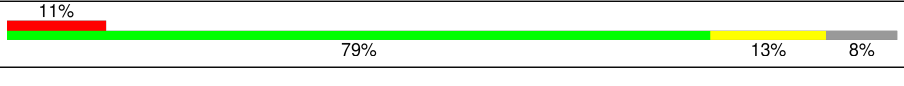
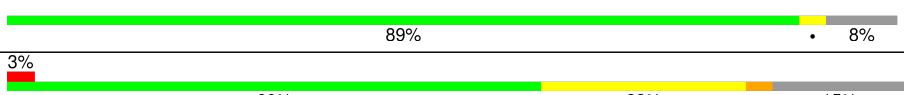
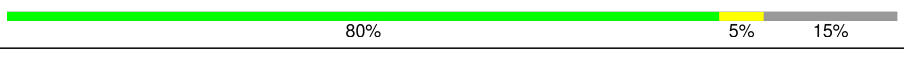
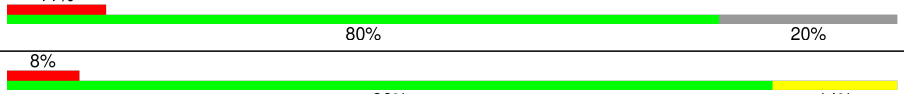
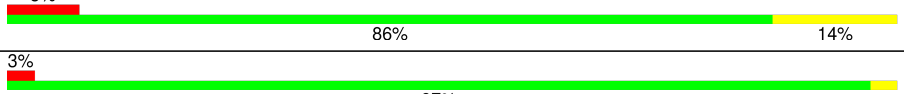
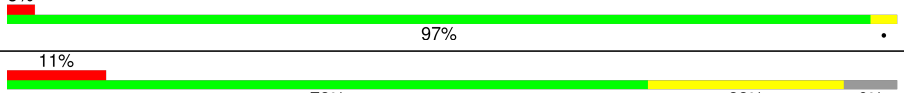
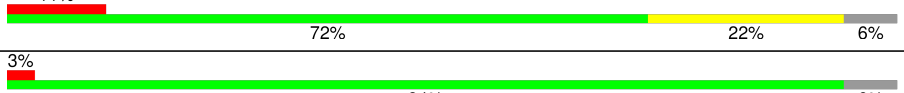
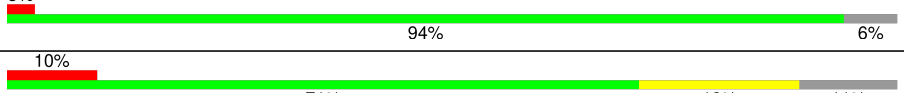
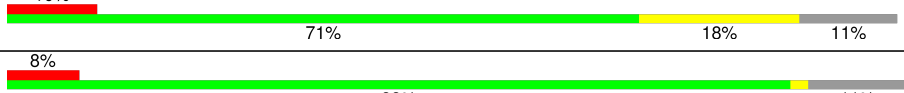
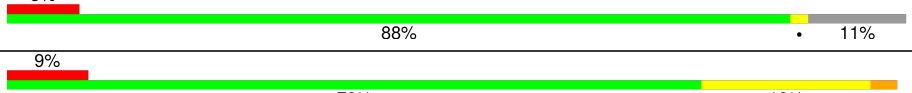
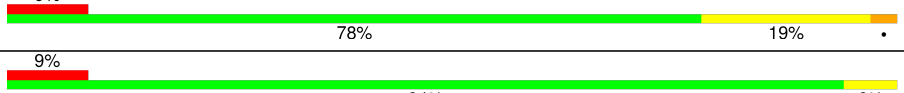
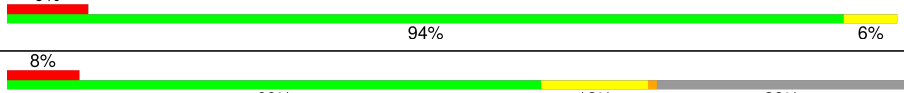
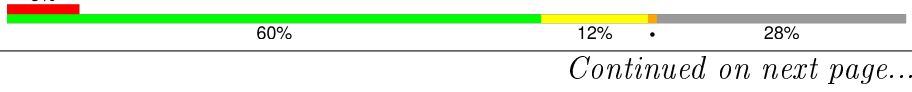
Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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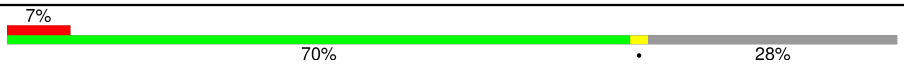
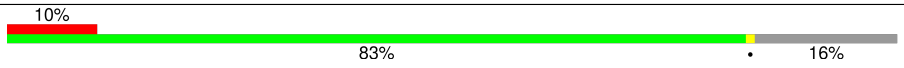
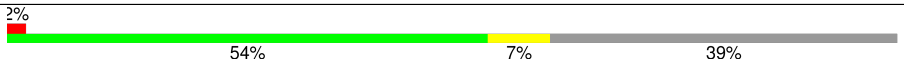
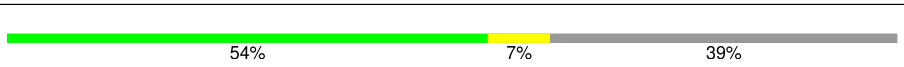
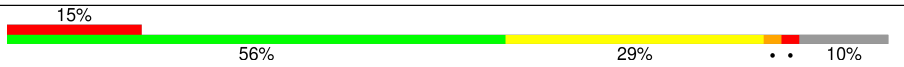
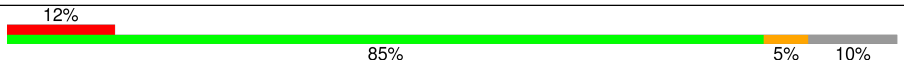
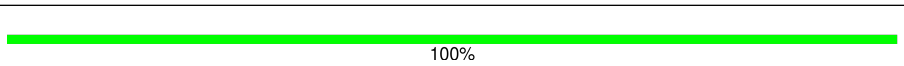
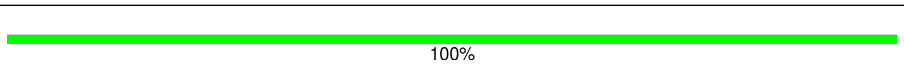
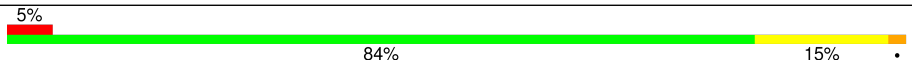
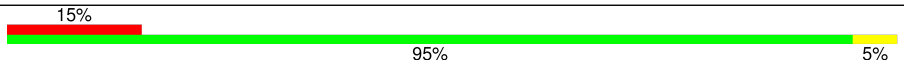
Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	X
22	CLA	A	403	X	-	-	X
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	X
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	X
22	CLA	B	604	X	-	-	X
22	CLA	B	605	X	-	-	X
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	X
22	CLA	B	608	X	-	-	X
22	CLA	B	609	X	-	-	X
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	X
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X
22	CLA	B	614	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	615	X	-	-	X
22	CLA	C	501	X	-	-	X
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	X
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	X
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	520	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	X
22	CLA	H	101	X	-	-	X
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	X
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	X
22	CLA	b	618	X	-	-	X
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	X
22	CLA	c	506	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	X
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	X
22	CLA	d	405	X	-	-	X
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	D	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	j	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	513	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	F	102	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	513	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	521	-	-	-	X
24	BCR	f	102	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	D	409	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	d	409	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	D	411	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	M	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	a	402	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	e	101	-	-	-	X
27	LMG	l	101	-	-	-	X
27	LMG	m	101	-	-	-	X
29	OEX	A	412	-	-	-	X
29	OEX	a	414	-	-	-	X
30	SQD	B	622	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	103	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	d	402	-	-	-	X
30	SQD	f	103	-	-	-	X
31	LMT	B	624	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	102	-	-	-	X
31	LMT	M	103	-	-	-	X
31	LMT	b	603	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	410	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	d	401	-	-	-	X
33	BCT	d	403	-	-	-	X
34	HEM	F	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	v	201	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	x	37	Total	C	N	O	0	0	0
			270	182	41	47			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	G	28	Total	C	N	O	0	0	0
			140	84	28	28			

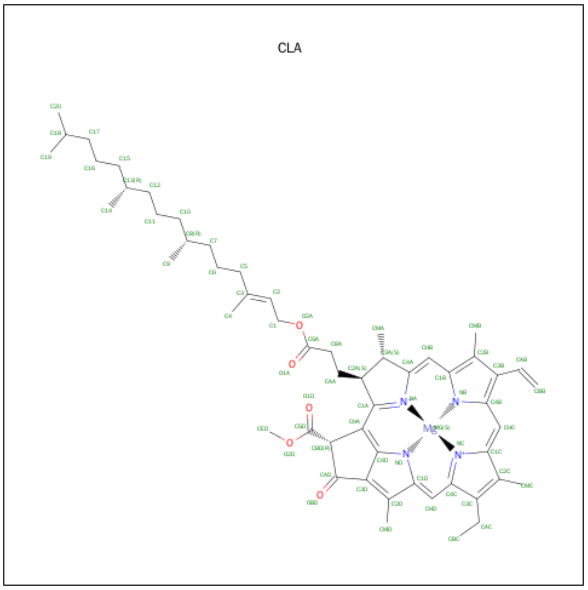
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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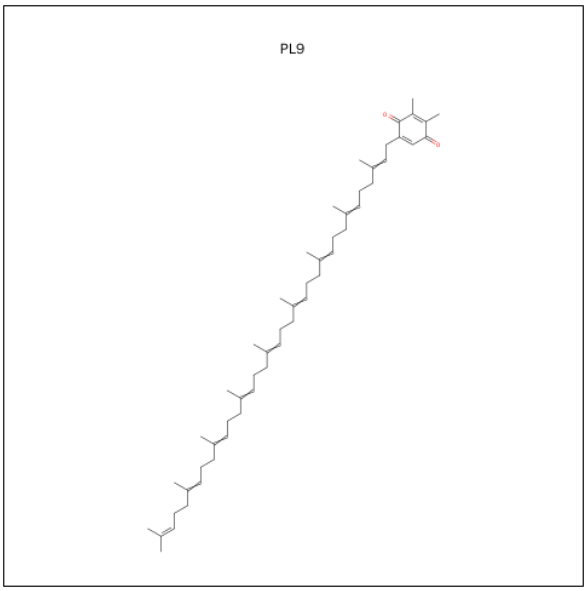
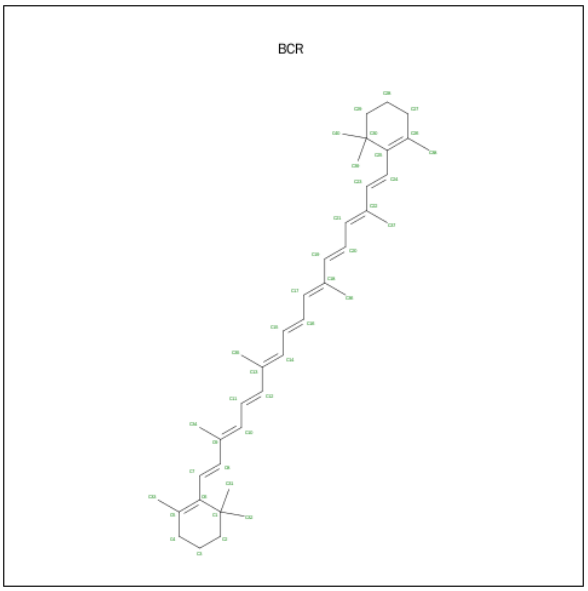
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	b	1	Total C Mg N O 65 55 1 4 5	0	0
22	b	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4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

- Molecule 23 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
23	A	1	Total C O 45 43 2	0	0
23	D	1	Total C O 55 53 2	0	0
23	J	1	Total C O 35 33 2	0	0
23	a	1	Total C O 45 43 2	0	0
23	d	1	Total C O 55 53 2	0	0
23	j	1	Total C O 35 33 2	0	0

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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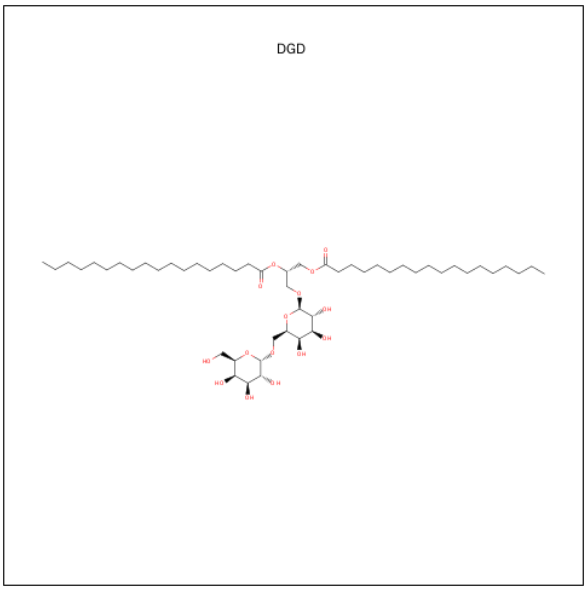
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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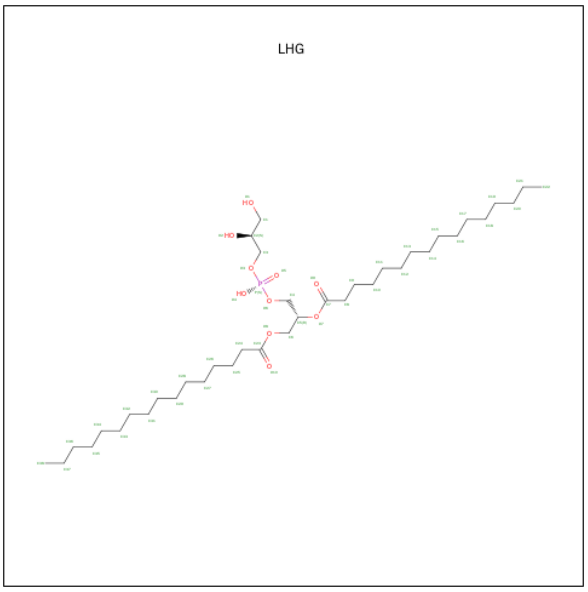
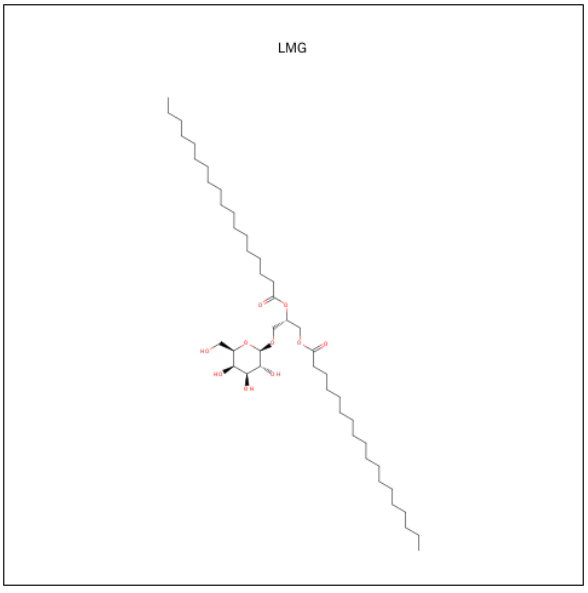
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 58 43 15	0	0
25	B	1	Total C O 52 37 15	0	0
25	C	1	Total C O 53 38 15	0	0
25	C	1	Total C O 62 47 15	0	0
25	C	1	Total C O 66 51 15	0	0
25	D	1	Total C O 63 48 15	0	0
25	a	1	Total C O 56 41 15	0	0
25	b	1	Total C O 52 37 15	0	0
25	b	1	Total C O 58 43 15	0	0
25	c	1	Total C O 53 38 15	0	0
25	c	1	Total C O 62 47 15	0	0
25	c	1	Total C O 66 51 15	0	0
25	d	1	Total C O 63 48 15	0	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

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

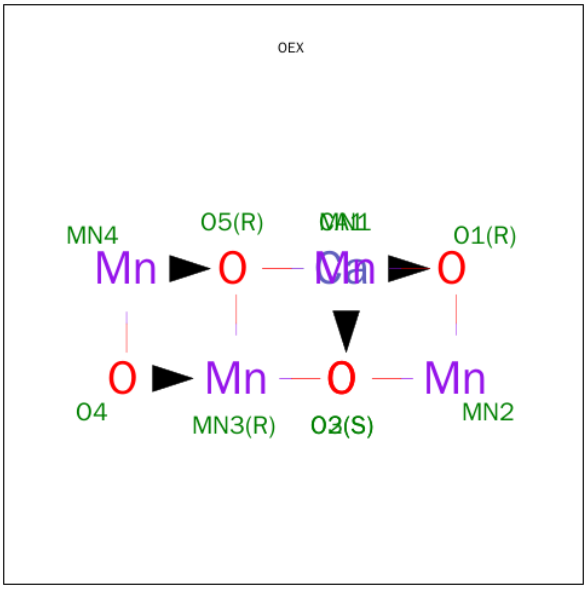


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 51 41 10	0	0
27	A	1	Total C O 42 32 10	0	0
27	B	1	Total C O 49 39 10	0	0
27	C	1	Total C O 45 35 10	0	0
27	C	1	Total C O 48 38 10	0	0
27	D	1	Total C O 49 39 10	0	0
27	D	1	Total C O 48 38 10	0	0
27	D	1	Total C O 46 36 10	0	0
27	E	1	Total C O 44 34 10	0	0
27	I	1	Total C O 43 33 10	0	0
27	M	1	Total C O 42 32 10	0	0
27	a	1	Total C O 42 32 10	0	0
27	b	1	Total C O 49 39 10	0	0
27	c	1	Total C O 45 35 10	0	0
27	c	1	Total C O 48 38 10	0	0
27	d	1	Total C O 49 39 10	0	0
27	d	1	Total C O 48 38 10	0	0
27	d	1	Total C O 46 36 10	0	0
27	e	1	Total C O 44 34 10	0	0
27	i	1	Total C O 43 33 10	0	0
27	l	1	Total C O 51 41 10	0	0
27	m	1	Total C O 42 32 10	0	0

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

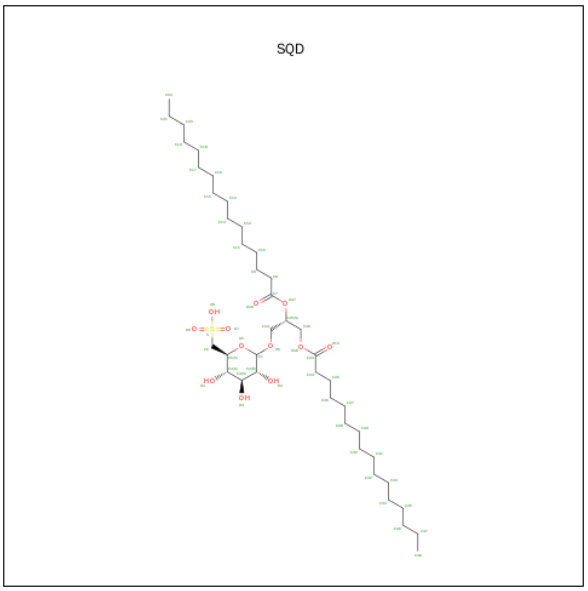
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Cl 1 1	0	0
28	a	1	Total Cl 1 1	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



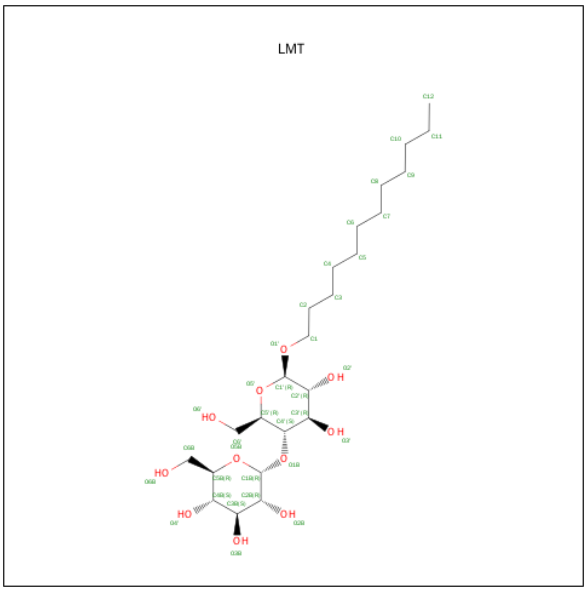
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0	0
29	a	1	Total Ca Mn O 10 1 4 5	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



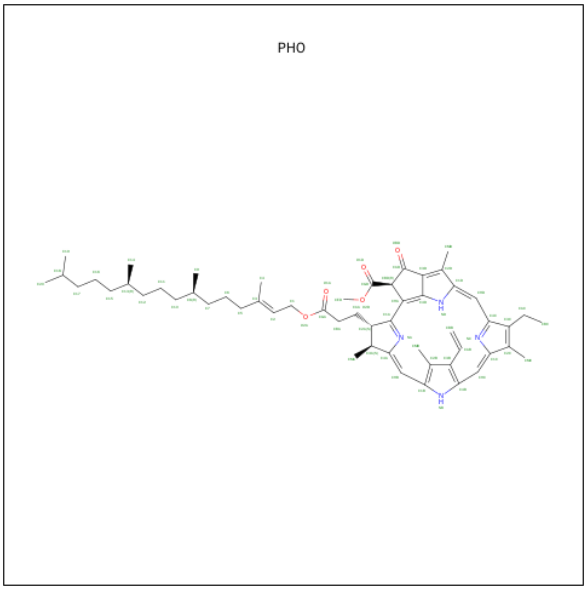
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



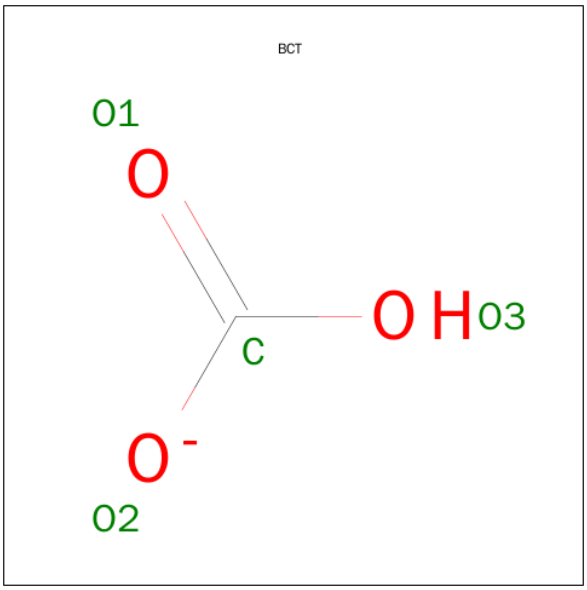
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	D	1	Total C O 31 20 11	0	0
31	I	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	d	1	Total C O 31 20 11	0	0
31	i	1	Total C O 35 24 11	0	0

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



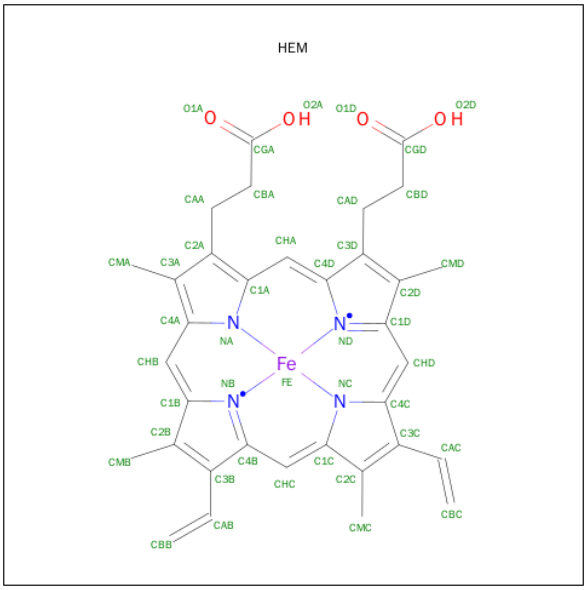
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 4 1 3	0	0
33	d	1	Total C O 4 1 3	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	F	1	Total C Fe N O 43 34 1 4 4	0	0
34	V	1	Total C Fe N O 43 34 1 4 4	0	0
34	f	1	Total C Fe N O 43 34 1 4 4	0	0
34	v	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	o	1	Total Ca 1 1	0	0
35	O	1	Total Ca 1 1	0	0
35	K	1	Total Ca 1 1	0	0

Continued on next page...

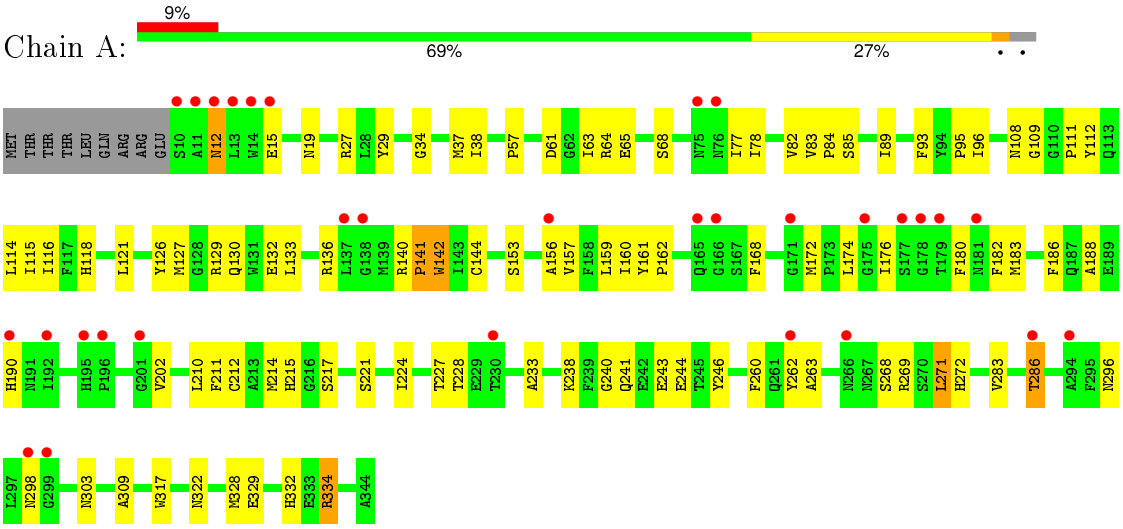
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	k	1	Total	Ca	0	0
			1	1		

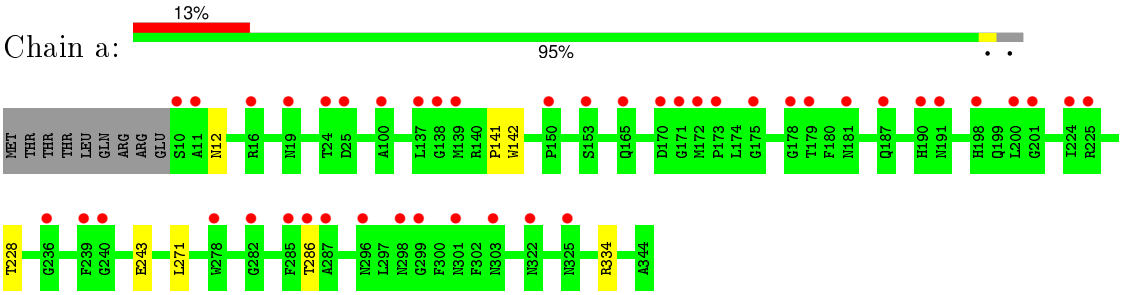
3 Residue-property plots (i)

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.

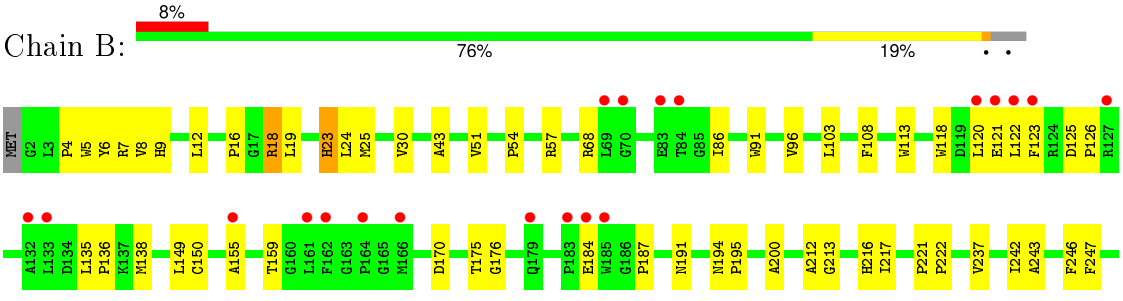
- Molecule 1: Photosystem Q(B) protein 1

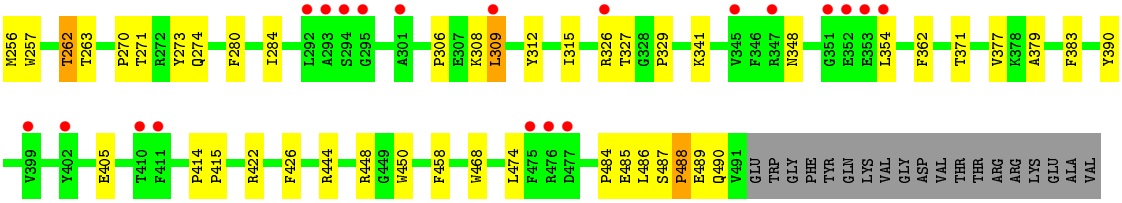


- Molecule 1: Photosystem Q(B) protein 1



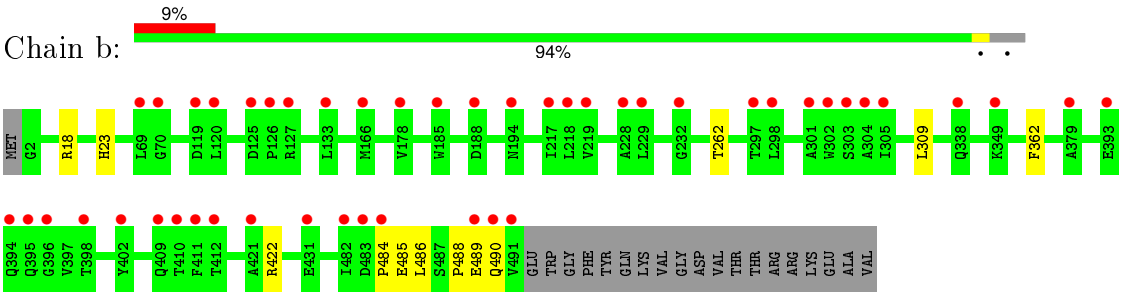
- Molecule 2: Photosystem II core light harvesting protein





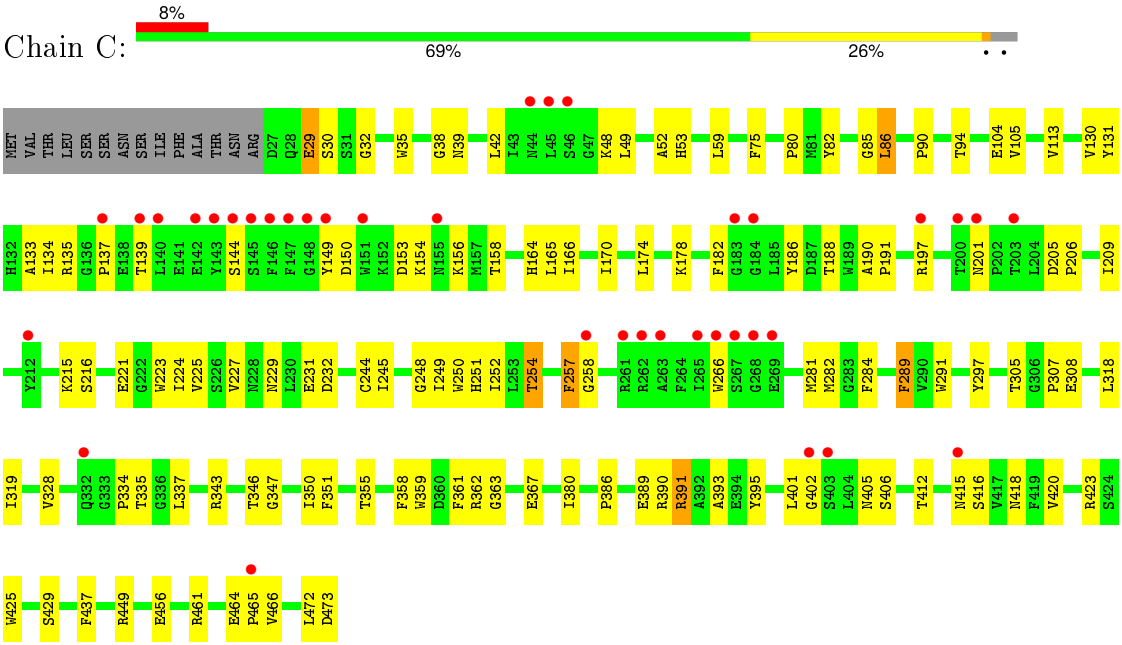
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



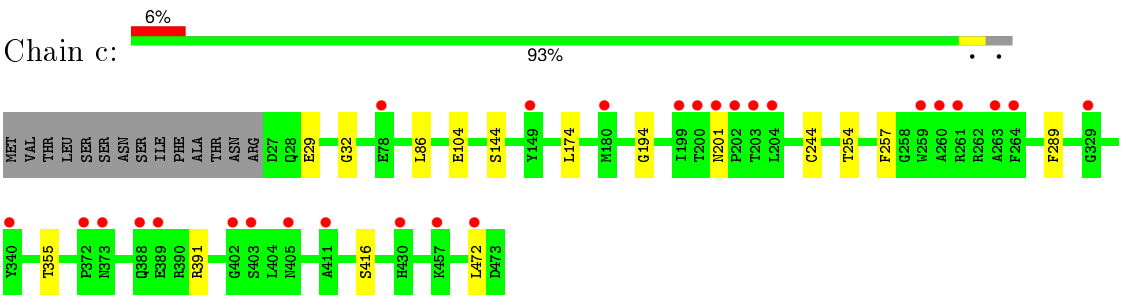
• Molecule 3: Photosystem II CP43 protein

Chain C:

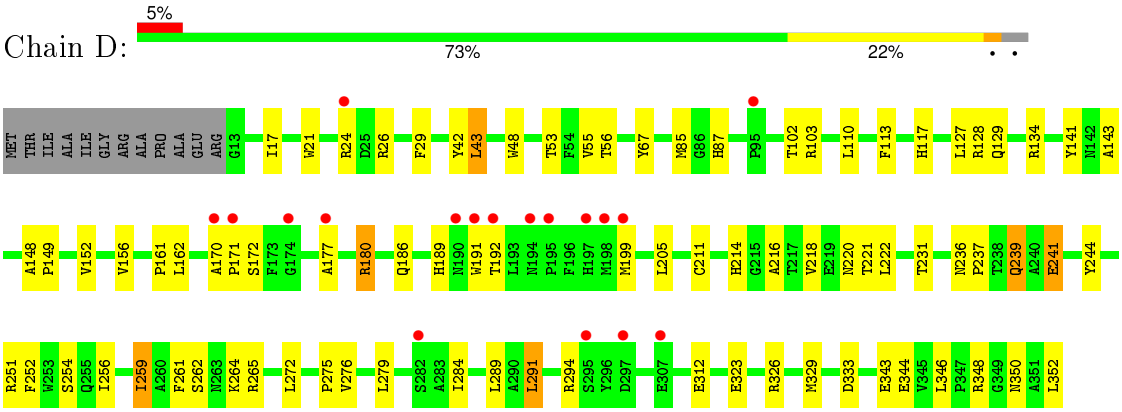


• Molecule 3: Photosystem II CP43 protein

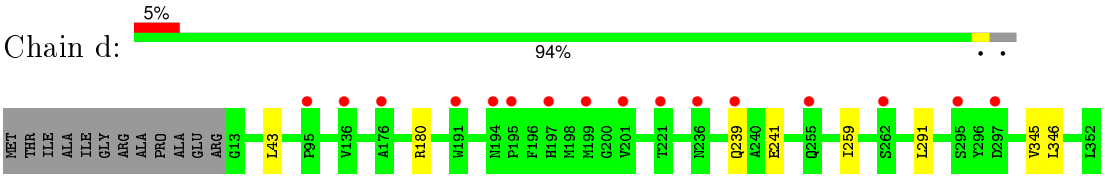
Chain c:



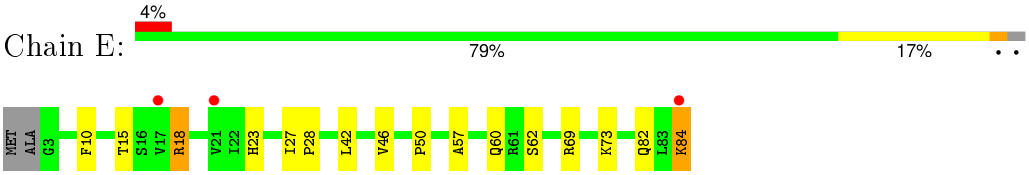
• Molecule 4: Photosystem II D2 protein



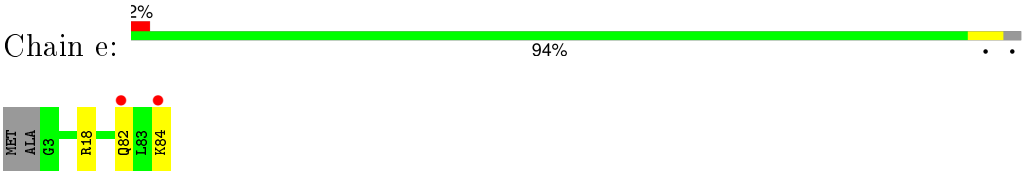
- Molecule 4: Photosystem II D2 protein



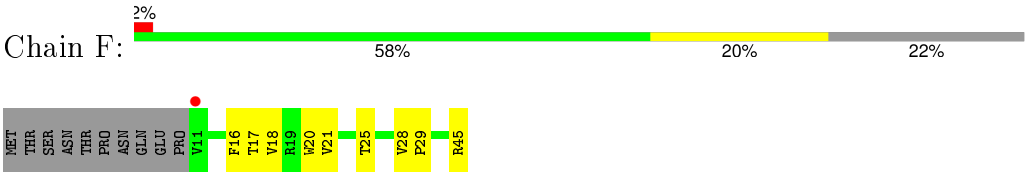
- Molecule 5: Cytochrome b559 subunit alpha



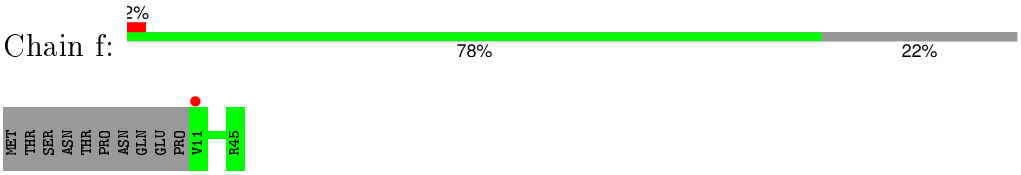
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

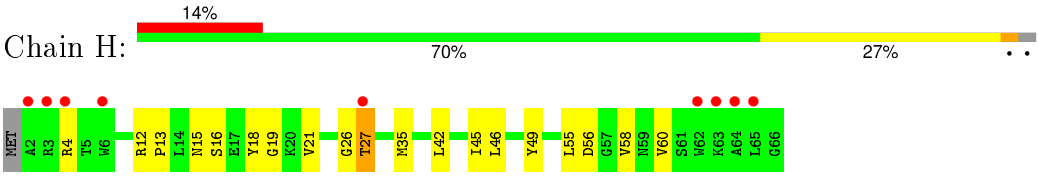


- Molecule 6: Cytochrome b559 subunit beta



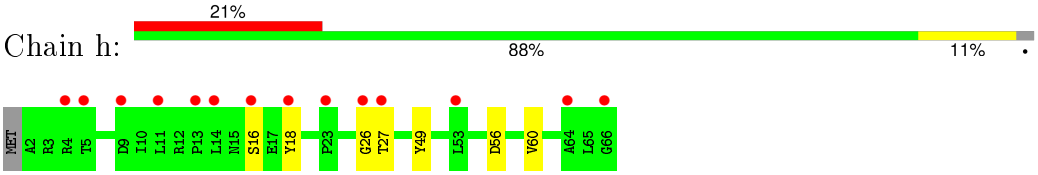
- Molecule 7: Photosystem II reaction center protein H

Chain H:



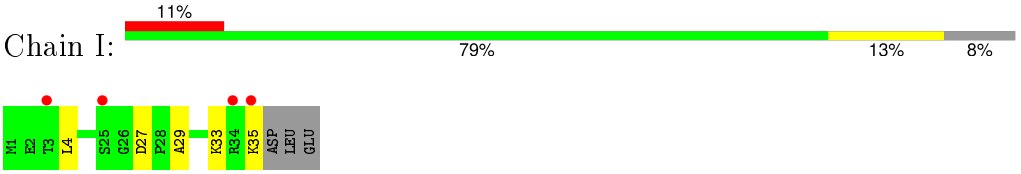
• Molecule 7: Photosystem II reaction center protein H

Chain h:



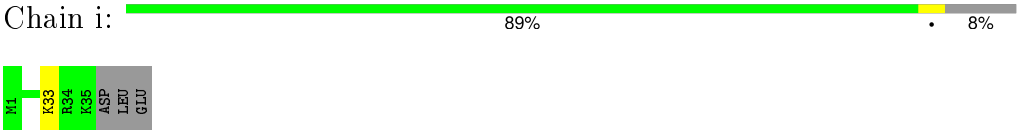
• Molecule 8: Photosystem II reaction center protein I

Chain I:



• Molecule 8: Photosystem II reaction center protein I

Chain i:

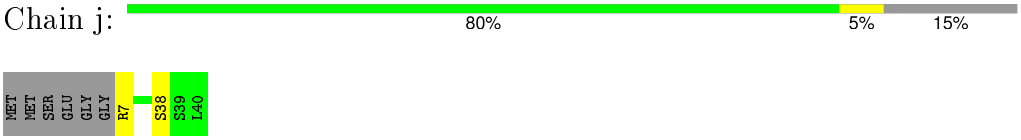


• Molecule 9: Photosystem II reaction center protein J

Chain J:

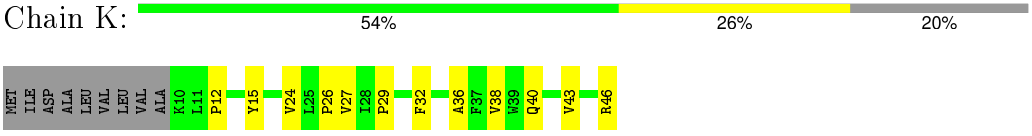
• Molecule 9: Photosystem II reaction center protein J

Chain j:



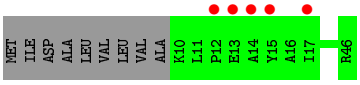
• Molecule 10: Photosystem II reaction center protein K

Chain K:



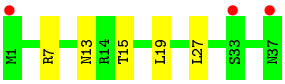
• Molecule 10: Photosystem II reaction center protein K

Chain k:



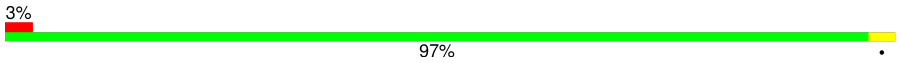
• Molecule 11: Photosystem II reaction center protein L

Chain L:



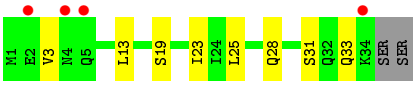
• Molecule 11: Photosystem II reaction center protein L

Chain l:



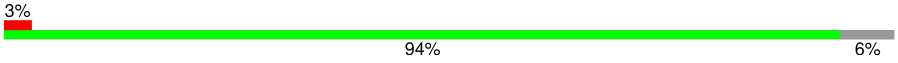
• Molecule 12: Photosystem II reaction center protein M

Chain M:



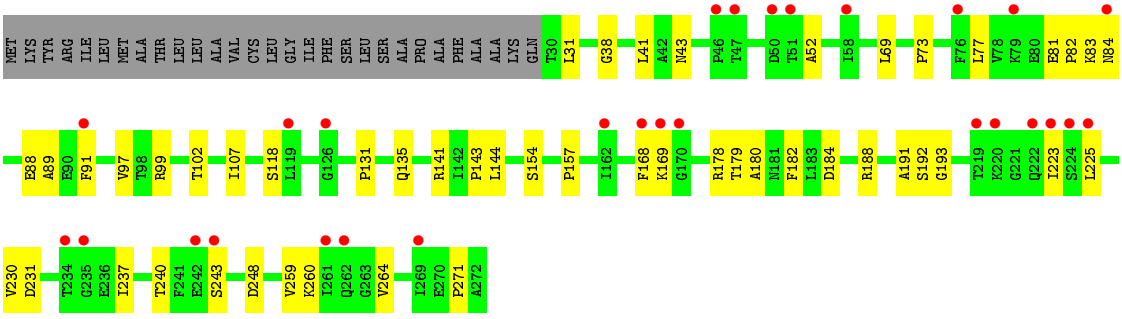
• Molecule 12: Photosystem II reaction center protein M

Chain m:



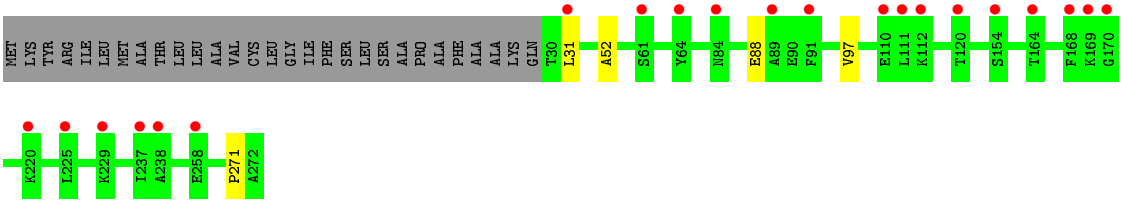
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

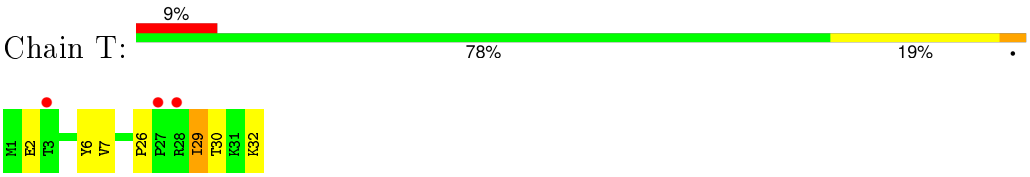


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

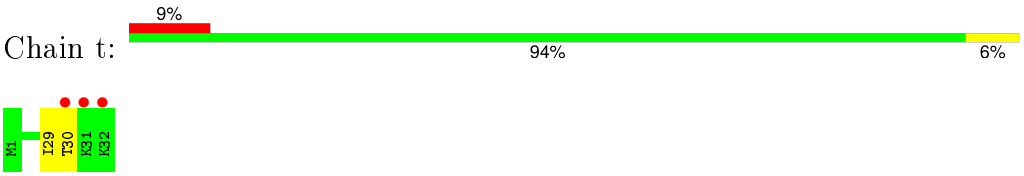
Chain o:



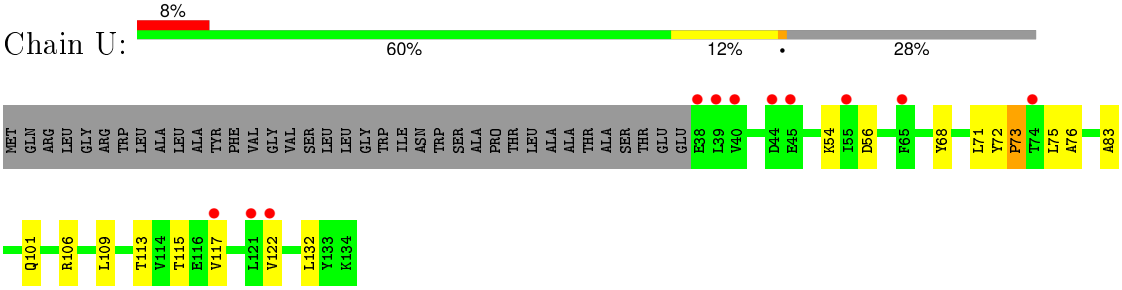
• Molecule 14: Photosystem II reaction center protein T



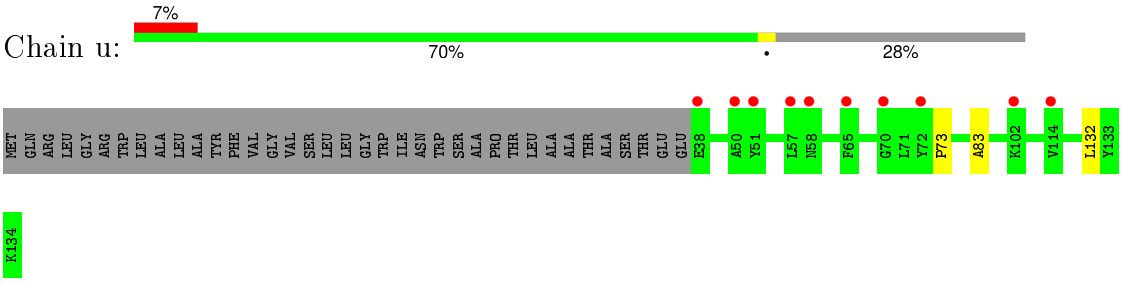
• Molecule 14: Photosystem II reaction center protein T



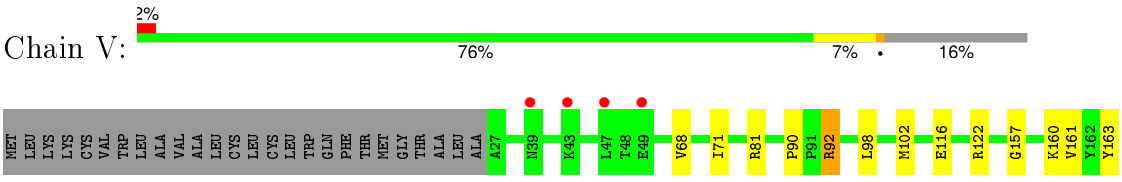
• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

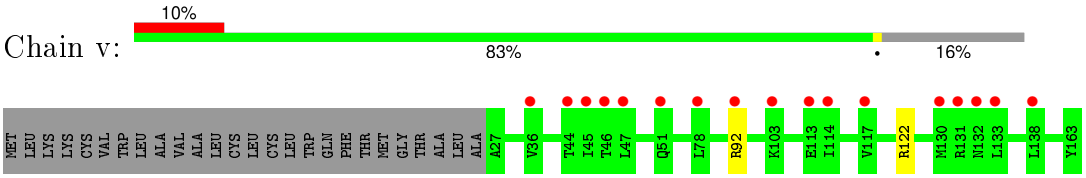


• Molecule 16: Cytochrome c-550



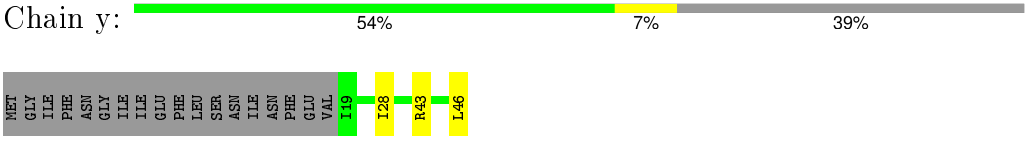
• Molecule 16: Cytochrome c-550

Chain v:



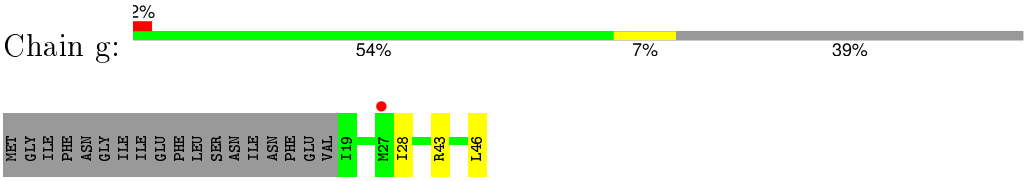
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



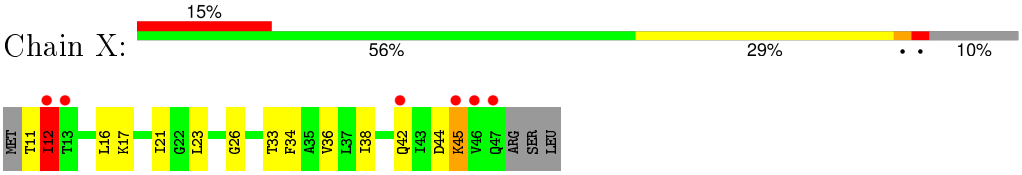
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



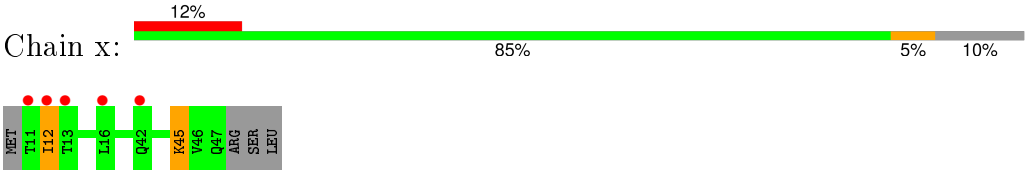
• Molecule 18: Photosystem II reaction center X protein

Chain X:



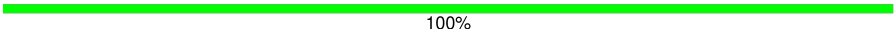
• Molecule 18: Photosystem II reaction center X protein

Chain x:



• Molecule 19: Photosystem II reaction center protein Y

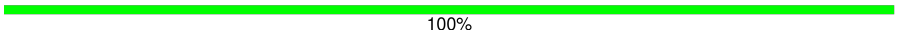
Chain Y:



There are no outlier residues recorded for this chain.

• Molecule 19: Photosystem II reaction center protein Y

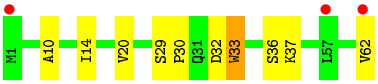
Chain G:



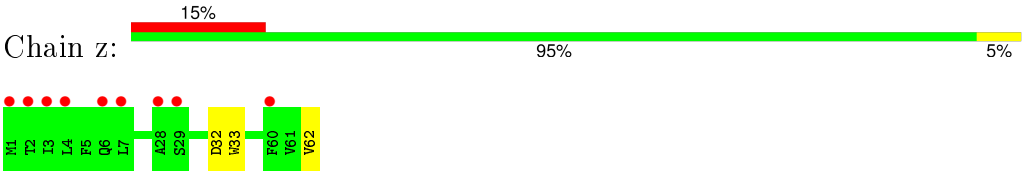
There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Z

Chain Z:



• Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.88Å 229.03Å 307.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 4.90 72.93 – 4.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (72.93-4.90) 97.8 (72.93-4.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.281 , 0.292 0.296 , 0.292	Depositor DCC
R_{free} test set	2096 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	173.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 154.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Outliers	0 of 42966 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å^2)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, BCT, HEM, LMG, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.23	0/3556	0.41	0/4842
3	c	0.23	0/3556	0.41	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.43	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.46	0/709
7	h	0.23	0/520	0.46	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.21	0/255	0.40	0/346
9	j	0.21	0/255	0.40	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.44	0/367
12	m	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.24	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.43	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	g	0.21	0/202	0.46	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	0/57100

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	85	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	89	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	88	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	71	0
4	d	2706	0	2608	0	0
5	E	666	0	651	12	0
5	e	666	0	651	0	0
6	F	282	0	291	7	0
6	f	282	0	291	0	0
7	H	507	0	521	18	0
7	h	507	0	521	0	0
8	I	286	0	308	3	0
8	i	286	0	308	0	0
9	J	249	0	262	7	0
9	j	249	0	262	0	0
10	K	293	0	305	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	5	0
11	l	304	0	316	0	0
12	M	267	0	289	8	0
12	m	267	0	289	0	0
13	O	1845	0	1801	31	0
13	o	1845	0	1801	0	0
14	T	275	0	288	6	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	6	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	46	0
22	B	975	0	1080	97	0
22	C	845	0	936	49	0
22	D	130	0	144	14	0
22	H	65	0	72	11	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	5	0
23	D	55	0	80	12	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	12	0
24	C	80	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	40	0	56	3	0
24	H	40	0	56	1	0
24	J	40	0	56	2	0
24	K	40	0	56	3	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	1	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	3	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	3	0
27	D	143	0	196	11	0
27	E	44	0	58	2	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	42	0	54	0	0
27	b	49	0	68	0	0
27	c	93	0	126	0	0
27	d	143	0	196	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	l	51	0	72	0	0
27	m	42	0	54	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	10	0	0	0	0
30	A	105	0	147	8	0
30	B	90	0	111	5	0
30	F	45	0	54	3	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	1	0
31	M	70	0	92	0	0
31	b	140	0	183	0	0
31	d	31	0	35	0	0
31	i	35	0	46	0	0
32	D	128	0	148	13	0
32	a	64	0	74	0	0
32	d	64	0	74	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51373	595	0

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

All (595) 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)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.56	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.82
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.53	0.80
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.66	0.78
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.71	0.74
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.71	0.73
22:B:605:CLA:H72	24:B:619:BCR:H311	1.71	0.73
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.55	0.72
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.76	0.71
4:D:199:MET:HG2	23:D:406:PL9:H322	1.75	0.71
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.73	0.71
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.73	0.70
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.72	0.70
4:D:29:PHE:O	4:D:128:ARG:NH2	2.25	0.69
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.74	0.69
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.69
22:C:506:CLA:H112	24:C:514:BCR:H362	1.75	0.69
4:D:259:ILE:HG12	27:D:408:LMG:H292	1.76	0.68
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.76	0.68
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.30	0.68
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.76	0.68
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.76	0.68
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.76	0.67
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.77	0.67
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.67
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.67
4:D:236:ASN:ND2	4:D:239:GLN:O	2.31	0.66
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.81	0.66
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.66	0.66
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.65
1:A:174:LEU:HD22	32:D:401:PHO:H151	1.79	0.65
27:D:408:LMG:HO4	27:D:408:LMG:HO5	1.54	0.64
30:B:622:SQD:H171	30:B:622:SQD:H301	1.80	0.64
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.78	0.64
3:C:291:TRP:O	3:C:305:THR:OG1	2.15	0.64
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.80	0.64
2:B:271:THR:HG22	2:B:273:TYR:H	1.64	0.64
12:M:31:SER:HA	27:M:101:LMG:HC1	1.82	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.82	0.63
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.79	0.63
3:C:250:TRP:O	3:C:254:THR:OG1	2.12	0.63
22:B:611:CLA:H42	4:D:127:LEU:HD11	29.91	0.63
22:A:404:CLA:H142	22:D:404:CLA:H151	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:607:CLA:HBA2	30:B:622:SQD:H101	1.81	0.63
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.64	0.62
22:A:404:CLA:HHC	22:A:404:CLA:HBB1	3.75	0.62
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
1:A:183:MET:HA	22:A:404:CLA:HMD2	12.62	0.62
1:A:183:MET:HB3	22:A:404:CLA:HBC2	14.90	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.62
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.62
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.86	0.62
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.81	0.62
4:D:24:ARG:NH2	18:X:44:ASP:O	2.33	0.61
4:D:186:GLN:HB2	22:D:404:CLA:HBC1	1.81	0.61
2:B:149:LEU:HG	22:B:606:CLA:HBC1	27.92	0.61
22:B:612:CLA:HMD1	7:H:27:THR:HB	39.61	0.61
30:A:413:SQD:H172	26:C:519:LHG:H172	1.83	0.60
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.82	0.60
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.82	0.60
3:C:406:SER:O	3:C:418:ASN:ND2	2.35	0.60
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.83	0.60
22:B:606:CLA:H193	7:H:42:LEU:HD12	33.87	0.60
4:D:216:ALA:O	4:D:220:ASN:ND2	2.33	0.60
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.83	0.60
1:A:329:GLU:O	1:A:332:HIS:ND1	2.37	0.60
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.35	0.60
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.84	0.60
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.83	0.60
22:A:404:CLA:H122	32:D:401:PHO:H3A	32.53	0.59
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.74	0.59
4:D:192:THR:HG23	22:D:404:CLA:HBC2	1.85	0.59
22:A:404:CLA:H71	22:A:405:CLA:HAB	47.00	0.59
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.59
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.83	0.58
22:B:605:CLA:OBD	31:B:623:LMT:O6'	2.20	0.58
2:B:262:THR:OG1	22:B:606:CLA:O1D	22.19	0.58
2:B:121:GLU:O	7:H:12:ARG:NH2	2.36	0.58
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.86	0.58
22:B:606:CLA:C2D	22:B:608:CLA:H2	39.98	0.58
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.93	0.58
32:D:402:PHO:H151	22:D:404:CLA:H172	1.85	0.58
22:H:101:CLA:HBD	22:H:101:CLA:H2	1.89	0.58
1:A:217:SER:HA	4:D:272:LEU:HD12	1.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.85	0.58
1:A:29:TYR:O	1:A:129:ARG:NH1	2.55	0.58
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.24	0.58
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.34	0.57
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.93	0.57
22:A:403:CLA:H203	32:D:401:PHO:H71	1.85	0.57
22:B:611:CLA:H151	22:B:612:CLA:H203	19.90	0.57
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.85	0.57
13:O:83:LYS:HG2	13:O:84:ASN:H	1.69	0.57
22:C:501:CLA:HMB3	24:C:514:BCR:H403	1.87	0.57
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.57
1:A:84:PRO:HA	1:A:112:TYR:CG	2.39	0.57
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.85	0.57
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.86	0.57
2:B:12:LEU:HB2	22:B:615:CLA:HMC2	13.40	0.57
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.90	0.57
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.30	0.56
26:C:519:LHG:H271	26:C:519:LHG:H101	1.86	0.56
4:D:214:HIS:ND1	23:D:406:PL9:O2	2.26	0.56
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.70	0.56
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.56
27:D:408:LMG:O6	11:L:15:THR:HG21	2.05	0.56
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.88	0.56
1:A:224:ILE:O	4:D:265:ARG:NH2	2.46	0.56
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.34	0.56
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.56
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.88	0.56
2:B:327:THR:HG21	27:B:621:LMG:H111	1.87	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.24	0.56
2:B:262:THR:HG22	2:B:263:THR:HG23	1.87	0.56
2:B:256:MET:O	2:B:448:ARG:NH1	2.34	0.55
22:B:607:CLA:HBD	22:B:608:CLA:H43	4.12	0.55
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.36	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.88	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.55
30:B:626:SQD:H1	30:B:626:SQD:H462	1.88	0.55
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.78	0.55
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.38	0.55
2:B:474:LEU:O	4:D:134:ARG:NH1	2.47	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:404:CLA:H93	22:D:404:CLA:H152	1.89	0.55
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.88	0.55
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.94	0.55
22:B:606:CLA:C3D	22:B:608:CLA:H2	40.21	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.91	0.55
1:A:64:ARG:O	13:O:178:ARG:NH2	2.40	0.55
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.42	0.55
24:A:407:BCR:H321	30:A:414:SQD:H321	1.89	0.54
2:B:184:GLU:H	2:B:200:ALA:HB2	1.72	0.54
2:B:458:PHE:HB3	22:B:607:CLA:HBC2	12.95	0.54
22:C:510:CLA:HMB2	24:C:513:BCR:H382	1.88	0.54
22:A:405:CLA:H203	32:D:401:PHO:H71	33.20	0.54
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.42	0.54
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.88	0.54
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.89	0.54
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.90	0.54
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.93	0.54
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.54
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.39	0.54
2:B:271:THR:HB	2:B:274:GLN:HG3	1.90	0.54
1:A:268:SER:O	1:A:272:HIS:ND1	2.38	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.54
22:D:405:CLA:H42	18:X:26:GLY:HA3	1.90	0.54
22:D:405:CLA:H43	18:X:23:LEU:HA	1.90	0.53
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.53
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.44	0.53
24:A:407:BCR:H342	30:A:414:SQD:H311	1.90	0.53
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.91	0.53
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.89	0.53
22:A:405:CLA:HED1	23:D:406:PL9:H372	28.92	0.53
2:B:150:CYS:HB2	22:B:606:CLA:HMC3	24.94	0.53
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.91	0.53
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.61	0.53
13:O:73:PRO:HG2	13:O:102:THR:HB	1.91	0.53
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.91	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.91	0.53
22:A:402:CLA:H122	32:D:401:PHO:H3A	1.90	0.53
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:403:CLA:HED1	23:D:406:PL9:H372	1.90	0.53
22:B:607:CLA:H151	22:B:608:CLA:H203	1.91	0.53
22:A:403:CLA:HMA2	23:D:406:PL9:H411	1.90	0.53
27:A:410:LMG:H231	23:D:406:PL9:H352	1.91	0.52
31:B:627:LMT:H62	8:I:4:LEU:HD22	82.16	0.52
22:B:608:CLA:H202	22:B:612:CLA:HBB2	21.91	0.52
2:B:103:LEU:HD21	22:B:608:CLA:HMC3	26.61	0.52
25:B:625:DGD:O2D	25:B:625:DGD:O1B	2.27	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.94	0.52
3:C:85:GLY:N	25:C:516:DGD:HE4	2.24	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.42	0.52
2:B:212:ALA:HB2	22:B:612:CLA:HMC3	27.30	0.52
30:A:413:SQD:H311	22:C:507:CLA:H71	1.92	0.52
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.91	0.52
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.95	0.52
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	2.06	0.52
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.73	0.52
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.49	0.52
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.93	0.51
27:A:415:LMG:H112	2:B:43:ALA:HA	42.20	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.98	0.51
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.51
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.41	0.51
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.51
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.96	0.51
4:D:275:PRO:O	4:D:279:LEU:HD23	2.14	0.51
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.92	0.51
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.91	0.51
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.92	0.50
22:B:611:CLA:H51	22:B:612:CLA:H101	17.99	0.50
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.92	0.50
22:B:612:CLA:H51	27:D:407:LMG:H231	1.93	0.50
1:A:210:LEU:HG	32:D:402:PHO:NC	2.27	0.50
22:C:504:CLA:HBD	22:C:504:CLA:HBA1	1.93	0.50
1:A:132:GLU:O	1:A:136:ARG:HG2	2.12	0.50
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.93	0.50
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.96	0.50
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.95	0.50
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.97	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.88	0.50
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.92	0.50
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.50
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.42	0.50
1:A:153:SER:HB3	22:A:404:CLA:HED1	19.23	0.50
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.94	0.50
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.76	0.50
1:A:211:PHE:HA	1:A:214:MET:HB2	1.93	0.50
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.76	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.49
13:O:118:SER:HB3	13:O:157:PRO:HA	1.98	0.49
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.47	0.49
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.02	0.49
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.49
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.96	0.49
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.95	0.49
30:A:413:SQD:H223	25:C:517:DGD:HAE1	1.93	0.49
2:B:327:THR:HG22	22:B:610:CLA:H12	26.95	0.49
3:C:158:THR:O	3:C:251:HIS:HB3	2.13	0.49
27:D:411:LMG:H171	24:F:102:BCR:H383	1.96	0.49
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.28	0.49
2:B:150:CYS:HA	22:B:606:CLA:HBC2	29.85	0.49
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.49
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.72	0.49
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.80	0.49
30:F:103:SQD:H162	18:X:33:THR:HA	1.94	0.49
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.95	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.49
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.95	0.49
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.14	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
1:A:244:GLU:HG3	1:A:246:TYR:H	1.78	0.48
27:D:408:LMG:H111	11:L:19:LEU:HD21	1.99	0.48
1:A:78:ILE:O	1:A:176:ILE:HB	2.13	0.48
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.53	0.48
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.76	0.48
5:E:15:THR:HG23	9:J:8:ILE:O	2.14	0.48
22:A:405:CLA:H42	23:D:406:PL9:H162	36.94	0.48
26:A:409:LHG:H382	22:C:509:CLA:H93	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.95	0.48
4:D:102:THR:OG1	25:D:409:DGD:HD62	2.18	0.48
22:A:404:CLA:H161	23:A:406:PL9:H253	1.94	0.48
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.94	0.48
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.98	0.48
2:B:212:ALA:O	2:B:216:HIS:ND1	2.47	0.48
32:D:401:PHO:H41	32:D:401:PHO:H62	1.45	0.48
22:A:404:CLA:HAB	22:D:404:CLA:H72	1.96	0.48
13:O:240:THR:HA	13:O:264:VAL:HA	1.98	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.47
9:J:14:ALA:O	9:J:18:GLY:N	2.45	0.47
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.78	0.47
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.79	0.47
22:B:613:CLA:H51	24:B:616:BCR:H372	1.96	0.47
4:D:279:LEU:HG	32:D:402:PHO:HBC3	1.96	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.45	0.47
4:D:85:MET:HA	5:E:69:ARG:HB3	1.98	0.47
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.01	0.47
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.96	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.96	0.47
22:D:404:CLA:H61	22:D:404:CLA:H41	1.64	0.47
4:D:262:SER:N	27:D:408:LMG:O3	2.44	0.47
22:B:614:CLA:H172	22:B:614:CLA:H111	1.97	0.47
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.01	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.00	0.47
7:H:46:LEU:HD13	22:H:101:CLA:H72	1.98	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	2.01	0.47
1:A:202:VAL:HB	22:A:404:CLA:HMB3	13.00	0.47
2:B:222:PRO:HG3	7:H:27:THR:H	1.80	0.47
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.50	0.47
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.47
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.79	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
9:J:38:SER:OG	9:J:39:SER:N	2.47	0.47
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.99	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.97	0.46
24:B:616:BCR:H361	24:B:616:BCR:H20C	1.75	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.48	0.46
22:A:405:CLA:H162	22:A:405:CLA:H141	1.70	0.46
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.97	0.46
24:C:513:BCR:H343	24:C:513:BCR:H311	2.00	0.46
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.09	0.46
30:A:414:SQD:HO8	2:B:113:TRP:HE1	62.74	0.46
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.46
25:B:625:DGD:HD1	31:B:627:LMT:H32	1.97	0.46
4:D:48:TRP:CE2	32:D:402:PHO:H161	2.51	0.46
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.46
25:B:620:DGD:HAW2	22:H:101:CLA:H152	1.98	0.46
4:D:348:ARG:NH2	4:D:352:LEU:O	2.35	0.46
27:C:518:LMG:H292	27:C:518:LMG:H111	1.96	0.46
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.64	0.46
22:H:101:CLA:H62	22:H:101:CLA:H41	1.57	0.46
31:B:628:LMT:H122	14:T:7:VAL:HG12	34.43	0.46
3:C:224:ILE:O	3:C:227:VAL:HG23	2.16	0.46
1:A:114:LEU:O	1:A:118:HIS:ND1	2.45	0.46
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.00	0.46
22:A:402:CLA:HBA1	22:A:402:CLA:H3A	1.53	0.46
22:B:606:CLA:H2	22:B:608:CLA:H93	34.04	0.46
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.98	0.46
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.99	0.46
22:B:607:CLA:H51	22:B:608:CLA:H101	1.97	0.46
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.98	0.46
22:A:403:CLA:H42	23:D:406:PL9:H162	1.96	0.46
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.46
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.98	0.46
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.51	0.46
24:B:618:BCR:H361	24:B:618:BCR:H20C	1.82	0.46
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.45
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.33	0.45
22:H:101:CLA:H162	22:H:101:CLA:H122	1.51	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.17	0.45
27:I:101:LMG:H181	31:I:102:LMT:H42	2.06	0.45
22:C:510:CLA:H61	22:C:510:CLA:H93	1.81	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.52	0.45
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.98	0.45
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.45
2:B:213:GLY:O	2:B:217:ILE:HG13	2.15	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.85	0.45
22:B:611:CLA:H162	22:B:611:CLA:H122	1.75	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
27:D:408:LMG:O9	27:D:408:LMG:HC1	2.20	0.45
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.53	0.45
2:B:329:PRO:HB3	22:B:606:CLA:HED1	1.99	0.45
22:B:607:CLA:H18	22:B:608:CLA:H192	1.99	0.45
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.45
25:B:620:DGD:HA71	22:H:101:CLA:H193	1.99	0.45
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.03	0.45
3:C:318:LEU:HD21	3:C:380:ILE:HG23	1.99	0.45
1:A:202:VAL:HB	22:A:402:CLA:HMB3	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.99	0.45
2:B:150:CYS:HA	22:B:602:CLA:HBC2	2.00	0.44
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.21	0.44
24:C:513:BCR:H24C	24:C:513:BCR:H371	1.79	0.44
30:F:103:SQD:H131	18:X:36:VAL:HG11	2.00	0.44
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.99	0.44
15:U:106:ARG:HA	15:U:109:LEU:HG	1.98	0.44
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.21	0.44
2:B:327:THR:HG22	22:B:606:CLA:H12	1.99	0.44
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.06	0.44
22:C:506:CLA:H62	22:C:506:CLA:H92	1.75	0.44
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.70	0.44
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.44
3:C:245:ILE:O	3:C:249:ILE:HG12	2.19	0.44
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.01	0.44
1:A:238:LYS:O	1:A:241:GLN:HG3	2.17	0.44
22:A:402:CLA:H51	32:D:401:PHO:C3B	2.48	0.44
22:C:501:CLA:H193	22:C:506:CLA:H111	2.10	0.44
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.44
22:B:606:CLA:H41	22:B:606:CLA:H61	2.90	0.44
32:D:401:PHO:H102	32:D:401:PHO:H13	1.82	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
22:C:508:CLA:H11	22:C:508:CLA:H51	1.82	0.44
3:C:29:GLU:HB2	3:C:30:SER:H	1.65	0.44
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.78	0.44
22:B:602:CLA:H162	22:B:602:CLA:H192	1.76	0.44
22:B:613:CLA:H91	22:B:613:CLA:H112	1.82	0.44
24:C:514:BCR:H20C	24:C:514:BCR:H361	1.84	0.44
22:A:405:CLA:HMA2	23:D:406:PL9:H411	24.67	0.44
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.75	0.44
3:C:343:ARG:NH1	3:C:347:GLY:O	2.50	0.44
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.02	0.44
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.44
1:A:303:ASN:O	3:C:415:ASN:ND2	2.40	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.03	0.44
22:A:403:CLA:H51	22:A:403:CLA:H11	1.82	0.44
22:B:612:CLA:H171	27:D:407:LMG:H401	2.00	0.44
24:B:616:BCR:H341	24:B:616:BCR:H11C	1.90	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.44
22:B:603:CLA:HMD2	22:B:611:CLA:H193	2.00	0.43
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.53	0.43
1:A:111:PRO:O	1:A:115:ILE:HG13	2.20	0.43
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.43
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.83	0.43
13:O:192:SER:OG	13:O:193:GLY:N	2.51	0.43
2:B:170:ASP:OD1	2:B:175:THR:N	2.51	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.19	0.43
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.49	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.02	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.43
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.43
15:U:72:TYR:O	15:U:76:ALA:HB3	2.20	0.43
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.43
7:H:35:MET:HB2	7:H:35:MET:HE3	1.85	0.43
22:B:611:CLA:H18	22:B:612:CLA:H192	22.19	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.77	0.43
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.00	0.43
22:B:605:CLA:HBA2	22:B:605:CLA:H3A	1.25	0.43
30:A:414:SQD:H332	22:B:609:CLA:H203	66.19	0.43
22:D:404:CLA:HBA1	22:D:404:CLA:H3A	1.84	0.43
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.90	0.43
22:C:512:CLA:H3A	22:C:512:CLA:HBA2	1.75	0.43
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:405:CLA:H51	22:A:405:CLA:H11	4.35	0.43
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.17	0.43
16:V:90:PRO:O	16:V:92:ARG:HD3	2.18	0.43
3:C:456:GLU:N	3:C:456:GLU:OE1	2.51	0.43
4:D:261:PHE:HB2	23:D:406:PL9:H522	2.01	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.70	0.43
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.03	0.43
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.01	0.43
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.76	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.02	0.43
22:B:615:CLA:H162	22:B:615:CLA:H122	5.18	0.43
22:C:504:CLA:H11	24:C:514:BCR:H312	2.04	0.43
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.01	0.43
24:J:102:BCR:H11C	24:J:102:BCR:H341	1.80	0.43
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.54	0.43
2:B:86:ILE:H	2:B:86:ILE:HG13	1.75	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.43
22:B:615:CLA:H12	22:B:615:CLA:H72	2.01	0.42
22:C:501:CLA:H162	22:C:501:CLA:H141	1.79	0.42
1:A:38:ILE:HD13	30:A:414:SQD:H121	2.01	0.42
22:A:404:CLA:H143	22:A:404:CLA:H161	1.85	0.42
1:A:176:ILE:HD12	22:A:405:CLA:HED3	23.97	0.42
22:B:613:CLA:H152	22:B:613:CLA:H112	1.85	0.42
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.54	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.23	0.42
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.78	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.78	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
31:B:628:LMT:H1B	31:B:628:LMT:H3'	1.53	0.42
23:D:406:PL9:H421	23:D:406:PL9:H401	1.85	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.03	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.19	0.42
3:C:248:GLY:O	3:C:252:ILE:HG12	2.20	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.06	0.42
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.01	0.42
22:A:402:CLA:H102	22:A:402:CLA:H62	1.88	0.42
22:B:614:CLA:H52	22:B:614:CLA:H12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:622:SQD:H111	30:B:622:SQD:H241	2.02	0.42
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.42
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.62	0.42
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.02	0.42
1:A:61:ASP:HB2	1:A:63:ILE:HG12	2.08	0.42
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.91	0.42
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.55	0.42
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.20	0.42
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.06	0.42
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.02	0.42
22:C:503:CLA:HMD2	22:C:503:CLA:H201	2.02	0.42
7:H:12:ARG:HD3	7:H:12:ARG:O	2.20	0.42
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.01	0.42
1:A:262:TYR:HB3	27:E:101:LMG:H112	2.09	0.42
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.13	0.42
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.83	0.42
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.92	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.42
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.42
22:A:403:CLA:H202	22:A:403:CLA:H162	1.75	0.42
1:A:153:SER:HB2	22:A:404:CLA:H43	19.21	0.42
2:B:6:TYR:OH	27:D:407:LMG:HC5	2.23	0.42
3:C:282:MET:HG2	22:C:501:CLA:H61	2.07	0.42
22:D:404:CLA:H62	22:D:404:CLA:H92	1.81	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.95	0.42
1:A:238:LYS:HD2	14:T:32:LYS:HB3	2.03	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.19	0.42
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.02	0.42
1:A:180:PHE:HA	1:A:183:MET:HE2	2.09	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.01	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.87	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.42
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.02	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.64	0.42
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.86	0.42
22:C:505:CLA:H202	22:C:505:CLA:H161	1.86	0.42
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.57	0.42
22:C:512:CLA:HAB	24:K:102:BCR:H24C	2.02	0.42
4:D:252:PHE:O	4:D:256:ILE:HG22	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.05	0.41
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.41
1:A:127:MET:HG3	1:A:144:CYS:HB2	2.08	0.41
1:A:141:PRO:HB2	1:A:142:TRP:H	1.68	0.41
22:B:604:CLA:H202	22:B:604:CLA:H162	1.86	0.41
22:B:611:CLA:H143	22:B:611:CLA:H161	4.41	0.41
22:D:405:CLA:H41	22:D:405:CLA:H61	1.87	0.41
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.03	0.41
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.88	0.41
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.84	0.41
1:A:140:ARG:HH22	26:A:409:LHG:P	2.43	0.41
22:B:606:CLA:HBC3	24:B:618:BCR:HC8	2.01	0.41
22:B:608:CLA:H141	22:B:608:CLA:H161	4.19	0.41
22:C:520:CLA:H112	22:C:520:CLA:H142	1.76	0.41
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.41
1:A:298:ASN:ND2	3:C:402:GLY:O	2.55	0.41
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.03	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
1:A:27:ARG:NH1	4:D:254:SER:O	2.52	0.41
22:C:511:CLA:H61	22:C:511:CLA:H13	2.02	0.41
16:V:98:LEU:O	16:V:102:MET:HG3	2.21	0.41
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.41
22:A:405:CLA:H202	22:A:405:CLA:H162	3.74	0.41
2:B:108:PHE:HB2	30:B:626:SQD:H223	2.02	0.41
2:B:68:ARG:HH22	22:B:603:CLA:HED1	1.85	0.41
3:C:429:SER:HB3	25:C:516:DGD:HA81	2.02	0.41
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.03	0.41
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.60	0.41
1:A:182:PHE:O	1:A:186:PHE:HB2	2.22	0.41
1:A:121:LEU:HD13	25:A:408:DGD:HB92	2.03	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.93	0.41
22:B:602:CLA:H61	22:B:602:CLA:H41	1.66	0.41
22:B:607:CLA:H202	22:B:607:CLA:H161	4.72	0.41
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.41
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.95	0.41
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.41
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.03	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.49	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.41
1:A:240:GLY:HA3	14:T:29:ILE:HG22	2.02	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:19:SER:O	12:M:23:ILE:HG13	2.22	0.41
1:A:96:ILE:HD12	22:A:405:CLA:HMD1	2.02	0.41
7:H:12:ARG:N	7:H:13:PRO:HD2	2.36	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.29	0.41
22:C:508:CLA:H142	22:C:508:CLA:H112	1.84	0.41
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.35	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.85	0.41
22:B:605:CLA:C3D	31:B:623:LMT:H11	2.51	0.41
2:B:25:MET:HG2	24:B:616:BCR:H23C	2.02	0.41
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.03	0.41
12:M:31:SER:HA	27:M:101:LMG:HC5	2.09	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.43	0.41
6:F:16:PHE:HB3	30:F:103:SQD:H241	2.07	0.41
3:C:386:PRO:O	3:C:390:ARG:HG2	2.26	0.41
1:A:269:ARG:NH1	4:D:231:THR:HB	2.43	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.21	0.41
2:B:19:LEU:O	2:B:23:HIS:ND1	2.53	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.41
3:C:425:TRP:CZ2	22:C:520:CLA:HBA1	2.57	0.41
32:D:402:PHO:CHB	22:D:404:CLA:H101	2.51	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.05	0.41
24:F:102:BCR:H341	24:F:102:BCR:H11C	1.94	0.41
3:C:334:PRO:HA	13:O:179:THR:OG1	2.21	0.41
10:K:24:VAL:O	10:K:27:VAL:HG12	2.21	0.41
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.51	0.40
22:B:606:CLA:H41	22:B:606:CLA:H62	1.90	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.50	0.40
22:B:613:CLA:H12	22:B:613:CLA:H51	4.47	0.40
7:H:46:LEU:HB2	22:H:101:CLA:H61	2.06	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.95	0.40
3:C:257:PHE:HB3	3:C:258:GLY:H	1.63	0.40
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.81	0.40
22:B:602:CLA:HHB	22:H:101:CLA:O1D	2.21	0.40
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.40
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.58	0.40
6:F:21:VAL:O	6:F:25:THR:HG23	2.22	0.40
22:A:403:CLA:HMA1	22:A:403:CLA:H122	2.02	0.40
22:A:405:CLA:H122	22:A:405:CLA:HMA1	15.47	0.40
22:A:403:CLA:HAA1	23:D:406:PL9:H362	2.03	0.40
2:B:468:TRP:HH2	27:D:407:LMG:HO2	1.66	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.98	0.40
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.40	0.40
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
2:B:242:ILE:HG12	22:B:614:CLA:HBB1	23.30	0.40
2:B:91:TRP:CH2	22:B:605:CLA:H12	2.56	0.40
3:C:35:TRP:CZ2	26:C:519:LHG:H261	2.56	0.40
22:B:607:CLA:H172	22:D:405:CLA:H3A	2.03	0.40
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.60	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.22	0.40
4:D:329:MET:HG2	4:D:333:ASP:HB2	2.04	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.40
23:A:406:PL9:H301	4:D:42:TYR:HA	2.03	0.40
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.05	0.40
4:D:294:ARG:H	4:D:294:ARG:HG2	1.64	0.40
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.56	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	333/344 (97%)	312 (94%)	17 (5%)	4 (1%)	16	62
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	16	62
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	24	69
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	30	74
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	21	67
3	c	445/461 (96%)	405 (91%)	35 (8%)	5 (1%)	17	64
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	46	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	46 83
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15 60
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	15 60
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100 100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100 100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3 32
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3 32
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100 100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100 100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 43
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 43
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	16 62
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	16 62
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5 42
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5 42
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9 51
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9 51
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100 100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100 100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4 38
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4 38
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 28
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 28
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11 56
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5138/5618 (92%)	4678 (91%)	404 (8%)	56 (1%)	17 64

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
9	J	38	SER
14	T	30	THR
17	y	43	ARG
18	X	12	ILE
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
9	j	38	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
4	D	239	GLN
7	H	26	GLY
13	O	88	GLU
2	b	489	GLU
4	d	239	GLN
7	h	26	GLY
13	o	88	GLU
1	A	142	TRP
1	A	334	ARG

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Mol	Chain	Res	Type
2	B	489	GLU
3	C	32	GLY
5	E	82	GLN
13	O	271	PRO
1	a	334	ARG
3	c	32	GLY
5	e	82	GLN
13	o	271	PRO
7	H	16	SER
15	U	73	PRO
1	a	142	TRP
3	c	144	SER
7	h	16	SER
15	u	73	PRO
3	C	144	SER
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY
3	c	194	GLY

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	271/280 (97%)	267 (98%)	4 (2%)	72	89
1	a	271/280 (97%)	267 (98%)	4 (2%)	72	89
2	B	390/407 (96%)	381 (98%)	9 (2%)	58	83
2	b	390/407 (96%)	381 (98%)	9 (2%)	58	83
3	C	347/362 (96%)	336 (97%)	11 (3%)	46	77
3	c	347/362 (96%)	336 (97%)	11 (3%)	46	77
4	D	275/283 (97%)	269 (98%)	6 (2%)	60	84
4	d	275/283 (97%)	268 (98%)	7 (2%)	55	82
5	E	72/73 (99%)	70 (97%)	2 (3%)	51	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	e	72/73 (99%)	70 (97%)	2 (3%)	51 79
6	F	29/39 (74%)	29 (100%)	0	100 100
6	f	29/39 (74%)	29 (100%)	0	100 100
7	H	53/55 (96%)	49 (92%)	4 (8%)	17 55
7	h	53/55 (96%)	49 (92%)	4 (8%)	17 55
8	I	32/35 (91%)	31 (97%)	1 (3%)	47 78
8	i	32/35 (91%)	31 (97%)	1 (3%)	47 78
9	J	24/28 (86%)	23 (96%)	1 (4%)	36 71
9	j	24/28 (86%)	23 (96%)	1 (4%)	36 71
10	K	30/37 (81%)	30 (100%)	0	100 100
10	k	30/37 (81%)	30 (100%)	0	100 100
11	L	35/35 (100%)	34 (97%)	1 (3%)	50 79
11	l	35/35 (100%)	34 (97%)	1 (3%)	50 79
12	M	31/33 (94%)	31 (100%)	0	100 100
12	m	31/33 (94%)	31 (100%)	0	100 100
13	O	202/228 (89%)	200 (99%)	2 (1%)	82 92
13	o	202/228 (89%)	200 (99%)	2 (1%)	82 92
14	T	29/29 (100%)	28 (97%)	1 (3%)	44 76
14	t	29/29 (100%)	28 (97%)	1 (3%)	44 76
15	U	84/112 (75%)	83 (99%)	1 (1%)	78 90
15	u	84/112 (75%)	83 (99%)	1 (1%)	78 90
16	V	116/138 (84%)	114 (98%)	2 (2%)	68 88
16	v	116/138 (84%)	114 (98%)	2 (2%)	68 88
17	g	20/37 (54%)	18 (90%)	2 (10%)	9 41
17	y	20/37 (54%)	18 (90%)	2 (10%)	9 41
18	X	30/34 (88%)	28 (93%)	2 (7%)	20 59
18	x	30/34 (88%)	28 (93%)	2 (7%)	20 59
20	Z	52/52 (100%)	50 (96%)	2 (4%)	40 74
20	z	52/52 (100%)	50 (96%)	2 (4%)	40 74
All	All	4244/4594 (92%)	4141 (98%)	103 (2%)	57 83

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	346	LEU
5	E	18	ARG
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU

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Mol	Chain	Res	Type
16	V	92	ARG
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	45	LYS
20	Z	33	TRP
20	Z	62	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	472	LEU
4	d	43	LEU
4	d	180	ARG
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	84	LYS
7	h	27	THR

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Mol	Chain	Res	Type
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	132	LEU
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	45	LYS
20	z	33	TRP
20	z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
4	D	117	HIS
4	d	117	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	$\#\|Z\| > 2$
22	CLA	A	402	-	55,73,73	0.94	3 (5%)	61,113,113	1.18	6 (9%)
22	CLA	A	403	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	6 (9%)
22	CLA	A	404	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	A	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.18	7 (11%)
23	PL9	A	406	-	45,45,55	1.10	3 (6%)	56,57,69	1.60	11 (19%)
24	BCR	A	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	7 (12%)
25	DGD	A	408	-	57,57,67	0.91	0	71,71,81	1.43	8 (11%)
26	LHG	A	409	-	38,38,48	0.68	0	39,44,54	1.19	3 (7%)
27	LMG	A	410	-	51,51,55	0.74	1 (1%)	59,59,63	1.37	6 (10%)
29	OEX	A	412	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	A	413	-	50,51,54	0.95	3 (6%)	58,62,65	1.99	9 (15%)
30	SQD	A	414	-	53,54,54	0.94	3 (5%)	61,65,65	1.66	9 (14%)
27	LMG	A	415	-	42,42,55	0.82	0	50,50,63	1.27	4 (8%)
22	CLA	B	601	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	B	602	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	9 (14%)
22	CLA	B	603	-	55,73,73	0.95	3 (5%)	61,113,113	1.25	8 (13%)
22	CLA	B	604	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	6 (9%)
22	CLA	B	605	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	6 (9%)
22	CLA	B	606	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	B	607	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	B	608	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	B	609	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	6 (9%)
22	CLA	B	610	-	55,73,73	1.03	4 (7%)	61,113,113	1.35	7 (11%)
22	CLA	B	611	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	8 (13%)
22	CLA	B	612	-	55,73,73	0.92	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	B	613	-	55,73,73	0.93	3 (5%)	61,113,113	1.22	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	614	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	7 (11%)
22	CLA	B	615	-	55,73,73	0.95	4 (7%)	61,113,113	1.18	6 (9%)
24	BCR	B	616	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	6 (10%)
24	BCR	B	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	9 (16%)
24	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	10 (17%)
24	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	8 (14%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	7 (9%)
27	LMG	B	621	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	6 (10%)
30	SQD	B	622	-	42,43,54	1.04	3 (7%)	50,54,65	1.92	9 (18%)
31	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	1.01	2 (4%)
31	LMT	B	624	-	36,36,36	1.08	4 (11%)	47,47,47	1.04	3 (6%)
25	DGD	B	625	-	53,53,67	1.06	4 (7%)	67,67,81	1.34	7 (10%)
30	SQD	B	626	-	46,47,54	1.01	3 (6%)	54,58,65	1.97	9 (16%)
31	LMT	B	627	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
31	LMT	B	628	-	36,36,36	1.11	5 (13%)	47,47,47	1.07	1 (2%)
22	CLA	C	501	-	55,73,73	0.95	3 (5%)	61,113,113	1.16	7 (11%)
22	CLA	C	502	-	55,73,73	0.95	4 (7%)	61,113,113	1.23	8 (13%)
22	CLA	C	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.25	7 (11%)
22	CLA	C	504	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	8 (13%)
22	CLA	C	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	C	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	C	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.26	7 (11%)
22	CLA	C	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	C	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	C	510	3	55,73,73	0.94	3 (5%)	61,113,113	1.22	6 (9%)
22	CLA	C	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	C	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	8 (13%)
24	BCR	C	513	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	10 (17%)
24	BCR	C	514	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	8 (14%)
25	DGD	C	515	-	54,54,67	0.95	2 (3%)	68,68,81	1.28	8 (11%)
25	DGD	C	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.46	13 (16%)
25	DGD	C	517	-	67,67,67	0.88	2 (2%)	81,81,81	1.42	11 (13%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
26	LHG	C	519	-	36,36,48	0.69	0	37,42,54	1.27	4 (10%)
22	CLA	C	520	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LMG	C	521	-	48,48,55	0.75	0	56,56,63	1.30	6 (10%)
32	PHO	D	401	-	67,69,69	1.21	9 (13%)	84,99,99	1.01	5 (5%)
32	PHO	D	402	-	67,69,69	1.22	9 (13%)	84,99,99	1.00	4 (4%)
33	BCT	D	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	D	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	D	406	-	55,55,55	1.15	3 (5%)	68,69,69	1.58	15 (22%)
27	LMG	D	407	-	49,49,55	0.75	0	57,57,63	1.32	5 (8%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.38	4 (7%)
25	DGD	D	409	-	64,64,67	0.90	0	78,78,81	1.35	10 (12%)
31	LMT	D	410	-	32,32,36	1.16	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	D	411	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	5 (9%)
27	LMG	E	101	-	44,44,55	0.75	1 (2%)	52,52,63	1.29	5 (9%)
34	HEM	F	101	5,6	30,50,50	2.12	11 (36%)	24,82,82	2.32	9 (37%)
24	BCR	F	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
30	SQD	F	103	-	44,45,54	1.02	3 (6%)	52,56,65	1.77	9 (17%)
22	CLA	H	101	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
24	BCR	H	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	4 (7%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.27	5 (9%)
31	LMT	I	102	-	36,36,36	1.09	5 (13%)	47,47,47	1.08	2 (4%)
23	PL9	J	101	-	35,35,55	1.17	2 (5%)	44,45,69	1.55	6 (13%)
24	BCR	J	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.59	13 (23%)
24	BCR	K	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	9 (16%)
27	LMG	M	101	-	42,42,55	0.85	2 (4%)	50,50,63	1.23	4 (8%)
31	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	2 (4%)
31	LMT	M	103	-	36,36,36	1.11	5 (13%)	47,47,47	1.03	3 (6%)
34	HEM	V	201	16	30,50,50	2.24	11 (36%)	24,82,82	2.23	6 (25%)
30	SQD	a	401	-	53,54,54	0.94	3 (5%)	61,65,65	1.66	9 (14%)
27	LMG	a	402	-	42,42,55	0.82	0	50,50,63	1.26	5 (10%)
22	CLA	a	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	a	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	a	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
32	PHO	a	407	-	67,69,69	1.22	9 (13%)	84,99,99	1.00	4 (4%)
22	CLA	a	408	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	a	409	-	45,45,55	1.18	3 (6%)	56,57,69	1.60	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	a	410	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	7 (12%)
25	DGD	a	411	-	57,57,67	0.91	1 (1%)	71,71,81	1.41	7 (9%)
26	LHG	a	412	-	38,38,48	0.68	1 (2%)	39,44,54	1.20	3 (7%)
29	OEX	a	414	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	a	415	-	50,51,54	0.95	3 (6%)	58,62,65	1.99	9 (15%)
25	DGD	b	601	-	53,53,67	1.04	4 (7%)	67,67,81	1.36	7 (10%)
30	SQD	b	602	-	46,47,54	1.01	4 (8%)	54,58,65	1.98	9 (16%)
31	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	0.98	1 (2%)
31	LMT	b	604	-	36,36,36	1.11	5 (13%)	47,47,47	1.06	1 (2%)
22	CLA	b	605	-	55,73,73	0.95	4 (7%)	61,113,113	1.21	8 (13%)
22	CLA	b	606	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	b	607	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	608	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	b	609	-	55,73,73	0.93	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	b	610	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	b	611	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	b	612	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	8 (13%)
22	CLA	b	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	b	614	-	55,73,73	1.03	4 (7%)	61,113,113	1.34	7 (11%)
22	CLA	b	615	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	8 (13%)
22	CLA	b	616	-	55,73,73	0.94	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	617	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	8 (13%)
22	CLA	b	618	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	9 (14%)
22	CLA	b	619	-	55,73,73	0.95	4 (7%)	61,113,113	1.16	6 (9%)
24	BCR	b	620	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
24	BCR	b	621	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	9 (16%)
24	BCR	b	622	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	11 (19%)
24	BCR	b	623	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
25	DGD	b	624	-	59,59,67	0.89	0	73,73,81	1.36	6 (8%)
27	LMG	b	625	-	49,49,55	0.76	1 (2%)	57,57,63	1.33	6 (10%)
31	LMT	b	626	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
31	LMT	b	627	-	36,36,36	1.07	4 (11%)	47,47,47	1.03	2 (4%)
22	CLA	c	501	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	7 (11%)
22	CLA	c	502	-	55,73,73	0.96	4 (7%)	61,113,113	1.22	8 (13%)
22	CLA	c	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.23	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	504	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	c	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	7 (11%)
22	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	c	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.28	7 (11%)
22	CLA	c	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	6 (9%)
22	CLA	c	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	c	510	3	55,73,73	0.93	3 (5%)	61,113,113	1.21	6 (9%)
22	CLA	c	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	c	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	7 (11%)
24	BCR	c	513	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	11 (19%)
24	BCR	c	514	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	8 (14%)
25	DGD	c	515	-	54,54,67	0.94	1 (1%)	68,68,81	1.29	7 (10%)
25	DGD	c	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.45	13 (16%)
25	DGD	c	517	-	67,67,67	0.87	2 (2%)	81,81,81	1.42	8 (9%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.29	6 (11%)
26	LHG	c	519	-	36,36,48	0.72	0	37,42,54	1.26	4 (10%)
22	CLA	c	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
24	BCR	c	521	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	9 (16%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
32	PHO	d	401	-	67,69,69	1.20	9 (13%)	84,99,99	1.00	3 (3%)
30	SQD	d	402	-	42,43,54	1.03	3 (7%)	50,54,65	1.92	10 (20%)
33	BCT	d	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	404	-	55,73,73	0.96	4 (7%)	61,113,113	1.19	7 (11%)
22	CLA	d	405	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	d	406	-	55,55,55	1.15	3 (5%)	68,69,69	1.59	15 (22%)
27	LMG	d	407	-	49,49,55	0.76	0	57,57,63	1.30	4 (7%)
27	LMG	d	408	-	48,48,55	0.75	0	56,56,63	1.38	4 (7%)
25	DGD	d	409	-	64,64,67	0.91	1 (1%)	78,78,81	1.36	10 (12%)
31	LMT	d	410	-	32,32,36	1.15	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	d	411	-	46,46,55	0.77	0	54,54,63	1.30	5 (9%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.29	5 (9%)
34	HEM	f	101	5,6	30,50,50	2.10	12 (40%)	24,82,82	2.33	9 (37%)
24	BCR	f	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
30	SQD	f	103	-	44,45,54	1.02	3 (6%)	52,56,65	1.78	9 (17%)
24	BCR	g	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.31	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	h	101	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
27	LMG	i	101	-	43,43,55	0.81	0	51,51,63	1.27	5 (9%)
31	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.06	2 (4%)
23	PL9	j	101	-	35,35,55	1.13	1 (2%)	44,45,69	1.55	6 (13%)
24	BCR	j	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.58	13 (23%)
27	LMG	l	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.34	6 (10%)
27	LMG	m	101	-	42,42,55	0.85	2 (4%)	50,50,63	1.25	4 (8%)
34	HEM	v	201	16	30,50,50	2.23	11 (36%)	24,82,82	2.24	6 (25%)
24	BCR	x	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	5 (8%)
24	BCR	y	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.30	7 (12%)

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
22	CLA	A	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	BCR	A	407	-	-	0/29/63/63	0/2/2/2
25	DGD	A	408	-	-	0/45/85/95	0/2/2/2
26	LHG	A	409	-	-	0/43/43/53	0/0/0/0
27	LMG	A	410	-	-	0/46/66/70	0/1/1/1
29	OEX	A	412	1,3	-	0/0/68/68	0/0/6/6
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
30	SQD	A	414	-	-	0/49/69/69	0/1/1/1
27	LMG	A	415	-	-	0/37/57/70	0/1/1/1
22	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	B	616	-	-	0/29/63/63	0/2/2/2
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	DGD	B	620	-	-	0/47/87/95	0/2/2/2
27	LMG	B	621	-	-	0/44/64/70	0/1/1/1
30	SQD	B	622	-	-	1/38/58/69	0/1/1/1
31	LMT	B	623	-	-	0/21/61/61	0/2/2/2
31	LMT	B	624	-	-	0/21/61/61	0/2/2/2
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
30	SQD	B	626	-	-	0/42/62/69	0/1/1/1
31	LMT	B	627	-	-	0/21/61/61	0/2/2/2
31	LMT	B	628	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	C	513	-	-	0/29/63/63	0/2/2/2
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	DGD	C	515	-	-	0/42/82/95	0/2/2/2
25	DGD	C	516	-	-	1/51/91/95	0/2/2/2
25	DGD	C	517	-	-	0/55/95/95	0/2/2/2
27	LMG	C	518	-	-	0/40/60/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	C	519	-	-	0/41/41/53	0/0/0/0
22	CLA	C	520	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LMG	C	521	-	-	0/43/63/70	0/1/1/1
32	PHO	D	401	-	-	0/53/103/103	0/1/6/6
32	PHO	D	402	-	-	0/53/103/103	0/1/6/6
33	BCT	D	403	21	-	0/0/0/0	0/0/0/0
22	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	D	406	-	-	0/53/73/73	0/1/1/1
27	LMG	D	407	-	-	0/44/64/70	0/1/1/1
27	LMG	D	408	-	-	0/43/63/70	0/1/1/1
25	DGD	D	409	-	-	0/52/92/95	0/2/2/2
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
27	LMG	D	411	-	-	0/41/61/70	0/1/1/1
27	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
24	BCR	F	102	-	-	0/29/63/63	0/2/2/2
30	SQD	F	103	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	H	102	-	-	0/29/63/63	0/2/2/2
27	LMG	I	101	-	-	0/38/58/70	0/1/1/1
31	LMT	I	102	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
24	BCR	J	102	-	-	0/29/63/63	0/2/2/2
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	-	1/37/57/70	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/10/54/54	0/0/8/8
30	SQD	a	401	-	-	0/49/69/69	0/1/1/1
27	LMG	a	402	-	-	0/37/57/70	0/1/1/1
22	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
32	PHO	a	407	-	-	0/53/103/103	0/1/6/6
22	CLA	a	408	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	a	409	-	-	0/41/61/73	0/1/1/1
24	BCR	a	410	-	-	0/29/63/63	0/2/2/2
25	DGD	a	411	-	-	0/45/85/95	0/2/2/2
26	LHG	a	412	-	-	0/43/43/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
30	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2
30	SQD	b	602	-	-	0/42/62/69	0/1/1/1
31	LMT	b	603	-	-	0/21/61/61	0/2/2/2
31	LMT	b	604	-	-	0/21/61/61	0/2/2/2
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	DGD	b	624	-	-	0/47/87/95	0/2/2/2
27	LMG	b	625	-	-	0/44/64/70	0/1/1/1
31	LMT	b	626	-	-	0/21/61/61	0/2/2/2
31	LMT	b	627	-	-	0/21/61/61	0/2/2/2
22	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	513	-	-	0/29/63/63	0/2/2/2
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	DGD	c	515	-	-	0/42/82/95	0/2/2/2
25	DGD	c	516	-	-	1/51/91/95	0/2/2/2
25	DGD	c	517	-	-	0/55/95/95	0/2/2/2
27	LMG	c	518	-	-	0/40/60/70	0/1/1/1
26	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	LMG	c	522	-	-	0/43/63/70	0/1/1/1
32	PHO	d	401	-	-	0/53/103/103	0/1/6/6
30	SQD	d	402	-	-	1/38/58/69	0/1/1/1
33	BCT	d	403	21	-	0/0/0/0	0/0/0/0
22	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	405	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PL9	d	406	-	-	0/53/73/73	0/1/1/1
27	LMG	d	407	-	-	0/44/64/70	0/1/1/1
27	LMG	d	408	-	-	0/43/63/70	0/1/1/1
25	DGD	d	409	-	-	0/52/92/95	0/2/2/2
31	LMT	d	410	-	-	0/17/57/61	0/2/2/2
27	LMG	d	411	-	-	0/41/61/70	0/1/1/1
27	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
24	BCR	f	102	-	-	0/29/63/63	0/2/2/2
30	SQD	f	103	-	-	0/40/60/69	0/1/1/1
24	BCR	g	101	-	-	0/29/63/63	0/2/2/2
22	CLA	h	101	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LMG	i	101	-	-	0/38/58/70	0/1/1/1
31	LMT	i	102	-	-	0/21/61/61	0/2/2/2
23	PL9	j	101	-	-	0/29/49/73	0/1/1/1
24	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	LMG	l	101	-	-	0/46/66/70	0/1/1/1
27	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/10/54/54	0/0/8/8
24	BCR	x	101	-	-	0/29/63/63	0/2/2/2
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

All (496) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-7.31	1.45	1.51
34	v	201	HEM	C3B-C4B	-7.09	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.15	1.46	1.51
34	f	101	HEM	C3B-C4B	-6.09	1.46	1.51
34	F	101	HEM	C3D-C4D	-5.29	1.44	1.51
34	f	101	HEM	C3D-C4D	-5.22	1.44	1.51
23	d	406	PL9	C7-C3	-5.01	1.47	1.51
34	v	201	HEM	C3D-C4D	-4.95	1.45	1.51
34	V	201	HEM	C3D-C4D	-4.92	1.45	1.51
23	a	409	PL9	C7-C3	-4.85	1.47	1.51
23	D	406	PL9	C7-C3	-4.72	1.47	1.51
23	J	101	PL9	C7-C3	-4.50	1.48	1.51
23	A	406	PL9	C7-C3	-4.39	1.48	1.51
23	j	101	PL9	C7-C3	-4.35	1.48	1.51
34	V	201	HEM	C2C-C1C	-3.91	1.45	1.52
34	v	201	HEM	C2C-C1C	-3.84	1.45	1.52
22	b	614	CLA	CMB-C2B	-3.76	1.44	1.51
22	B	610	CLA	CMB-C2B	-3.68	1.44	1.51
24	g	101	BCR	C1-C6	-3.65	1.48	1.53
24	y	101	BCR	C1-C6	-3.60	1.48	1.53
34	F	101	HEM	C2C-C1C	-3.57	1.45	1.52
24	H	102	BCR	C1-C6	-3.53	1.48	1.53
34	f	101	HEM	C2C-C1C	-3.52	1.45	1.52
24	x	101	BCR	C1-C6	-3.52	1.48	1.53
24	F	102	BCR	C1-C6	-3.49	1.48	1.53
24	f	102	BCR	C1-C6	-3.47	1.48	1.53
24	C	514	BCR	C1-C6	-3.26	1.49	1.53
24	c	514	BCR	C1-C6	-3.25	1.49	1.53
24	b	620	BCR	C1-C6	-3.24	1.49	1.53
24	B	616	BCR	C1-C6	-3.24	1.49	1.53
24	g	101	BCR	C30-C25	-3.16	1.49	1.53
24	y	101	BCR	C30-C25	-3.15	1.49	1.53
24	J	102	BCR	C30-C25	-3.14	1.49	1.53
24	j	102	BCR	C30-C25	-3.14	1.49	1.53
24	b	622	BCR	C30-C25	-3.12	1.49	1.53
24	b	621	BCR	C1-C6	-3.11	1.49	1.53
24	C	513	BCR	C1-C6	-3.10	1.49	1.53
24	B	617	BCR	C1-C6	-3.10	1.49	1.53
24	F	102	BCR	C30-C25	-3.09	1.49	1.53
24	c	513	BCR	C1-C6	-3.08	1.49	1.53
24	B	618	BCR	C30-C25	-3.08	1.49	1.53
24	K	102	BCR	C30-C25	-3.07	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	623	BCR	C30-C25	-3.05	1.49	1.53
24	B	619	BCR	C30-C25	-3.05	1.49	1.53
24	f	102	BCR	C30-C25	-3.04	1.49	1.53
24	c	521	BCR	C30-C25	-3.02	1.49	1.53
24	a	410	BCR	C30-C25	-3.01	1.49	1.53
24	B	618	BCR	C1-C6	-3.00	1.49	1.53
24	A	407	BCR	C30-C25	-3.00	1.49	1.53
24	B	619	BCR	C1-C6	-3.00	1.49	1.53
24	b	623	BCR	C1-C6	-3.00	1.49	1.53
24	b	620	BCR	C30-C25	-3.00	1.49	1.53
24	b	622	BCR	C1-C6	-2.99	1.49	1.53
24	a	410	BCR	C1-C6	-2.98	1.49	1.53
24	B	616	BCR	C30-C25	-2.96	1.49	1.53
24	A	407	BCR	C1-C6	-2.94	1.49	1.53
24	K	102	BCR	C1-C6	-2.92	1.49	1.53
24	H	102	BCR	C30-C25	-2.91	1.49	1.53
24	C	513	BCR	C30-C25	-2.90	1.49	1.53
24	C	514	BCR	C30-C25	-2.90	1.49	1.53
24	x	101	BCR	C30-C25	-2.88	1.49	1.53
24	c	521	BCR	C1-C6	-2.86	1.49	1.53
24	c	514	BCR	C30-C25	-2.85	1.49	1.53
24	c	513	BCR	C30-C25	-2.74	1.49	1.53
24	J	102	BCR	C1-C6	-2.70	1.50	1.53
24	j	102	BCR	C1-C6	-2.69	1.50	1.53
24	b	621	BCR	C30-C25	-2.69	1.50	1.53
24	B	617	BCR	C30-C25	-2.68	1.50	1.53
22	C	507	CLA	CMB-C2B	-2.66	1.46	1.51
22	c	507	CLA	CMB-C2B	-2.63	1.46	1.51
22	B	611	CLA	CMD-C2D	-2.61	1.45	1.51
23	D	406	PL9	C3-C4	-2.60	1.45	1.49
23	a	409	PL9	C3-C4	-2.57	1.45	1.49
31	d	410	LMT	O3'-C3'	-2.57	1.36	1.43
31	b	627	LMT	O3'-C3'	-2.56	1.36	1.43
22	a	404	CLA	CMB-C2B	-2.56	1.46	1.51
31	D	410	LMT	O3'-C3'	-2.56	1.36	1.43
22	b	615	CLA	CMD-C2D	-2.55	1.46	1.51
31	M	102	LMT	O3'-C3'	-2.55	1.36	1.43
31	B	624	LMT	O3'-C3'	-2.55	1.36	1.43
22	C	509	CLA	CMB-C2B	-2.54	1.46	1.51
31	M	103	LMT	O3'-C3'	-2.53	1.36	1.43
22	c	509	CLA	CMB-C2B	-2.53	1.46	1.51
22	A	403	CLA	CMB-C2B	-2.53	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	603	LMT	O3'-C3'	-2.53	1.36	1.43
22	B	603	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.52	1.46	1.51
31	b	626	LMT	O3'-C3'	-2.52	1.36	1.43
31	i	102	LMT	O3'-C3'	-2.51	1.36	1.43
31	I	102	LMT	O3'-C3'	-2.51	1.36	1.43
22	B	601	CLA	CMB-C2B	-2.51	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.51	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.51	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.51	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.51	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.50	1.46	1.51
22	A	404	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.49	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.49	1.46	1.51
31	B	627	LMT	O3'-C3'	-2.49	1.37	1.43
22	c	505	CLA	CMB-C2B	-2.49	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.49	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.49	1.46	1.51
22	d	404	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.49	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.48	1.46	1.51
22	a	408	CLA	CMB-C2B	-2.48	1.46	1.51
31	B	623	LMT	O3'-C3'	-2.48	1.37	1.43
22	H	101	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.48	1.46	1.51
22	D	404	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	504	CLA	CMD-C2D	-2.47	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.47	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.47	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.47	1.46	1.51
31	b	604	LMT	O3'-C3'	-2.47	1.37	1.43
22	b	608	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.45	1.46	1.51
22	h	101	CLA	CMB-C2B	-2.45	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.45	1.46	1.51
23	d	406	PL9	C3-C4	-2.45	1.45	1.49
22	c	512	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.44	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.44	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	504	CLA	CMD-C2D	-2.44	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	509	CLA	CMD-C2D	-2.44	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.43	1.46	1.51
31	B	628	LMT	O3'-C3'	-2.42	1.37	1.43
22	b	612	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	611	CLA	CMD-C2D	-2.41	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.39	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.39	1.46	1.51
25	C	515	DGD	O2G-C2G	-2.38	1.40	1.46
22	B	603	CLA	CMD-C2D	-2.38	1.46	1.51
22	B	613	CLA	CMB-C2B	-2.38	1.46	1.51
22	A	402	CLA	CMD-C2D	-2.37	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.36	1.46	1.51
22	a	406	CLA	CMD-C2D	-2.36	1.46	1.51
22	b	614	CLA	C3B-C2B	-2.36	1.37	1.40
23	A	406	PL9	C3-C4	-2.35	1.45	1.49
22	a	404	CLA	CMD-C2D	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	CMD-C2D	-2.34	1.46	1.51
22	A	404	CLA	CMD-C2D	-2.33	1.46	1.51
31	I	102	LMT	O2B-C2B	-2.33	1.37	1.43
23	a	409	PL9	C53-C6	-2.33	1.46	1.50
22	B	615	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	619	CLA	CMD-C2D	-2.32	1.46	1.51
22	C	502	CLA	CMD-C2D	-2.31	1.46	1.51
31	I	102	LMT	O2'-C2'	-2.31	1.37	1.43
22	B	610	CLA	C3B-C2B	-2.31	1.37	1.40
22	C	508	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	602	CLA	CMD-C2D	-2.31	1.46	1.51
22	A	403	CLA	CMD-C2D	-2.30	1.46	1.51
22	a	405	CLA	CMD-C2D	-2.30	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.30	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.30	1.46	1.51
22	D	404	CLA	CMD-C2D	-2.29	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.29	1.46	1.51
31	i	102	LMT	O2B-C2B	-2.29	1.37	1.43
22	B	604	CLA	CMD-C2D	-2.29	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.29	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.28	1.46	1.51
22	h	101	CLA	CMD-C2D	-2.28	1.46	1.51
22	B	614	CLA	CMD-C2D	-2.28	1.46	1.51
22	b	616	CLA	CMD-C2D	-2.28	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.28	1.46	1.51
22	B	601	CLA	CMD-C2D	-2.28	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.28	1.46	1.51
32	D	401	PHO	C1C-NC	-2.27	1.33	1.38
22	H	101	CLA	CMD-C2D	-2.27	1.46	1.51
22	c	511	CLA	CMD-C2D	-2.27	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.27	1.46	1.51
22	C	520	CLA	CMD-C2D	-2.27	1.46	1.51
22	B	605	CLA	CMD-C2D	-2.27	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.27	1.46	1.51
22	B	609	CLA	CMD-C2D	-2.27	1.46	1.51
22	c	503	CLA	CMD-C2D	-2.27	1.46	1.51
31	i	102	LMT	O2'-C2'	-2.26	1.37	1.43
22	C	507	CLA	CMD-C2D	-2.26	1.46	1.51
22	d	404	CLA	CMD-C2D	-2.26	1.46	1.51
22	c	520	CLA	CMD-C2D	-2.26	1.46	1.51
22	a	408	CLA	CMD-C2D	-2.26	1.46	1.51
22	c	507	CLA	CMD-C2D	-2.26	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	103	LMT	O3B-C3B	-2.25	1.37	1.43
32	a	407	PHO	C1C-NC	-2.25	1.33	1.38
32	d	401	PHO	C1C-NC	-2.25	1.33	1.38
22	b	608	CLA	CMD-C2D	-2.25	1.46	1.51
22	b	606	CLA	CMD-C2D	-2.25	1.46	1.51
22	C	511	CLA	CMD-C2D	-2.25	1.46	1.51
22	b	618	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	612	CLA	CMD-C2D	-2.25	1.46	1.51
31	b	604	LMT	O3B-C3B	-2.25	1.37	1.43
22	C	503	CLA	CMD-C2D	-2.24	1.46	1.51
22	C	506	CLA	CMD-C2D	-2.24	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.24	1.46	1.51
22	c	510	CLA	CMD-C2D	-2.24	1.46	1.51
31	b	626	LMT	O2'-C2'	-2.24	1.37	1.43
22	d	405	CLA	CMD-C2D	-2.24	1.46	1.51
31	I	102	LMT	O3B-C3B	-2.24	1.37	1.43
22	c	505	CLA	CMD-C2D	-2.24	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.24	1.46	1.51
31	b	627	LMT	O3B-C3B	-2.24	1.37	1.43
22	c	512	CLA	CMD-C2D	-2.24	1.46	1.51
31	B	628	LMT	O3B-C3B	-2.23	1.37	1.43
22	D	405	CLA	CMD-C2D	-2.23	1.46	1.51
32	D	402	PHO	C1C-NC	-2.23	1.33	1.38
31	b	603	LMT	O3B-C3B	-2.23	1.37	1.43
22	c	506	CLA	CMD-C2D	-2.23	1.46	1.51
31	B	627	LMT	O2B-C2B	-2.23	1.37	1.43
25	c	515	DGD	O2G-C2G	-2.23	1.40	1.46
22	b	613	CLA	CMD-C2D	-2.23	1.46	1.51
31	B	623	LMT	O2'-C2'	-2.23	1.37	1.43
31	M	103	LMT	O2'-C2'	-2.22	1.37	1.43
31	D	410	LMT	O3B-C3B	-2.22	1.37	1.43
22	c	501	CLA	CMD-C2D	-2.22	1.46	1.51
31	M	102	LMT	O3B-C3B	-2.22	1.37	1.43
31	B	628	LMT	O2'-C2'	-2.22	1.37	1.43
31	B	624	LMT	O3B-C3B	-2.21	1.37	1.43
31	b	603	LMT	O2'-C2'	-2.21	1.37	1.43
22	C	510	CLA	CMD-C2D	-2.21	1.46	1.51
22	C	512	CLA	CMD-C2D	-2.21	1.46	1.51
31	M	102	LMT	O2'-C2'	-2.21	1.37	1.43
31	b	603	LMT	O2B-C2B	-2.21	1.37	1.43
31	i	102	LMT	O3B-C3B	-2.21	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	627	LMT	O2'-C2'	-2.20	1.37	1.43
31	B	628	LMT	O2B-C2B	-2.20	1.37	1.43
31	d	410	LMT	O3B-C3B	-2.20	1.37	1.43
22	B	610	CLA	CMD-C2D	-2.20	1.46	1.51
31	B	623	LMT	O3B-C3B	-2.19	1.37	1.43
22	C	501	CLA	CMD-C2D	-2.19	1.46	1.51
31	B	627	LMT	O3B-C3B	-2.19	1.37	1.43
31	M	103	LMT	O2B-C2B	-2.19	1.37	1.43
31	B	624	LMT	O2'-C2'	-2.19	1.37	1.43
31	b	626	LMT	O3B-C3B	-2.18	1.37	1.43
22	b	614	CLA	CMD-C2D	-2.18	1.46	1.51
31	D	410	LMT	O2B-C2B	-2.17	1.37	1.43
31	M	102	LMT	O2B-C2B	-2.17	1.37	1.43
31	b	604	LMT	O2'-C2'	-2.17	1.37	1.43
31	D	410	LMT	O2'-C2'	-2.17	1.37	1.43
23	A	406	PL9	C53-C6	-2.17	1.46	1.50
34	F	101	HEM	C2B-C1B	-2.17	1.44	1.51
31	b	626	LMT	O2B-C2B	-2.16	1.37	1.43
31	d	410	LMT	O2B-C2B	-2.15	1.37	1.43
30	B	626	SQD	O2-C2	-2.15	1.37	1.43
30	b	602	SQD	O2-C2	-2.15	1.37	1.43
34	f	101	HEM	C2B-C1B	-2.15	1.44	1.51
31	b	627	LMT	O2'-C2'	-2.15	1.37	1.43
31	b	604	LMT	O2B-C2B	-2.15	1.37	1.43
26	a	412	LHG	O7-C5	-2.13	1.41	1.46
25	C	515	DGD	O1G-C1G	-2.13	1.40	1.45
31	B	623	LMT	O2B-C2B	-2.13	1.37	1.43
27	D	411	LMG	O7-C8	-2.12	1.41	1.46
31	d	410	LMT	O2'-C2'	-2.12	1.37	1.43
25	c	516	DGD	O2G-C2G	-2.10	1.41	1.46
24	g	101	BCR	C33-C5	-2.10	1.47	1.51
22	b	619	CLA	CMC-C2C	-2.09	1.46	1.50
34	V	201	HEM	C2D-C1D	-2.08	1.45	1.51
30	a	401	SQD	O3-C3	-2.07	1.38	1.43
32	D	402	PHO	CMC-C2C	-2.07	1.46	1.50
24	y	101	BCR	C33-C5	-2.07	1.47	1.51
30	A	414	SQD	O3-C3	-2.07	1.38	1.43
32	d	401	PHO	CMC-C2C	-2.07	1.46	1.50
25	a	411	DGD	O1G-C1G	-2.06	1.40	1.45
32	a	407	PHO	CMC-C2C	-2.06	1.46	1.50
22	C	502	CLA	CMC-C2C	-2.06	1.46	1.50
31	B	627	LMT	O4'-C4B	-2.06	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	516	DGD	O2G-C2G	-2.05	1.41	1.46
31	B	624	LMT	O2B-C2B	-2.05	1.38	1.43
30	B	622	SQD	O2-C2	-2.05	1.38	1.43
31	B	628	LMT	O4'-C4B	-2.04	1.38	1.43
31	M	102	LMT	O4'-C4B	-2.04	1.38	1.43
31	M	103	LMT	O4'-C4B	-2.04	1.38	1.43
22	B	615	CLA	CMC-C2C	-2.04	1.46	1.50
31	I	102	LMT	O4'-C4B	-2.03	1.38	1.43
31	b	627	LMT	O2B-C2B	-2.03	1.38	1.43
34	f	101	HEM	C2D-C1D	-2.03	1.45	1.51
30	a	415	SQD	O2-C2	-2.03	1.38	1.43
31	d	410	LMT	O4'-C4B	-2.03	1.38	1.43
32	D	401	PHO	CMC-C2C	-2.03	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.03	1.46	1.50
31	D	410	LMT	O4'-C4B	-2.03	1.38	1.43
30	A	413	SQD	O2-C2	-2.03	1.38	1.43
31	b	604	LMT	O4'-C4B	-2.02	1.38	1.43
30	f	103	SQD	O3-C3	-2.02	1.38	1.43
32	d	401	PHO	CMD-C2D	-2.02	1.46	1.50
31	b	603	LMT	O4'-C4B	-2.02	1.38	1.43
23	D	406	PL9	C53-C6	-2.02	1.46	1.50
24	C	514	BCR	C38-C26	-2.02	1.47	1.51
34	F	101	HEM	C2D-C1D	-2.02	1.45	1.51
22	B	614	CLA	CMC-C2C	-2.02	1.46	1.50
22	b	605	CLA	CMC-C2C	-2.02	1.46	1.50
30	d	402	SQD	O2-C2	-2.01	1.38	1.43
32	D	402	PHO	CMD-C2D	-2.01	1.46	1.50
23	J	101	PL9	C53-C6	-2.01	1.46	1.50
24	c	514	BCR	C38-C26	-2.01	1.47	1.51
34	v	201	HEM	C2D-C1D	-2.01	1.45	1.51
23	d	406	PL9	C53-C6	-2.01	1.46	1.50
30	F	103	SQD	O3-C3	-2.00	1.38	1.43
32	D	401	PHO	CMD-C2D	-2.00	1.46	1.50
32	a	407	PHO	CMD-C2D	-2.00	1.46	1.50
22	c	502	CLA	CMC-C2C	-2.00	1.46	1.50
22	d	404	CLA	CMC-C2C	-2.00	1.46	1.50
31	b	626	LMT	O4'-C4B	-2.00	1.38	1.43
30	b	602	SQD	O3-C3	-2.00	1.38	1.43
25	B	620	DGD	O2G-C2G	-2.00	1.41	1.46
27	E	101	LMG	C7-C8	2.01	1.56	1.50
34	f	101	HEM	C3B-CAB	2.02	1.55	1.51
27	m	101	LMG	C7-C8	2.02	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	C4C-NC	2.02	1.38	1.36
34	F	101	HEM	C3B-CAB	2.03	1.55	1.51
34	V	201	HEM	FE-NB	2.03	2.08	1.97
34	V	201	HEM	C1C-NC	2.07	1.38	1.36
34	F	101	HEM	C1C-NC	2.07	1.38	1.36
34	f	101	HEM	C1C-NC	2.07	1.38	1.36
32	d	401	PHO	CHD-C1D	2.07	1.42	1.38
25	c	517	DGD	C3G-C2G	2.07	1.56	1.50
27	m	101	LMG	C4-C5	2.07	1.57	1.53
27	M	101	LMG	C7-C8	2.07	1.56	1.50
25	b	601	DGD	C1G-C2G	2.08	1.56	1.50
34	F	101	HEM	FE-NB	2.08	2.08	1.97
34	f	101	HEM	FE-NB	2.08	2.08	1.97
25	c	517	DGD	C1G-C2G	2.09	1.56	1.50
25	B	625	DGD	C1G-C2G	2.11	1.56	1.50
25	d	409	DGD	C1D-C2D	2.11	1.58	1.52
27	A	410	LMG	C7-C8	2.11	1.56	1.50
34	v	201	HEM	C1C-NC	2.12	1.38	1.36
25	b	601	DGD	C4D-C5D	2.13	1.57	1.53
32	d	401	PHO	C4C-C3C	2.15	1.49	1.45
27	M	101	LMG	C4-C5	2.16	1.57	1.53
25	C	517	DGD	C3G-C2G	2.17	1.56	1.50
22	b	614	CLA	CHC-C1C	2.17	1.42	1.35
27	B	621	LMG	C4-C5	2.17	1.57	1.53
27	b	625	LMG	C4-C5	2.18	1.57	1.53
22	B	610	CLA	CHC-C1C	2.19	1.42	1.35
34	v	201	HEM	FE-NB	2.19	2.09	1.97
34	V	201	HEM	C3C-CAC	2.20	1.55	1.51
25	b	601	DGD	C3G-C2G	2.22	1.57	1.50
34	v	201	HEM	C3C-CAC	2.22	1.55	1.51
32	D	402	PHO	C4C-C3C	2.23	1.49	1.45
32	D	401	PHO	CHD-C1D	2.23	1.43	1.38
27	l	101	LMG	C7-C8	2.25	1.57	1.50
25	C	517	DGD	C1G-C2G	2.25	1.57	1.50
34	V	201	HEM	C4C-NC	2.25	1.38	1.36
32	D	401	PHO	C4C-C3C	2.26	1.49	1.45
32	a	407	PHO	C4C-C3C	2.26	1.49	1.45
32	D	402	PHO	C1A-NA	2.26	1.42	1.37
34	F	101	HEM	C3C-CAC	2.26	1.55	1.51
32	a	407	PHO	C1A-NA	2.27	1.42	1.37
32	D	401	PHO	C1A-NA	2.27	1.42	1.37
32	d	401	PHO	C1A-NA	2.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3B-CAB	2.30	1.55	1.51
34	V	201	HEM	C3B-CAB	2.32	1.55	1.51
32	D	402	PHO	CHD-C1D	2.32	1.43	1.38
34	v	201	HEM	C4C-NC	2.33	1.38	1.36
34	f	101	HEM	C3C-CAC	2.33	1.55	1.51
32	a	407	PHO	CHD-C1D	2.34	1.43	1.38
22	a	405	CLA	CHC-C1C	2.37	1.42	1.35
22	B	615	CLA	CHC-C1C	2.37	1.42	1.35
25	B	625	DGD	C3G-C2G	2.38	1.57	1.50
25	B	625	DGD	C4D-C5D	2.38	1.58	1.53
22	B	611	CLA	CHC-C1C	2.39	1.42	1.35
22	b	619	CLA	CHC-C1C	2.40	1.42	1.35
22	C	507	CLA	CHC-C1C	2.40	1.42	1.35
22	C	501	CLA	CHC-C1C	2.41	1.42	1.35
22	b	610	CLA	CHC-C1C	2.41	1.42	1.35
22	A	405	CLA	CHC-C1C	2.41	1.42	1.35
22	b	615	CLA	CHC-C1C	2.42	1.42	1.35
22	A	402	CLA	CHC-C1C	2.42	1.42	1.35
22	B	605	CLA	CHC-C1C	2.42	1.42	1.35
22	D	405	CLA	CHC-C1C	2.42	1.42	1.35
22	c	501	CLA	CHC-C1C	2.42	1.42	1.35
22	c	520	CLA	CHC-C1C	2.42	1.42	1.35
22	B	601	CLA	CHC-C1C	2.42	1.42	1.35
34	f	101	HEM	FE-NC	2.42	2.05	1.95
22	c	506	CLA	CHC-C1C	2.43	1.42	1.35
22	b	609	CLA	CHC-C1C	2.43	1.42	1.35
22	C	506	CLA	CHC-C1C	2.44	1.42	1.35
22	B	604	CLA	CHC-C1C	2.44	1.42	1.35
22	C	502	CLA	CHC-C1C	2.44	1.42	1.35
22	b	613	CLA	CHC-C1C	2.44	1.42	1.35
22	B	612	CLA	CHC-C1C	2.44	1.42	1.35
22	b	605	CLA	CHC-C1C	2.44	1.42	1.35
22	b	608	CLA	CHC-C1C	2.44	1.42	1.35
22	A	403	CLA	CHC-C1C	2.44	1.42	1.35
22	C	510	CLA	CHC-C1C	2.44	1.42	1.35
22	B	606	CLA	CHC-C1C	2.45	1.43	1.35
22	C	503	CLA	CHC-C1C	2.45	1.43	1.35
22	C	504	CLA	CHC-C1C	2.45	1.43	1.35
22	c	510	CLA	CHC-C1C	2.45	1.43	1.35
22	c	504	CLA	CHC-C1C	2.45	1.43	1.35
22	C	509	CLA	CHC-C1C	2.46	1.43	1.35
22	A	404	CLA	CHC-C1C	2.46	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	CHC-C1C	2.46	1.43	1.35
22	b	607	CLA	CHC-C1C	2.46	1.43	1.35
22	C	508	CLA	CHC-C1C	2.46	1.43	1.35
22	c	503	CLA	CHC-C1C	2.46	1.43	1.35
22	C	520	CLA	CHC-C1C	2.46	1.43	1.35
22	C	505	CLA	CHC-C1C	2.47	1.43	1.35
22	c	508	CLA	CHC-C1C	2.47	1.43	1.35
22	a	406	CLA	CHC-C1C	2.47	1.43	1.35
34	v	201	HEM	FE-ND	2.47	2.10	1.97
22	b	616	CLA	CHC-C1C	2.47	1.43	1.35
22	D	404	CLA	CHC-C1C	2.47	1.43	1.35
34	F	101	HEM	FE-NC	2.47	2.05	1.95
22	d	405	CLA	CHC-C1C	2.47	1.43	1.35
22	a	408	CLA	CHC-C1C	2.47	1.43	1.35
22	c	507	CLA	CHC-C1C	2.48	1.43	1.35
22	B	609	CLA	CHC-C1C	2.48	1.43	1.35
22	B	603	CLA	CHC-C1C	2.48	1.43	1.35
22	B	602	CLA	CHC-C1C	2.48	1.43	1.35
22	b	618	CLA	CHC-C1C	2.48	1.43	1.35
22	C	512	CLA	CHC-C1C	2.48	1.43	1.35
22	d	404	CLA	CHC-C1C	2.48	1.43	1.35
22	c	509	CLA	CHC-C1C	2.49	1.43	1.35
22	B	607	CLA	CHC-C1C	2.49	1.43	1.35
22	c	511	CLA	CHC-C1C	2.49	1.43	1.35
22	c	505	CLA	CHC-C1C	2.49	1.43	1.35
34	V	201	HEM	FE-ND	2.50	2.10	1.97
22	a	404	CLA	CHC-C1C	2.50	1.43	1.35
34	V	201	HEM	FE-NC	2.50	2.05	1.95
22	C	511	CLA	CHC-C1C	2.50	1.43	1.35
32	D	401	PHO	C4C-NC	2.51	1.42	1.37
22	b	606	CLA	CHC-C1C	2.51	1.43	1.35
22	h	101	CLA	CHC-C1C	2.52	1.43	1.35
22	c	512	CLA	CHC-C1C	2.52	1.43	1.35
22	c	502	CLA	CHC-C1C	2.53	1.43	1.35
22	b	617	CLA	CHC-C1C	2.53	1.43	1.35
22	H	101	CLA	CHC-C1C	2.54	1.43	1.35
32	d	401	PHO	C4C-NC	2.54	1.42	1.37
22	b	611	CLA	CHC-C1C	2.55	1.43	1.35
22	B	613	CLA	CHC-C1C	2.56	1.43	1.35
22	B	608	CLA	CHC-C1C	2.57	1.43	1.35
32	D	402	PHO	C4C-NC	2.57	1.42	1.37
22	b	612	CLA	CHC-C1C	2.58	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	101	HEM	FE-ND	2.58	2.11	1.97
32	a	407	PHO	C4C-NC	2.59	1.42	1.37
34	f	101	HEM	FE-ND	2.62	2.11	1.97
30	f	103	SQD	O47-C7	2.66	1.42	1.34
30	b	602	SQD	O47-C7	2.69	1.42	1.34
30	B	626	SQD	O47-C7	2.69	1.42	1.34
30	a	415	SQD	O47-C7	2.70	1.42	1.34
34	v	201	HEM	FE-NC	2.71	2.06	1.95
30	B	622	SQD	O47-C7	2.72	1.42	1.34
30	F	103	SQD	O47-C7	2.72	1.42	1.34
30	a	401	SQD	O47-C7	2.73	1.42	1.34
30	A	413	SQD	O47-C7	2.73	1.42	1.34
25	B	625	DGD	C1E-C2E	2.73	1.60	1.52
30	d	402	SQD	O47-C7	2.76	1.42	1.34
30	A	414	SQD	O47-C7	2.77	1.42	1.34
32	D	401	PHO	CHC-C1C	2.80	1.44	1.38
32	d	401	PHO	CHC-C1C	2.81	1.44	1.38
25	b	601	DGD	C1E-C2E	2.83	1.61	1.52
32	D	401	PHO	C3B-C4B	2.93	1.50	1.43
32	d	401	PHO	C3B-C4B	2.94	1.50	1.43
32	a	407	PHO	CHC-C1C	2.95	1.44	1.38
32	D	402	PHO	CHC-C1C	2.96	1.44	1.38
30	A	413	SQD	O48-C23	2.97	1.42	1.33
30	a	415	SQD	O48-C23	3.00	1.42	1.33
30	F	103	SQD	O48-C23	3.03	1.42	1.33
30	f	103	SQD	O48-C23	3.04	1.42	1.33
30	B	622	SQD	O48-C23	3.05	1.42	1.33
30	d	402	SQD	O48-C23	3.05	1.42	1.33
30	A	414	SQD	O48-C23	3.05	1.42	1.33
32	D	402	PHO	C3B-C4B	3.06	1.50	1.43
30	a	401	SQD	O48-C23	3.06	1.42	1.33
30	b	602	SQD	O48-C23	3.07	1.42	1.33
32	a	407	PHO	C3B-C4B	3.07	1.50	1.43
30	B	626	SQD	O48-C23	3.08	1.42	1.33

All (1177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	j	101	PL9	C7-C3-C2	-6.13	118.34	123.42
23	J	101	PL9	C7-C3-C2	-6.12	118.35	123.42
23	d	406	PL9	C7-C3-C2	-5.83	118.58	123.42
23	A	406	PL9	C7-C3-C2	-5.77	118.63	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	409	PL9	C7-C3-C2	-5.62	118.76	123.42
23	D	406	PL9	C7-C3-C2	-5.62	118.76	123.42
22	b	614	CLA	CMB-C2B-C1B	-4.81	120.40	128.36
25	a	411	DGD	O3G-C3G-C2G	-4.81	99.54	110.99
25	A	408	DGD	O3G-C3G-C2G	-4.77	99.65	110.99
22	B	610	CLA	CMB-C2B-C1B	-4.75	120.51	128.36
25	C	517	DGD	O3G-C3G-C2G	-4.37	100.60	110.99
25	c	517	DGD	O3G-C3G-C2G	-4.21	100.97	110.99
27	d	408	LMG	C1-C2-C3	-4.07	101.95	109.97
27	D	408	LMG	C1-C2-C3	-4.06	101.97	109.97
22	c	507	CLA	CMB-C2B-C1B	-3.86	121.98	128.36
25	c	516	DGD	O5D-C6D-C5D	-3.85	102.11	109.08
22	C	507	CLA	CMB-C2B-C1B	-3.82	122.04	128.36
24	J	102	BCR	C11-C10-C9	-3.80	121.71	127.20
25	C	516	DGD	O5D-C6D-C5D	-3.78	102.22	109.08
22	b	616	CLA	CMB-C2B-C1B	-3.76	122.14	128.36
22	B	612	CLA	CMB-C2B-C1B	-3.75	122.15	128.36
25	c	516	DGD	O3G-C3G-C2G	-3.75	102.08	110.99
25	C	516	DGD	O3G-C3G-C2G	-3.72	102.14	110.99
24	j	102	BCR	C11-C10-C9	-3.66	121.91	127.20
25	d	409	DGD	O6D-C1D-O3G	-3.63	101.31	110.05
24	B	617	BCR	C33-C5-C6	-3.61	121.06	124.61
25	D	409	DGD	O6D-C1D-O3G	-3.59	101.41	110.05
22	b	611	CLA	CMB-C2B-C1B	-3.53	122.52	128.36
30	F	103	SQD	O9-S-O7	-3.52	100.64	113.48
30	f	103	SQD	O9-S-O7	-3.52	100.64	113.48
24	b	621	BCR	C33-C5-C6	-3.52	121.15	124.61
30	d	402	SQD	O9-S-O7	-3.48	100.81	113.48
30	A	413	SQD	O9-S-O7	-3.47	100.85	113.48
24	x	101	BCR	C33-C5-C6	-3.46	121.21	124.61
25	b	624	DGD	O3G-C3G-C2G	-3.45	102.77	110.99
30	a	415	SQD	O9-S-O7	-3.44	100.93	113.48
24	f	102	BCR	C33-C5-C6	-3.44	121.22	124.61
24	F	102	BCR	C33-C5-C6	-3.44	121.23	124.61
25	c	515	DGD	O3G-C3G-C2G	-3.44	102.81	110.99
24	J	102	BCR	C3-C4-C5	-3.44	108.42	113.87
30	B	622	SQD	O9-S-O7	-3.44	100.96	113.48
25	C	515	DGD	O3G-C3G-C2G	-3.43	102.82	110.99
30	a	401	SQD	O9-S-O7	-3.42	101.03	113.48
24	H	102	BCR	C33-C5-C6	-3.40	121.26	124.61
22	c	510	CLA	CMB-C2B-C1B	-3.40	122.73	128.36
24	j	102	BCR	C3-C4-C5	-3.40	108.47	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	CMB-C2B-C1B	-3.40	122.74	128.36
30	B	626	SQD	O9-S-O7	-3.39	101.12	113.48
22	b	615	CLA	CMB-C2B-C1B	-3.39	122.76	128.36
22	B	613	CLA	CMB-C2B-C1B	-3.39	122.76	128.36
30	b	602	SQD	O9-S-O7	-3.38	101.16	113.48
22	b	613	CLA	CMB-C2B-C1B	-3.38	122.77	128.36
22	b	617	CLA	CMB-C2B-C1B	-3.37	122.79	128.36
22	C	503	CLA	CMB-C2B-C1B	-3.37	122.80	128.36
22	C	505	CLA	CMB-C2B-C1B	-3.36	122.81	128.36
25	B	620	DGD	O3G-C3G-C2G	-3.35	103.01	110.99
22	B	602	CLA	CMB-C2B-C1B	-3.35	122.82	128.36
30	A	414	SQD	O9-S-O7	-3.34	101.29	113.48
22	B	611	CLA	CMB-C2B-C1B	-3.34	122.84	128.36
22	c	512	CLA	CMB-C2B-C1B	-3.34	122.84	128.36
22	C	512	CLA	CMB-C2B-C1B	-3.31	122.88	128.36
22	C	506	CLA	CMB-C2B-C1B	-3.31	122.88	128.36
22	B	609	CLA	CMB-C2B-C1B	-3.31	122.89	128.36
22	b	606	CLA	CMB-C2B-C1B	-3.31	122.89	128.36
22	c	503	CLA	CMB-C2B-C1B	-3.31	122.89	128.36
22	C	502	CLA	CMB-C2B-C1B	-3.30	122.90	128.36
22	c	506	CLA	CMB-C2B-C1B	-3.29	122.93	128.36
22	c	505	CLA	CMB-C2B-C1B	-3.28	122.93	128.36
25	D	409	DGD	O3G-C3G-C2G	-3.27	103.20	110.99
22	A	405	CLA	CMB-C2B-C1B	-3.27	122.95	128.36
22	C	510	CLA	CMB-C2B-C1B	-3.27	122.96	128.36
22	B	601	CLA	CMB-C2B-C1B	-3.26	122.96	128.36
22	a	404	CLA	CMB-C2B-C1B	-3.25	122.99	128.36
22	c	502	CLA	CMB-C2B-C1B	-3.24	123.01	128.36
22	c	511	CLA	CMB-C2B-C1B	-3.23	123.02	128.36
25	d	409	DGD	O3G-C3G-C2G	-3.23	103.31	110.99
22	c	509	CLA	CMB-C2B-C1B	-3.23	123.03	128.36
22	C	511	CLA	CMB-C2B-C1B	-3.22	123.03	128.36
22	a	408	CLA	CMB-C2B-C1B	-3.22	123.04	128.36
22	A	402	CLA	CMB-C2B-C1B	-3.21	123.06	128.36
22	a	405	CLA	CMB-C2B-C1B	-3.20	123.07	128.36
24	g	101	BCR	C33-C5-C6	-3.20	121.46	124.61
22	C	509	CLA	CMB-C2B-C1B	-3.20	123.07	128.36
22	B	604	CLA	CMB-C2B-C1B	-3.19	123.08	128.36
24	y	101	BCR	C38-C26-C25	-3.17	121.49	124.61
24	g	101	BCR	C38-C26-C25	-3.17	121.49	124.61
31	B	628	LMT	C1'-O5'-C5'	-3.17	107.59	113.75
25	b	624	DGD	O6D-C1D-O3G	-3.16	102.44	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	608	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
22	B	614	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
22	c	520	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
22	D	404	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
22	b	605	CLA	CMB-C2B-C1B	-3.15	123.15	128.36
22	B	605	CLA	CMB-C2B-C1B	-3.15	123.15	128.36
22	D	405	CLA	CMB-C2B-C1B	-3.15	123.16	128.36
25	B	620	DGD	O6D-C1D-O3G	-3.14	102.49	110.05
24	b	620	BCR	C33-C5-C6	-3.14	121.52	124.61
22	C	520	CLA	CMB-C2B-C1B	-3.14	123.17	128.36
24	B	616	BCR	C33-C5-C6	-3.13	121.53	124.61
22	d	404	CLA	CMB-C2B-C1B	-3.13	123.19	128.36
22	b	618	CLA	CMB-C2B-C1B	-3.13	123.19	128.36
22	d	405	CLA	CMB-C2B-C1B	-3.12	123.20	128.36
22	c	508	CLA	CMB-C2B-C1B	-3.11	123.22	128.36
22	A	404	CLA	CMB-C2B-C1B	-3.11	123.22	128.36
24	J	102	BCR	C24-C23-C22	-3.11	121.48	126.22
23	A	406	PL9	C22-C23-C24	-3.10	121.02	127.76
22	C	508	CLA	CMB-C2B-C1B	-3.09	123.25	128.36
22	c	503	CLA	O2D-CGD-O1D	-3.09	117.42	123.79
25	c	516	DGD	O6D-C1D-O3G	-3.09	102.62	110.05
22	A	403	CLA	CMB-C2B-C1B	-3.08	123.26	128.36
25	C	516	DGD	O6D-C1D-O3G	-3.08	102.64	110.05
24	y	101	BCR	C33-C5-C6	-3.08	121.58	124.61
31	b	604	LMT	C1'-O5'-C5'	-3.07	107.79	113.75
22	B	603	CLA	CMB-C2B-C1B	-3.07	123.29	128.36
23	a	409	PL9	C22-C23-C24	-3.06	121.11	127.76
22	h	101	CLA	CMB-C2B-C1B	-3.06	123.30	128.36
22	H	101	CLA	CMB-C2B-C1B	-3.06	123.30	128.36
22	B	613	CLA	O2D-CGD-O1D	-3.06	117.47	123.79
22	b	610	CLA	CMB-C2B-C1B	-3.06	123.31	128.36
25	c	517	DGD	C1D-C2D-C3D	-3.05	103.95	109.97
22	b	607	CLA	CMB-C2B-C1B	-3.05	123.31	128.36
22	b	609	CLA	CMB-C2B-C1B	-3.05	123.32	128.36
22	a	406	CLA	CMB-C2B-C1B	-3.05	123.32	128.36
24	j	102	BCR	C24-C23-C22	-3.05	121.57	126.22
24	b	622	BCR	C24-C23-C22	-3.04	121.59	126.22
22	B	615	CLA	CMB-C2B-C1B	-3.03	123.35	128.36
22	B	603	CLA	O2D-CGD-O1D	-3.02	117.55	123.79
24	b	623	BCR	C3-C4-C5	-3.02	109.08	113.87
25	b	601	DGD	C1D-C2D-C3D	-3.02	104.03	109.97
24	B	619	BCR	C3-C4-C5	-3.01	109.08	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	605	CLA	O2D-CGD-O1D	-3.01	117.58	123.79
23	D	406	PL9	C22-C23-C24	-3.01	121.22	127.76
22	C	503	CLA	O2D-CGD-O1D	-2.99	117.61	123.79
22	B	606	CLA	CMB-C2B-C1B	-2.99	123.41	128.36
24	B	617	BCR	C15-C16-C17	-2.99	116.79	123.39
25	A	408	DGD	O6D-C1D-O3G	-2.98	102.89	110.05
22	b	617	CLA	O2D-CGD-O1D	-2.97	117.65	123.79
22	b	619	CLA	CMB-C2B-C1B	-2.97	123.46	128.36
25	a	411	DGD	O6D-C1D-O3G	-2.96	102.92	110.05
22	b	606	CLA	O2D-CGD-O1D	-2.96	117.69	123.79
23	d	406	PL9	C22-C23-C24	-2.95	121.36	127.76
24	c	514	BCR	C33-C5-C6	-2.95	121.71	124.61
22	B	608	CLA	CMB-C2B-C1B	-2.94	123.49	128.36
22	b	609	CLA	O2D-CGD-O1D	-2.94	117.71	123.79
24	B	617	BCR	C28-C27-C26	-2.94	109.20	113.87
24	C	514	BCR	C33-C5-C6	-2.94	121.72	124.61
22	c	507	CLA	O2D-CGD-O1D	-2.93	117.74	123.79
22	B	608	CLA	O2D-CGD-O1D	-2.93	117.74	123.79
25	b	601	DGD	C3G-C2G-C1G	-2.92	105.23	112.07
27	D	407	LMG	O6-C1-O1	-2.92	103.03	110.05
25	b	601	DGD	O3G-C3G-C2G	-2.92	104.05	110.99
27	d	407	LMG	O6-C1-O1	-2.91	103.05	110.05
24	b	621	BCR	C28-C27-C26	-2.91	109.25	113.87
22	c	504	CLA	O2D-CGD-O1D	-2.91	117.79	123.79
25	C	515	DGD	O6D-C1D-O3G	-2.91	103.06	110.05
22	C	504	CLA	O2D-CGD-O1D	-2.89	117.82	123.79
25	c	515	DGD	O6D-C1D-O3G	-2.89	103.10	110.05
24	j	102	BCR	C7-C8-C9	-2.89	121.81	126.22
24	j	102	BCR	C38-C26-C25	-2.89	121.77	124.61
25	C	517	DGD	CDB-CCB-CBB	-2.88	99.64	114.53
25	c	517	DGD	CDB-CCB-CBB	-2.88	99.68	114.53
22	c	505	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
22	b	607	CLA	O2D-CGD-O1D	-2.87	117.86	123.79
25	c	517	DGD	O5D-C6D-C5D	-2.87	103.87	109.08
31	B	624	LMT	C3'-C4'-C5'	-2.87	104.34	110.84
22	b	612	CLA	CMB-C2B-C1B	-2.87	123.61	128.36
22	C	502	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
23	J	101	PL9	C22-C23-C24	-2.86	121.53	127.76
25	C	517	DGD	C1D-C2D-C3D	-2.86	104.33	109.97
24	J	102	BCR	C38-C26-C25	-2.86	121.80	124.61
24	J	102	BCR	C7-C8-C9	-2.86	121.86	126.22
22	b	612	CLA	O2D-CGD-O1D	-2.85	117.91	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	O2D-CGD-O1D	-2.85	117.91	123.79
22	B	606	CLA	O2D-CGD-O1D	-2.83	117.94	123.79
22	B	604	CLA	O2D-CGD-O1D	-2.83	117.94	123.79
23	j	101	PL9	C22-C23-C24	-2.83	121.61	127.76
24	c	514	BCR	C28-C27-C26	-2.83	109.38	113.87
24	b	621	BCR	C15-C16-C17	-2.83	117.14	123.39
25	c	516	DGD	CDB-CCB-CBB	-2.82	99.95	114.53
25	C	517	DGD	O5D-C6D-C5D	-2.82	103.97	109.08
22	c	502	CLA	O2D-CGD-O1D	-2.82	117.97	123.79
25	B	625	DGD	C1D-C2D-C3D	-2.81	104.42	109.97
25	B	625	DGD	O3G-C3G-C2G	-2.81	104.30	110.99
22	a	404	CLA	O2D-CGD-O1D	-2.81	117.98	123.79
22	b	610	CLA	O2D-CGD-O1D	-2.81	117.98	123.79
25	C	516	DGD	CDB-CCB-CBB	-2.81	100.04	114.53
22	b	605	CLA	O2D-CGD-O1D	-2.80	118.00	123.79
22	a	406	CLA	O2D-CGD-O1D	-2.80	118.01	123.79
22	b	613	CLA	O2D-CGD-O1D	-2.79	118.03	123.79
22	b	611	CLA	O2D-CGD-O1D	-2.79	118.03	123.79
24	B	618	BCR	C24-C23-C22	-2.78	121.98	126.22
22	b	608	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
22	B	602	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
23	j	101	PL9	C7-C8-C9	-2.78	121.99	126.70
22	c	512	CLA	O2D-CGD-O1D	-2.77	118.06	123.79
22	A	402	CLA	O2D-CGD-O1D	-2.77	118.07	123.79
24	C	514	BCR	C28-C27-C26	-2.76	109.48	113.87
22	B	609	CLA	O2D-CGD-O1D	-2.76	118.09	123.79
22	C	504	CLA	CMB-C2B-C1B	-2.76	123.80	128.36
22	C	506	CLA	O2D-CGD-O1D	-2.76	118.09	123.79
22	C	507	CLA	O2D-CGD-O1D	-2.76	118.09	123.79
22	c	510	CLA	O2D-CGD-O1D	-2.76	118.10	123.79
27	C	518	LMG	O6-C1-O1	-2.75	103.44	110.05
22	c	520	CLA	O2D-CGD-O1D	-2.74	118.12	123.79
24	a	410	BCR	C33-C5-C6	-2.74	121.91	124.61
31	b	627	LMT	C3'-C4'-C5'	-2.74	104.64	110.84
25	D	409	DGD	CDB-CCB-CBB	-2.74	100.38	114.53
24	J	102	BCR	C35-C13-C14	-2.74	118.86	122.90
23	J	101	PL9	C7-C8-C9	-2.74	122.06	126.70
22	A	403	CLA	O2D-CGD-O1D	-2.74	118.14	123.79
22	C	501	CLA	O2D-CGD-O1D	-2.73	118.14	123.79
22	c	504	CLA	CMB-C2B-C1B	-2.73	123.84	128.36
25	d	409	DGD	CDB-CCB-CBB	-2.73	100.43	114.53
22	c	511	CLA	O2D-CGD-O1D	-2.73	118.16	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	DGD	O5D-C6D-C5D	-2.73	104.14	109.08
22	h	101	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
25	B	625	DGD	C3G-C2G-C1G	-2.72	105.70	112.07
22	B	612	CLA	O2D-CGD-O1D	-2.71	118.19	123.79
22	H	101	CLA	O2D-CGD-O1D	-2.71	118.19	123.79
31	M	102	LMT	C1'-O5'-C5'	-2.71	108.48	113.75
22	d	405	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
24	B	618	BCR	C11-C10-C9	-2.71	123.29	127.20
22	B	607	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
22	D	404	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
22	c	506	CLA	O2D-CGD-O1D	-2.70	118.21	123.79
24	j	102	BCR	C35-C13-C14	-2.70	118.91	122.90
23	D	406	PL9	C27-C28-C29	-2.70	121.89	127.76
22	b	616	CLA	O2D-CGD-O1D	-2.70	118.21	123.79
22	C	512	CLA	O2D-CGD-O1D	-2.70	118.21	123.79
22	A	404	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
25	c	517	DGD	C1D-O6D-C5D	-2.70	108.51	113.75
22	C	510	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
23	d	406	PL9	C7-C8-C9	-2.69	122.14	126.70
22	C	520	CLA	O2D-CGD-O1D	-2.69	118.24	123.79
27	i	101	LMG	O6-C1-O1	-2.69	103.59	110.05
27	I	101	LMG	O6-C1-O1	-2.68	103.60	110.05
24	b	621	BCR	C15-C14-C13	-2.68	123.33	127.20
27	c	518	LMG	O6-C1-O1	-2.68	103.61	110.05
22	c	501	CLA	O2D-CGD-O1D	-2.68	118.26	123.79
24	g	101	BCR	C7-C8-C9	-2.68	122.14	126.22
22	B	601	CLA	O2D-CGD-O1D	-2.68	118.27	123.79
22	D	405	CLA	O2D-CGD-O1D	-2.67	118.28	123.79
22	d	404	CLA	O2D-CGD-O1D	-2.67	118.28	123.79
24	K	102	BCR	C33-C5-C6	-2.67	121.98	124.61
24	A	407	BCR	C33-C5-C6	-2.67	121.99	124.61
24	y	101	BCR	C7-C8-C9	-2.66	122.17	126.22
22	B	610	CLA	O2D-CGD-O1D	-2.64	118.33	123.79
24	B	619	BCR	C38-C26-C25	-2.64	122.01	124.61
32	D	402	PHO	O2D-CGD-O1D	-2.64	118.33	123.79
22	a	408	CLA	O2D-CGD-O1D	-2.64	118.34	123.79
24	b	623	BCR	C38-C26-C25	-2.64	122.02	124.61
22	b	618	CLA	O2D-CGD-O1D	-2.64	118.35	123.79
24	c	521	BCR	C33-C5-C6	-2.63	122.02	124.61
24	c	514	BCR	C11-C10-C9	-2.63	123.39	127.20
23	a	409	PL9	C27-C28-C29	-2.62	122.06	127.76
27	E	101	LMG	C1-C2-C3	-2.62	104.81	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	409	DGD	C3G-C2G-C1G	-2.62	105.94	112.07
24	C	514	BCR	C15-C16-C17	-2.62	117.60	123.39
27	b	625	LMG	C1-C2-C3	-2.62	104.81	109.97
31	B	623	LMT	C1'-O5'-C5'	-2.62	108.67	113.75
24	J	102	BCR	C15-C14-C13	-2.61	123.43	127.20
24	j	102	BCR	C15-C14-C13	-2.60	123.44	127.20
27	B	621	LMG	C1-C2-C3	-2.60	104.84	109.97
22	c	501	CLA	CMB-C2B-C1B	-2.60	124.06	128.36
22	B	614	CLA	O2D-CGD-O1D	-2.60	118.42	123.79
24	c	521	BCR	C15-C16-C17	-2.60	117.64	123.39
23	d	406	PL9	C27-C28-C29	-2.60	122.11	127.76
24	B	617	BCR	C15-C14-C13	-2.60	123.44	127.20
22	C	511	CLA	O2D-CGD-O1D	-2.59	118.43	123.79
23	A	406	PL9	C27-C28-C29	-2.59	122.13	127.76
32	d	401	PHO	O2D-CGD-O1D	-2.59	118.45	123.79
22	a	405	CLA	O2D-CGD-O1D	-2.58	118.45	123.79
22	A	405	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
23	D	406	PL9	C7-C8-C9	-2.58	122.33	126.70
25	C	517	DGD	C1D-O6D-C5D	-2.58	108.74	113.75
23	D	406	PL9	C37-C38-C39	-2.58	122.16	127.76
22	C	509	CLA	O2D-CGD-O1D	-2.57	118.48	123.79
24	C	514	BCR	C38-C26-C25	-2.56	122.09	124.61
24	c	513	BCR	C7-C8-C9	-2.56	122.31	126.22
24	C	513	BCR	C24-C23-C22	-2.56	122.32	126.22
23	d	406	PL9	C37-C38-C39	-2.55	122.21	127.76
31	M	103	LMT	C1'-O5'-C5'	-2.55	108.79	113.75
25	c	516	DGD	C3G-C2G-C1G	-2.55	106.11	112.07
22	C	501	CLA	CMB-C2B-C1B	-2.55	124.15	128.36
25	a	411	DGD	O5D-C6D-C5D	-2.54	104.47	109.08
25	D	409	DGD	CFB-CEB-CDB	-2.53	101.44	114.53
22	b	614	CLA	O2D-CGD-O1D	-2.53	118.56	123.79
25	c	515	DGD	C3G-C2G-C1G	-2.53	106.14	112.07
32	D	401	PHO	O2D-CGD-O1D	-2.53	118.56	123.79
22	c	509	CLA	O2D-CGD-O1D	-2.53	118.57	123.79
23	D	406	PL9	C32-C33-C34	-2.52	122.28	127.76
24	c	514	BCR	C38-C26-C25	-2.52	122.14	124.61
25	C	515	DGD	C3G-C2G-C1G	-2.52	106.19	112.07
24	b	622	BCR	C33-C5-C6	-2.51	122.14	124.61
25	C	516	DGD	C3G-C2G-C1G	-2.51	106.19	112.07
25	d	409	DGD	CFB-CEB-CDB	-2.51	101.58	114.53
24	J	102	BCR	C33-C5-C6	-2.51	122.14	124.61
24	A	407	BCR	C38-C26-C25	-2.50	122.15	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	407	PHO	O2D-CGD-O1D	-2.50	118.62	123.79
31	b	626	LMT	C1'-O5'-C5'	-2.50	108.90	113.75
23	d	406	PL9	C32-C33-C34	-2.50	122.33	127.76
24	b	622	BCR	C11-C10-C9	-2.50	123.59	127.20
25	D	409	DGD	C3G-C2G-C1G	-2.49	106.24	112.07
32	a	407	PHO	CBD-CHA-C4D	-2.49	105.67	108.46
23	d	406	PL9	C31-C32-C33	-2.49	105.18	111.69
24	K	102	BCR	C15-C16-C17	-2.49	117.90	123.39
27	A	415	LMG	O6-C1-O1	-2.48	104.07	110.05
24	B	618	BCR	C15-C14-C13	-2.48	123.61	127.20
23	a	409	PL9	C7-C8-C9	-2.48	122.49	126.70
27	a	402	LMG	O6-C1-O1	-2.48	104.08	110.05
27	D	411	LMG	C38-C37-C36	-2.48	101.72	114.53
27	M	101	LMG	C1-C2-C3	-2.48	105.08	109.97
27	d	411	LMG	C38-C37-C36	-2.47	101.77	114.53
27	D	411	LMG	C1-C2-C3	-2.47	105.10	109.97
24	c	513	BCR	C24-C23-C22	-2.47	122.45	126.22
25	A	408	DGD	CBB-CAB-C9B	-2.46	101.83	114.53
27	d	408	LMG	C38-C37-C36	-2.46	101.83	114.53
24	a	410	BCR	C38-C26-C25	-2.46	122.19	124.61
25	C	516	DGD	O6E-C1E-O5D	-2.46	104.14	110.05
24	C	514	BCR	C15-C14-C13	-2.45	123.65	127.20
24	j	102	BCR	C33-C5-C6	-2.45	122.20	124.61
24	b	623	BCR	C7-C8-C9	-2.45	122.48	126.22
24	B	618	BCR	C33-C5-C6	-2.45	122.20	124.61
27	m	101	LMG	C1-C2-C3	-2.45	105.15	109.97
32	d	401	PHO	CBD-CHA-C4D	-2.45	105.72	108.46
27	m	101	LMG	O2-C2-C1	-2.45	104.66	110.02
31	d	410	LMT	C3'-C4'-C5'	-2.44	105.32	110.84
31	M	103	LMT	C3'-C4'-C5'	-2.44	105.32	110.84
24	B	619	BCR	C33-C5-C6	-2.44	122.21	124.61
24	b	623	BCR	C33-C5-C6	-2.44	122.21	124.61
25	a	411	DGD	CBB-CAB-C9B	-2.44	101.94	114.53
22	c	508	CLA	O2D-CGD-O1D	-2.44	118.76	123.79
27	A	410	LMG	C40-C39-C38	-2.43	101.96	114.53
27	l	101	LMG	C40-C39-C38	-2.43	101.96	114.53
22	b	619	CLA	O2D-CGD-O1D	-2.43	118.77	123.79
25	B	620	DGD	CBB-CAB-C9B	-2.43	101.97	114.53
24	C	513	BCR	C3-C4-C5	-2.43	110.01	113.87
25	b	624	DGD	CBB-CAB-C9B	-2.43	101.99	114.53
25	c	516	DGD	O6E-C1E-O5D	-2.43	104.21	110.05
32	D	401	PHO	CBD-CHA-C4D	-2.42	105.75	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	411	DGD	C3G-C2G-C1G	-2.42	106.41	112.07
31	D	410	LMT	C1'-O5'-C5'	-2.42	109.05	113.75
25	A	408	DGD	C3G-C2G-C1G	-2.42	106.41	112.07
24	c	514	BCR	C15-C16-C17	-2.42	118.05	123.39
25	C	517	DGD	CFB-CEB-CDB	-2.42	102.05	114.53
27	D	408	LMG	C38-C37-C36	-2.42	102.06	114.53
24	c	513	BCR	C3-C4-C5	-2.41	110.04	113.87
22	B	615	CLA	O2D-CGD-O1D	-2.41	118.81	123.79
27	D	407	LMG	C38-C37-C36	-2.41	102.07	114.53
27	A	410	LMG	O3-C3-C2	-2.41	104.92	110.34
31	D	410	LMT	C3'-C4'-C5'	-2.41	105.40	110.84
26	C	519	LHG	C11-C10-C9	-2.40	102.13	114.53
27	e	101	LMG	C1-C2-C3	-2.40	105.24	109.97
24	b	622	BCR	C15-C14-C13	-2.40	123.73	127.20
27	A	410	LMG	C1-C2-C3	-2.40	105.25	109.97
27	d	407	LMG	C38-C37-C36	-2.39	102.17	114.53
24	B	618	BCR	C15-C16-C17	-2.39	118.10	123.39
23	D	406	PL9	C31-C32-C33	-2.39	105.43	111.69
31	B	627	LMT	C1'-O5'-C5'	-2.39	109.11	113.75
27	D	408	LMG	O6-C1-C2	-2.39	105.38	110.28
27	c	522	LMG	C40-C39-C38	-2.38	102.22	114.53
27	c	522	LMG	O2-C2-C1	-2.38	104.79	110.02
25	c	517	DGD	CFB-CEB-CDB	-2.38	102.23	114.53
27	d	411	LMG	C1-C2-C3	-2.38	105.28	109.97
32	D	402	PHO	CBD-CHA-C4D	-2.38	105.80	108.46
27	l	101	LMG	C1-C2-C3	-2.38	105.28	109.97
23	A	406	PL9	C7-C8-C9	-2.38	122.67	126.70
26	c	519	LHG	C11-C10-C9	-2.38	102.25	114.53
24	b	622	BCR	C15-C16-C17	-2.38	118.13	123.39
24	y	101	BCR	C1-C6-C5	-2.38	119.17	122.66
24	C	513	BCR	C15-C14-C13	-2.38	123.77	127.20
24	c	513	BCR	C15-C14-C13	-2.38	123.77	127.20
25	b	624	DGD	C1D-C2D-C3D	-2.38	105.29	109.97
27	D	407	LMG	O2-C2-C1	-2.37	104.82	110.02
27	c	522	LMG	O6-C1-O1	-2.37	104.34	110.05
24	C	513	BCR	C7-C8-C9	-2.37	122.60	126.22
25	c	516	DGD	CFB-CEB-CDB	-2.37	102.29	114.53
24	c	514	BCR	C15-C14-C13	-2.37	123.78	127.20
31	b	603	LMT	C1'-O5'-C5'	-2.36	109.16	113.75
31	M	102	LMT	C3'-C4'-C5'	-2.36	105.50	110.84
27	C	521	LMG	C40-C39-C38	-2.36	102.33	114.53
24	A	407	BCR	C15-C14-C13	-2.36	123.79	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	BCR	C38-C26-C25	-2.36	122.29	124.61
24	K	102	BCR	C38-C26-C25	-2.35	122.30	124.61
27	i	101	LMG	O2-C2-C1	-2.35	104.86	110.02
24	C	514	BCR	C11-C10-C9	-2.35	123.80	127.20
27	e	101	LMG	O6-C1-O1	-2.35	104.40	110.05
27	M	101	LMG	O2-C2-C1	-2.35	104.88	110.02
27	d	407	LMG	O2-C2-C1	-2.34	104.88	110.02
27	B	621	LMG	O6-C1-O1	-2.34	104.42	110.05
31	i	102	LMT	C1'-O5'-C5'	-2.34	109.20	113.75
24	B	619	BCR	C7-C8-C9	-2.34	122.65	126.22
24	b	621	BCR	C35-C13-C14	-2.34	119.45	122.90
27	C	518	LMG	C38-C37-C36	-2.34	102.45	114.53
27	b	625	LMG	O2-C2-C1	-2.34	104.90	110.02
22	b	615	CLA	O2D-CGD-O1D	-2.34	118.96	123.79
27	I	101	LMG	O2-C2-C1	-2.34	104.90	110.02
24	C	513	BCR	C15-C16-C17	-2.33	118.23	123.39
27	A	410	LMG	C38-C37-C36	-2.33	102.50	114.53
24	g	101	BCR	C1-C6-C5	-2.33	119.24	122.66
27	b	625	LMG	C40-C39-C38	-2.33	102.51	114.53
22	C	511	CLA	O2A-CGA-O1A	-2.33	117.48	123.49
24	y	101	BCR	C3-C2-C1	-2.33	106.22	114.83
22	c	511	CLA	O2A-CGA-O1A	-2.33	117.49	123.49
24	b	623	BCR	C11-C10-C9	-2.33	123.84	127.20
25	B	620	DGD	C3G-C2G-C1G	-2.33	106.63	112.07
25	C	515	DGD	C1D-C2D-C3D	-2.32	105.39	109.97
25	C	516	DGD	CFB-CEB-CDB	-2.32	102.54	114.53
24	c	521	BCR	C15-C14-C13	-2.32	123.84	127.20
27	l	101	LMG	C38-C37-C36	-2.32	102.56	114.53
22	C	508	CLA	O2D-CGD-O1D	-2.32	119.01	123.79
27	A	415	LMG	O1-C7-C8	-2.31	105.48	110.99
27	D	411	LMG	O3-C3-C2	-2.31	105.13	110.34
27	C	521	LMG	O2-C2-C1	-2.31	104.95	110.02
25	b	624	DGD	C3G-C2G-C1G	-2.31	106.67	112.07
25	c	516	DGD	O3D-C3D-C4D	-2.31	105.14	110.34
25	d	409	DGD	C3D-C4D-C5D	-2.31	106.18	110.20
31	d	410	LMT	C1'-O5'-C5'	-2.30	109.28	113.75
24	g	101	BCR	C3-C2-C1	-2.30	106.31	114.83
24	b	621	BCR	C38-C26-C25	-2.30	122.35	124.61
27	c	518	LMG	O2-C2-C1	-2.30	104.98	110.02
27	c	518	LMG	C38-C37-C36	-2.30	102.66	114.53
27	B	621	LMG	C40-C39-C38	-2.29	102.68	114.53
23	d	406	PL9	C46-C47-C48	-2.29	105.69	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	102	BCR	C11-C10-C9	-2.29	123.89	127.20
25	a	411	DGD	C1D-C2D-C3D	-2.29	105.46	109.97
24	c	513	BCR	C11-C10-C9	-2.28	123.90	127.20
24	c	513	BCR	C15-C16-C17	-2.28	118.35	123.39
27	E	101	LMG	O6-C1-O1	-2.28	104.57	110.05
27	C	521	LMG	O6-C1-O1	-2.27	104.58	110.05
27	d	411	LMG	O6-C1-O1	-2.27	104.58	110.05
27	m	101	LMG	C1-O6-C5	-2.27	109.34	113.75
24	c	521	BCR	C38-C26-C25	-2.27	122.38	124.61
27	A	410	LMG	O1-C1-C2	-2.27	105.18	108.04
23	j	101	PL9	O2-C1-C2	-2.26	116.79	121.89
24	C	513	BCR	C38-C26-C25	-2.26	122.39	124.61
34	f	101	HEM	C3B-C4B-NB	-2.26	107.31	111.63
25	b	601	DGD	O6D-C1D-O3G	-2.26	104.62	110.05
23	D	406	PL9	C46-C47-C48	-2.26	105.78	111.69
24	b	620	BCR	C38-C26-C25	-2.26	122.39	124.61
24	J	102	BCR	C15-C16-C17	-2.26	118.41	123.39
27	b	625	LMG	C38-C37-C36	-2.25	102.89	114.53
23	d	406	PL9	O2-C1-C2	-2.25	116.82	121.89
27	d	407	LMG	O3-C3-C2	-2.25	105.27	110.34
24	b	620	BCR	C11-C10-C9	-2.25	123.95	127.20
25	c	515	DGD	O5D-C6D-C5D	-2.25	105.00	109.08
27	C	521	LMG	C38-C37-C36	-2.25	102.92	114.53
27	D	407	LMG	O3-C3-C2	-2.25	105.27	110.34
27	e	101	LMG	O3-C3-C2	-2.25	105.28	110.34
24	K	102	BCR	C24-C23-C22	-2.25	122.79	126.22
27	B	621	LMG	O2-C2-C1	-2.24	105.10	110.02
24	f	102	BCR	C38-C26-C25	-2.24	122.40	124.61
27	a	402	LMG	O1-C7-C8	-2.24	105.66	110.99
34	F	101	HEM	C3B-C4B-NB	-2.24	107.35	111.63
27	C	518	LMG	O2-C2-C1	-2.24	105.11	110.02
25	c	515	DGD	C1D-C2D-C3D	-2.24	105.56	109.97
27	b	625	LMG	O3-C3-C2	-2.24	105.30	110.34
24	B	618	BCR	C7-C8-C9	-2.24	122.81	126.22
23	J	101	PL9	O2-C1-C2	-2.23	116.86	121.89
27	c	522	LMG	C38-C37-C36	-2.23	102.99	114.53
27	I	101	LMG	O3-C3-C2	-2.23	105.31	110.34
22	B	611	CLA	O2D-CGD-O1D	-2.23	119.18	123.79
23	d	406	PL9	C12-C13-C14	-2.23	122.91	127.76
24	j	102	BCR	C15-C16-C17	-2.23	118.46	123.39
31	B	624	LMT	C1'-O5'-C5'	-2.23	109.42	113.75
27	d	411	LMG	O3-C3-C2	-2.23	105.32	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	102	BCR	C15-C14-C13	-2.23	123.98	127.20
23	J	101	PL9	C12-C13-C14	-2.23	122.92	127.76
27	l	101	LMG	O2-C2-C1	-2.23	105.14	110.02
31	I	102	LMT	C1'-O5'-C5'	-2.23	109.42	113.75
23	D	406	PL9	C12-C13-C14	-2.23	122.92	127.76
34	F	101	HEM	CAA-CBA-CGA	-2.22	108.67	112.75
25	B	625	DGD	O6D-C1D-O3G	-2.22	104.70	110.05
24	B	617	BCR	C38-C26-C25	-2.22	122.42	124.61
27	B	621	LMG	O3-C3-C2	-2.22	105.33	110.34
23	j	101	PL9	C12-C13-C14	-2.22	122.93	127.76
27	C	518	LMG	O3-C3-C2	-2.22	105.34	110.34
25	c	516	DGD	C3D-C4D-C5D	-2.22	106.33	110.20
25	C	516	DGD	O3D-C3D-C4D	-2.22	105.34	110.34
27	B	621	LMG	C38-C37-C36	-2.22	103.07	114.53
24	c	513	BCR	C38-C26-C25	-2.22	122.43	124.61
27	l	101	LMG	O3-C3-C2	-2.22	105.34	110.34
27	A	410	LMG	O2-C2-C1	-2.22	105.16	110.02
23	A	406	PL9	C31-C32-C33	-2.22	105.89	111.69
25	B	620	DGD	C1D-C2D-C3D	-2.21	105.61	109.97
27	b	625	LMG	O6-C1-O1	-2.21	104.73	110.05
23	a	409	PL9	C31-C32-C33	-2.21	105.90	111.69
25	C	516	DGD	C3D-C4D-C5D	-2.21	106.35	110.20
23	A	406	PL9	O2-C1-C2	-2.20	116.93	121.89
24	F	102	BCR	C38-C26-C25	-2.20	122.44	124.61
24	B	619	BCR	C24-C23-C22	-2.20	122.86	126.22
23	a	409	PL9	C32-C33-C34	-2.20	122.98	127.76
24	F	102	BCR	C11-C10-C9	-2.20	124.02	127.20
23	D	406	PL9	O2-C1-C2	-2.19	116.95	121.89
27	a	402	LMG	O3-C3-C2	-2.19	105.40	110.34
27	a	402	LMG	O2-C2-C1	-2.19	105.21	110.02
24	B	616	BCR	C11-C10-C9	-2.19	124.03	127.20
24	B	617	BCR	C35-C13-C14	-2.19	119.67	122.90
25	C	516	DGD	CBB-CAB-C9B	-2.19	103.24	114.53
23	A	406	PL9	C11-C12-C13	-2.19	105.96	111.69
24	c	521	BCR	C24-C23-C22	-2.18	122.89	126.22
23	a	409	PL9	C11-C12-C13	-2.18	105.97	111.69
27	D	408	LMG	O6-C1-O1	-2.18	104.80	110.05
27	d	411	LMG	O2-C2-C1	-2.18	105.24	110.02
25	c	516	DGD	O2D-C2D-C1D	-2.18	105.24	110.02
27	c	518	LMG	O3-C3-C2	-2.18	105.43	110.34
27	c	522	LMG	O3-C3-C2	-2.18	105.43	110.34
31	b	627	LMT	C1'-O5'-C5'	-2.18	109.52	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	DGD	CAB-C9B-C8B	-2.18	103.30	114.53
23	a	409	PL9	O2-C1-C2	-2.17	117.00	121.89
24	b	621	BCR	C11-C10-C9	-2.17	124.06	127.20
24	A	407	BCR	C15-C16-C17	-2.17	118.59	123.39
34	f	101	HEM	CAA-CBA-CGA	-2.17	108.77	112.75
27	d	408	LMG	O6-C1-O1	-2.17	104.83	110.05
25	c	516	DGD	CBB-CAB-C9B	-2.17	103.33	114.53
27	d	408	LMG	O6-C1-C2	-2.17	105.83	110.28
27	A	415	LMG	O2-C2-C1	-2.17	105.27	110.02
27	i	101	LMG	O3-C3-C2	-2.17	105.46	110.34
24	b	622	BCR	C38-C26-C25	-2.17	122.48	124.61
27	i	101	LMG	O1-C7-C8	-2.17	105.83	110.99
27	E	101	LMG	O3-C3-C2	-2.17	105.46	110.34
25	a	411	DGD	CAB-C9B-C8B	-2.16	103.35	114.53
25	D	409	DGD	C3D-C4D-C5D	-2.16	106.43	110.20
24	B	616	BCR	C15-C14-C13	-2.16	124.08	127.20
27	D	411	LMG	O6-C1-O1	-2.16	104.85	110.05
27	A	415	LMG	O3-C3-C2	-2.16	105.47	110.34
23	A	406	PL9	C12-C13-C14	-2.16	123.07	127.76
27	C	521	LMG	O3-C3-C2	-2.16	105.48	110.34
25	A	408	DGD	C1D-C2D-C3D	-2.15	105.73	109.97
25	C	515	DGD	O5D-C6D-C5D	-2.15	105.18	109.08
24	b	620	BCR	C15-C14-C13	-2.15	124.09	127.20
22	b	614	CLA	C4B-CHC-C1C	-2.15	124.64	129.26
25	C	517	DGD	CBB-CAB-C9B	-2.15	103.43	114.53
25	b	601	DGD	CBB-CAB-C9B	-2.15	103.43	114.53
24	B	619	BCR	C11-C10-C9	-2.15	124.10	127.20
26	a	412	LHG	C27-C26-C25	-2.14	103.46	114.53
25	B	625	DGD	CBB-CAB-C9B	-2.14	103.46	114.53
23	d	406	PL9	C36-C34-C33	-2.14	116.99	121.05
24	H	102	BCR	C38-C26-C25	-2.14	122.50	124.61
27	c	518	LMG	O1-C7-C8	-2.14	105.89	110.99
25	c	517	DGD	CBB-CAB-C9B	-2.14	103.48	114.53
22	B	610	CLA	C4B-CHC-C1C	-2.14	124.67	129.26
26	A	409	LHG	C27-C26-C25	-2.13	103.51	114.53
25	C	516	DGD	O2D-C2D-C1D	-2.13	105.34	110.02
27	I	101	LMG	O1-C1-C2	-2.13	105.35	108.04
23	a	409	PL9	C3-C2-C1	-2.13	121.67	122.97
24	C	513	BCR	C11-C10-C9	-2.13	124.12	127.20
24	b	622	BCR	C7-C8-C9	-2.13	122.97	126.22
23	d	406	PL9	C3-C2-C1	-2.13	121.67	122.97
25	C	516	DGD	CAB-C9B-C8B	-2.12	103.56	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	409	PL9	C12-C13-C14	-2.12	123.14	127.76
25	d	409	DGD	C5B-C4B-C3B	-2.12	103.57	114.53
27	D	411	LMG	O2-C2-C1	-2.12	105.37	110.02
27	m	101	LMG	O3-C3-C2	-2.12	105.56	110.34
24	c	521	BCR	C11-C10-C9	-2.12	124.13	127.20
24	b	623	BCR	C24-C23-C22	-2.12	122.98	126.22
25	b	601	DGD	CAB-C9B-C8B	-2.11	103.61	114.53
25	B	625	DGD	CAB-C9B-C8B	-2.11	103.62	114.53
24	c	513	BCR	C8-C7-C6	-2.11	120.98	127.32
23	D	406	PL9	C42-C43-C44	-2.11	123.18	127.76
27	e	101	LMG	O1-C7-C8	-2.11	105.97	110.99
23	A	406	PL9	C32-C33-C34	-2.11	123.18	127.76
27	M	101	LMG	O3-C3-C2	-2.11	105.59	110.34
24	f	102	BCR	C11-C10-C9	-2.11	124.16	127.20
27	C	521	LMG	C1-C2-C3	-2.11	105.82	109.97
24	j	102	BCR	C20-C21-C22	-2.10	124.16	127.20
24	K	102	BCR	C7-C8-C9	-2.10	123.01	126.22
24	b	621	BCR	C7-C8-C9	-2.10	123.01	126.22
24	A	407	BCR	C24-C23-C22	-2.10	123.02	126.22
24	g	101	BCR	C15-C16-C17	-2.10	118.75	123.39
24	a	410	BCR	C15-C14-C13	-2.10	124.17	127.20
27	e	101	LMG	O2-C2-C1	-2.10	105.42	110.02
22	b	615	CLA	O2A-CGA-O1A	-2.09	118.08	123.49
24	a	410	BCR	C15-C16-C17	-2.09	118.77	123.39
27	i	101	LMG	O1-C1-C2	-2.09	105.40	108.04
24	g	101	BCR	C24-C23-C22	-2.09	123.03	126.22
24	J	102	BCR	C20-C21-C22	-2.09	124.18	127.20
25	c	517	DGD	CAB-C9B-C8B	-2.09	103.75	114.53
24	B	618	BCR	C38-C26-C25	-2.08	122.56	124.61
24	C	514	BCR	C24-C23-C22	-2.08	123.04	126.22
27	C	518	LMG	O1-C7-C8	-2.08	106.04	110.99
24	C	513	BCR	C8-C7-C6	-2.08	121.08	127.32
25	D	409	DGD	C5B-C4B-C3B	-2.08	103.81	114.53
24	x	101	BCR	C38-C26-C25	-2.07	122.57	124.61
27	M	101	LMG	C1-O6-C5	-2.07	109.72	113.75
23	D	406	PL9	C11-C12-C13	-2.07	106.26	111.69
25	D	409	DGD	CAB-C9B-C8B	-2.07	103.83	114.53
26	C	519	LHG	C27-C26-C25	-2.07	103.84	114.53
27	E	101	LMG	O1-C7-C8	-2.07	106.06	110.99
25	C	517	DGD	CAB-C9B-C8B	-2.07	103.85	114.53
26	c	519	LHG	C27-C26-C25	-2.07	103.85	114.53
27	E	101	LMG	O2-C2-C1	-2.07	105.49	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	f	102	BCR	C15-C16-C17	-2.07	118.82	123.39
25	c	516	DGD	CAB-C9B-C8B	-2.07	103.87	114.53
25	c	515	DGD	O2D-C2D-C1D	-2.06	105.50	110.02
27	D	407	LMG	O1-C1-C2	-2.06	105.44	108.04
24	a	410	BCR	C24-C23-C22	-2.06	123.07	126.22
24	F	102	BCR	C7-C8-C9	-2.06	123.08	126.22
24	B	617	BCR	C11-C10-C9	-2.06	124.23	127.20
22	b	618	CLA	O2A-CGA-O1A	-2.05	118.19	123.49
24	c	513	BCR	C33-C5-C6	-2.05	122.59	124.61
22	B	603	CLA	O2A-CGA-O1A	-2.05	118.19	123.49
25	d	409	DGD	CAB-C9B-C8B	-2.05	103.95	114.53
24	y	101	BCR	C15-C16-C17	-2.05	118.86	123.39
24	F	102	BCR	C15-C16-C17	-2.05	118.86	123.39
23	D	406	PL9	C3-C2-C1	-2.05	121.72	122.97
23	d	406	PL9	C11-C12-C13	-2.05	106.33	111.69
25	D	409	DGD	CBB-CAB-C9B	-2.04	103.98	114.53
22	C	506	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
27	I	101	LMG	O1-C7-C8	-2.04	106.13	110.99
25	C	515	DGD	C5B-C4B-C3B	-2.04	104.00	114.53
25	A	408	DGD	C5B-C4B-C3B	-2.04	104.00	114.53
25	d	409	DGD	CBB-CAB-C9B	-2.04	104.00	114.53
27	c	518	LMG	O1-C1-C2	-2.04	105.47	108.04
25	C	515	DGD	O3E-C3E-C2E	-2.04	105.75	110.34
25	B	620	DGD	C4E-C3E-C2E	-2.03	107.00	110.79
25	c	515	DGD	C5B-C4B-C3B	-2.03	104.05	114.53
25	b	624	DGD	CAB-C9B-C8B	-2.03	104.06	114.53
24	c	514	BCR	C24-C23-C22	-2.03	123.13	126.22
24	c	521	BCR	C7-C8-C9	-2.02	123.13	126.22
22	c	509	CLA	O2A-CGA-O1A	-2.02	118.27	123.49
25	c	516	DGD	C1D-O6D-C5D	-2.02	109.82	113.75
24	B	617	BCR	C24-C23-C22	-2.02	123.13	126.22
25	C	515	DGD	O2D-C2D-C1D	-2.02	105.59	110.02
22	c	506	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
23	a	409	PL9	C36-C37-C38	-2.02	106.40	111.69
22	C	512	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
25	C	516	DGD	C5B-C4B-C3B	-2.01	104.14	114.53
22	c	512	CLA	O2A-CGA-O1A	-2.01	118.31	123.49
25	C	517	DGD	C5B-C4B-C3B	-2.01	104.16	114.53
24	x	101	BCR	C28-C27-C26	-2.01	110.68	113.87
25	B	620	DGD	C5B-C4B-C3B	-2.01	104.17	114.53
22	B	611	CLA	O2A-CGA-O1A	-2.01	118.31	123.49
27	a	402	LMG	C1-C2-C3	-2.01	106.02	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	O2A-CGA-O1A	-2.01	118.32	123.49
22	B	601	CLA	O2A-CGA-O1A	-2.00	118.33	123.49
24	b	622	BCR	C20-C21-C22	-2.00	124.31	127.20
27	l	101	LMG	O1-C1-C2	-2.00	105.51	108.04
22	b	607	CLA	CMD-C2D-C3D	2.00	129.00	125.09
22	c	520	CLA	CMD-C2D-C3D	2.00	129.01	125.09
22	b	618	CLA	O2D-CGD-CBD	2.01	114.05	111.30
22	C	505	CLA	O1D-CGD-CBD	2.01	127.50	124.62
32	D	401	PHO	CHB-C1B-NB	2.01	128.43	124.66
31	B	627	LMT	O1'-C1'-C2'	2.01	110.58	108.04
22	C	509	CLA	CMD-C2D-C3D	2.01	129.03	125.09
22	c	504	CLA	CBA-CAA-C2A	2.02	119.42	113.73
32	a	407	PHO	C1B-NB-C4B	2.02	110.50	106.51
22	C	520	CLA	O1D-CGD-CBD	2.02	127.51	124.62
22	c	520	CLA	O1D-CGD-CBD	2.02	127.51	124.62
32	D	401	PHO	C1B-NB-C4B	2.02	110.51	106.51
22	C	511	CLA	O2D-CGD-CBD	2.03	114.08	111.30
22	b	608	CLA	O1D-CGD-CBD	2.03	127.54	124.62
22	C	504	CLA	CBA-CAA-C2A	2.03	119.47	113.73
32	D	402	PHO	C1B-NB-C4B	2.04	110.55	106.51
22	b	616	CLA	CMD-C2D-C3D	2.04	129.08	125.09
25	C	517	DGD	C3G-O3G-C1D	2.04	118.11	113.82
22	b	619	CLA	O2D-CGD-CBD	2.04	114.10	111.30
30	A	413	SQD	C4-C3-C2	2.05	114.62	110.79
22	B	615	CLA	O2D-CGD-CBD	2.05	114.11	111.30
22	b	606	CLA	O1D-CGD-CBD	2.05	127.56	124.62
22	B	602	CLA	O1D-CGD-CBD	2.05	127.57	124.62
22	c	505	CLA	CMD-C2D-C3D	2.05	129.11	125.09
22	b	618	CLA	CMD-C2D-C3D	2.06	129.11	125.09
22	c	503	CLA	CMD-C2D-C3D	2.06	129.11	125.09
22	c	511	CLA	O2D-CGD-CBD	2.06	114.12	111.30
22	b	612	CLA	O1D-CGD-CBD	2.06	127.58	124.62
22	b	605	CLA	O1D-CGD-CBD	2.07	127.58	124.62
22	C	520	CLA	CMD-C2D-C3D	2.07	129.13	125.09
22	B	608	CLA	O1D-CGD-CBD	2.07	127.59	124.62
22	C	505	CLA	CMD-C2D-C3D	2.07	129.15	125.09
22	B	610	CLA	C4A-NA-C1A	2.07	109.04	106.36
22	b	618	CLA	O1D-CGD-CBD	2.08	127.60	124.62
22	C	501	CLA	CMB-C2B-C3B	2.08	129.16	125.09
22	B	614	CLA	O1D-CGD-CBD	2.08	127.61	124.62
22	c	506	CLA	CMD-C2D-C3D	2.08	129.16	125.09
22	H	101	CLA	CMD-C2D-C3D	2.08	129.16	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	512	CLA	CMD-C2D-C3D	2.09	129.17	125.09
30	a	415	SQD	C4-C3-C2	2.10	114.70	110.79
22	B	614	CLA	CMD-C2D-C3D	2.10	129.20	125.09
22	C	506	CLA	O2D-CGD-CBD	2.10	114.18	111.30
30	F	103	SQD	O48-C23-C24	2.10	118.31	111.90
30	d	402	SQD	C4-C3-C2	2.10	114.72	110.79
25	D	409	DGD	O5D-C1E-C2E	2.10	110.70	108.04
25	C	517	DGD	O5D-C1E-C2E	2.11	110.70	108.04
22	a	406	CLA	O1D-CGD-CBD	2.11	127.64	124.62
22	b	606	CLA	CMD-C2D-C3D	2.11	129.22	125.09
22	c	501	CLA	CMD-C2D-C3D	2.12	129.24	125.09
22	B	603	CLA	CMD-C2D-C3D	2.12	129.24	125.09
22	b	613	CLA	CMD-C2D-C3D	2.13	129.25	125.09
22	B	613	CLA	CMD-C2D-C3D	2.13	129.26	125.09
22	a	405	CLA	O2D-CGD-CBD	2.13	114.22	111.30
22	b	605	CLA	CMD-C2D-C3D	2.14	129.26	125.09
22	B	612	CLA	CMD-C2D-C3D	2.14	129.27	125.09
22	b	617	CLA	O1D-CGD-CBD	2.14	127.69	124.62
24	x	101	BCR	C27-C26-C25	2.14	125.51	122.78
22	C	503	CLA	CMD-C2D-C3D	2.14	129.28	125.09
22	C	506	CLA	CMD-C2D-C3D	2.14	129.28	125.09
22	C	501	CLA	CMD-C2D-C3D	2.15	129.28	125.09
22	C	502	CLA	O1D-CGD-CBD	2.15	127.70	124.62
22	b	614	CLA	C4A-NA-C1A	2.15	109.14	106.36
22	C	520	CLA	O2D-CGD-CBD	2.15	114.25	111.30
22	b	613	CLA	O1D-CGD-CBD	2.15	127.71	124.62
22	h	101	CLA	CMD-C2D-C3D	2.16	129.30	125.09
22	c	511	CLA	O1D-CGD-CBD	2.16	127.71	124.62
22	b	613	CLA	O2D-CGD-CBD	2.16	114.26	111.30
22	C	506	CLA	O1D-CGD-CBD	2.16	127.72	124.62
22	c	502	CLA	O1D-CGD-CBD	2.16	127.72	124.62
22	c	501	CLA	CMB-C2B-C3B	2.17	129.32	125.09
22	C	507	CLA	CMD-C2D-C3D	2.17	129.32	125.09
24	H	102	BCR	C29-C30-C25	2.17	113.80	110.36
30	f	103	SQD	O48-C23-C24	2.17	118.51	111.90
22	B	607	CLA	CMD-C2D-C3D	2.17	129.34	125.09
22	B	601	CLA	CMD-C2D-C3D	2.18	129.36	125.09
22	D	405	CLA	CMD-C2D-C3D	2.18	129.36	125.09
31	b	626	LMT	O1'-C1'-C2'	2.19	110.80	108.04
22	b	617	CLA	CMD-C2D-C3D	2.19	129.37	125.09
22	b	611	CLA	CMD-C2D-C3D	2.19	129.38	125.09
24	J	102	BCR	C29-C30-C25	2.19	113.84	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	502	CLA	O2D-CGD-CBD	2.20	114.31	111.30
22	C	508	CLA	O1D-CGD-CBD	2.20	127.77	124.62
24	j	102	BCR	C29-C30-C25	2.20	113.84	110.36
22	B	613	CLA	O1D-CGD-CBD	2.20	127.77	124.62
22	A	405	CLA	CMD-C2D-C3D	2.20	129.40	125.09
22	B	602	CLA	CMD-C2D-C3D	2.20	129.40	125.09
34	V	201	HEM	C2D-C3D-C4D	2.20	105.24	101.50
22	d	405	CLA	CMD-C2D-C3D	2.21	129.40	125.09
22	B	601	CLA	O1D-CGD-CBD	2.21	127.79	124.62
22	A	404	CLA	O2D-CGD-CBD	2.21	114.33	111.30
22	d	404	CLA	CHB-C4A-NA	2.21	127.57	124.51
22	D	404	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	a	406	CLA	O2D-CGD-CBD	2.22	114.34	111.30
34	v	201	HEM	C2D-C3D-C4D	2.22	105.27	101.50
24	H	102	BCR	C27-C26-C25	2.23	125.62	122.78
24	B	618	BCR	C27-C26-C25	2.23	125.62	122.78
22	c	509	CLA	O1D-CGD-CBD	2.23	127.82	124.62
22	b	612	CLA	CMD-C2D-C3D	2.23	129.46	125.09
22	c	520	CLA	O2D-CGD-CBD	2.23	114.36	111.30
22	B	608	CLA	CMD-C2D-C3D	2.24	129.47	125.09
24	x	101	BCR	C29-C30-C25	2.24	113.91	110.36
22	B	602	CLA	O2D-CGD-CBD	2.25	114.38	111.30
22	C	509	CLA	O1D-CGD-CBD	2.25	127.84	124.62
23	A	406	PL9	C41-C39-C40	2.25	120.18	114.64
30	F	103	SQD	C3-C4-C5	2.26	114.13	110.20
22	C	502	CLA	CMD-C2D-C3D	2.26	129.51	125.09
22	c	504	CLA	CMB-C2B-C3B	2.26	129.51	125.09
22	c	507	CLA	CMD-C2D-C3D	2.26	129.51	125.09
22	B	611	CLA	CMD-C2D-C3D	2.26	129.51	125.09
31	B	624	LMT	O1'-C1'-C2'	2.27	110.90	108.04
22	a	408	CLA	CMD-C2D-C3D	2.27	129.52	125.09
30	A	414	SQD	C1-O5-C5	2.27	118.14	113.75
22	b	608	CLA	O2D-CGD-CBD	2.27	114.41	111.30
22	c	506	CLA	O1D-CGD-CBD	2.27	127.88	124.62
22	b	605	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	b	605	CLA	O2D-CGD-CBD	2.27	114.41	111.30
30	a	401	SQD	O6-C1-C2	2.28	110.92	108.04
22	C	502	CLA	O2D-CGD-CBD	2.28	114.43	111.30
22	b	616	CLA	O1D-CGD-CBD	2.28	127.89	124.62
34	f	101	HEM	C2D-C3D-C4D	2.29	105.38	101.50
22	b	615	CLA	CMD-C2D-C3D	2.29	129.57	125.09
34	F	101	HEM	C2D-C3D-C4D	2.29	105.39	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	622	BCR	C27-C26-C25	2.29	125.70	122.78
22	C	509	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	A	405	CLA	O1D-CGD-CBD	2.31	127.93	124.62
22	c	508	CLA	O1D-CGD-CBD	2.31	127.94	124.62
22	C	504	CLA	CMB-C2B-C3B	2.31	129.61	125.09
23	a	409	PL9	C41-C39-C40	2.32	120.33	114.64
30	A	414	SQD	O6-C1-C2	2.32	110.96	108.04
31	M	103	LMT	O1'-C1'-C2'	2.32	110.97	108.04
22	c	504	CLA	CMD-C2D-C3D	2.32	129.63	125.09
22	b	615	CLA	O1D-CGD-CBD	2.32	127.95	124.62
22	d	404	CLA	CMD-C2D-C3D	2.33	129.64	125.09
30	f	103	SQD	C3-C4-C5	2.33	114.25	110.20
22	A	403	CLA	O2D-CGD-CBD	2.33	114.50	111.30
22	b	619	CLA	CMB-C2B-C3B	2.34	129.66	125.09
30	B	626	SQD	O48-C23-C24	2.34	119.03	111.90
22	c	502	CLA	CMD-C2D-C3D	2.34	129.67	125.09
22	B	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	b	612	CLA	O2D-CGD-CBD	2.34	114.52	111.30
22	B	612	CLA	O1D-CGD-CBD	2.35	127.99	124.62
22	C	502	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	b	619	CLA	CHB-C4A-NA	2.35	127.76	124.51
24	F	102	BCR	C27-C26-C25	2.35	125.78	122.78
22	D	404	CLA	CMD-C2D-C3D	2.35	129.69	125.09
30	b	602	SQD	O48-C23-C24	2.35	119.07	111.90
22	D	405	CLA	O1D-CGD-CBD	2.35	127.99	124.62
22	c	509	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	b	613	CLA	C4A-NA-C1A	2.36	109.41	106.36
22	A	402	CLA	CMB-C2B-C3B	2.36	129.71	125.09
30	a	401	SQD	C1-O5-C5	2.36	118.33	113.75
30	A	414	SQD	O48-C23-C24	2.36	119.10	111.90
22	A	402	CLA	C4A-NA-C1A	2.37	109.42	106.36
22	B	615	CLA	CMB-C2B-C3B	2.37	129.72	125.09
22	C	502	CLA	C4A-NA-C1A	2.37	109.42	106.36
25	d	409	DGD	O5D-C1E-C2E	2.37	111.04	108.04
22	A	405	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	B	617	BCR	C29-C30-C25	2.38	114.13	110.36
22	B	611	CLA	O1D-CGD-CBD	2.38	128.04	124.62
22	b	606	CLA	CHB-C4A-NA	2.38	127.81	124.51
30	F	103	SQD	C44-O6-C1	2.39	118.83	113.82
22	a	404	CLA	CMB-C2B-C3B	2.39	129.76	125.09
31	B	623	LMT	O1'-C1'-C2'	2.39	111.06	108.04
24	B	616	BCR	C2-C1-C6	2.39	114.15	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	405	CLA	O1D-CGD-CBD	2.39	128.05	124.62
22	B	604	CLA	O2D-CGD-CBD	2.39	114.58	111.30
22	b	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	b	620	BCR	C2-C1-C6	2.39	114.15	110.36
22	C	509	CLA	C4A-NA-C1A	2.40	109.46	106.36
22	C	505	CLA	O2D-CGD-CBD	2.40	114.59	111.30
22	B	609	CLA	O1D-CGD-CBD	2.40	128.06	124.62
22	a	404	CLA	C4A-NA-C1A	2.40	109.46	106.36
22	D	405	CLA	C4A-NA-C1A	2.40	109.46	106.36
22	C	511	CLA	CMD-C2D-C3D	2.40	129.78	125.09
22	B	606	CLA	O2D-CGD-CBD	2.40	114.59	111.30
22	A	402	CLA	CHB-C4A-NA	2.40	127.84	124.51
30	d	402	SQD	O48-C23-C24	2.41	119.23	111.90
22	D	404	CLA	C4A-NA-C1A	2.41	109.47	106.36
30	B	622	SQD	O48-C23-C24	2.41	119.23	111.90
22	C	507	CLA	O2D-CGD-CBD	2.41	114.60	111.30
30	a	401	SQD	O48-C23-C24	2.41	119.24	111.90
22	A	404	CLA	C4A-NA-C1A	2.41	109.47	106.36
22	b	606	CLA	C4A-NA-C1A	2.41	109.47	106.36
24	b	621	BCR	C29-C30-C25	2.41	114.18	110.36
22	b	605	CLA	CMB-C2B-C3B	2.42	129.81	125.09
22	C	507	CLA	CHB-C4A-NA	2.42	127.85	124.51
24	C	513	BCR	C27-C26-C25	2.42	125.86	122.78
22	b	610	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	c	509	CLA	C4A-NA-C1A	2.42	109.48	106.36
23	j	101	PL9	C20-C19-C21	2.42	119.10	115.41
22	c	511	CLA	CMD-C2D-C3D	2.42	129.82	125.09
22	B	615	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	c	501	CLA	O1D-CGD-CBD	2.42	128.09	124.62
22	C	508	CLA	CMB-C2B-C3B	2.42	129.82	125.09
22	b	616	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	H	101	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	B	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	b	612	CLA	CMB-C2B-C3B	2.43	129.84	125.09
22	b	612	CLA	C4A-NA-C1A	2.43	109.50	106.36
22	b	605	CLA	C4A-NA-C1A	2.43	109.50	106.36
22	c	502	CLA	C4A-NA-C1A	2.43	109.50	106.36
24	f	102	BCR	C27-C26-C25	2.43	125.88	122.78
22	h	101	CLA	O1D-CGD-CBD	2.43	128.11	124.62
22	d	405	CLA	C4A-NA-C1A	2.43	109.51	106.36
22	C	504	CLA	CMD-C2D-C3D	2.44	129.86	125.09
22	b	607	CLA	CMB-C2B-C3B	2.44	129.86	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	A	413	SQD	O48-C23-C24	2.44	119.34	111.90
22	B	610	CLA	CMD-C2D-C3D	2.44	129.87	125.09
22	C	501	CLA	O1D-CGD-CBD	2.45	128.13	124.62
22	c	502	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	c	508	CLA	CMB-C2B-C3B	2.45	129.87	125.09
22	c	510	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	A	404	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	c	507	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	601	CLA	C4A-NA-C1A	2.45	109.52	106.36
22	b	611	CLA	C4A-NA-C1A	2.45	109.52	106.36
22	B	608	CLA	CMB-C2B-C3B	2.45	129.88	125.09
22	b	610	CLA	C4A-NA-C1A	2.45	109.53	106.36
22	b	617	CLA	O2D-CGD-CBD	2.45	114.66	111.30
22	h	101	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	D	405	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	c	520	CLA	CMB-C2B-C3B	2.46	129.89	125.09
30	a	415	SQD	O48-C23-C24	2.46	119.38	111.90
22	b	610	CLA	O2D-CGD-CBD	2.46	114.67	111.30
22	B	608	CLA	O2D-CGD-CBD	2.46	114.67	111.30
22	a	408	CLA	O1D-CGD-CBD	2.46	128.14	124.62
22	b	611	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	c	513	BCR	C27-C26-C25	2.46	125.92	122.78
22	B	603	CLA	CMB-C2B-C3B	2.46	129.90	125.09
30	B	626	SQD	C4-C3-C2	2.46	115.39	110.79
22	a	406	CLA	CMB-C2B-C3B	2.46	129.90	125.09
22	b	614	CLA	CMD-C2D-C3D	2.46	129.90	125.09
22	A	403	CLA	CMB-C2B-C3B	2.46	129.91	125.09
22	c	508	CLA	C4A-NA-C1A	2.47	109.55	106.36
23	A	406	PL9	C20-C19-C21	2.47	119.17	115.41
22	B	608	CLA	C4A-NA-C1A	2.47	109.56	106.36
22	c	510	CLA	O1D-CGD-CBD	2.47	128.17	124.62
23	J	101	PL9	C20-C19-C21	2.47	119.19	115.41
22	B	612	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	C	505	CLA	C4A-NA-C1A	2.48	109.56	106.36
22	B	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	C	508	CLA	C4A-NA-C1A	2.48	109.56	106.36
22	B	606	CLA	CMB-C2B-C3B	2.48	129.94	125.09
22	d	405	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	B	611	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	b	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	a	406	CLA	C4A-NA-C1A	2.49	109.57	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	406	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	613	CLA	C4A-NA-C1A	2.49	109.58	106.36
22	B	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	b	617	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	f	103	SQD	C44-O6-C1	2.49	119.05	113.82
22	H	101	CLA	CMB-C2B-C3B	2.49	129.96	125.09
22	c	505	CLA	O2D-CGD-CBD	2.49	114.72	111.30
22	b	609	CLA	CMB-C2B-C3B	2.49	129.96	125.09
22	B	606	CLA	C4A-NA-C1A	2.49	109.58	106.36
22	C	510	CLA	O1D-CGD-CBD	2.50	128.20	124.62
22	B	602	CLA	C4A-NA-C1A	2.50	109.58	106.36
22	d	404	CLA	C4A-NA-C1A	2.50	109.58	106.36
22	C	509	CLA	CMB-C2B-C3B	2.50	129.97	125.09
23	d	406	PL9	C20-C19-C21	2.50	119.22	115.41
22	B	607	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	A	404	CLA	CMB-C2B-C3B	2.50	129.97	125.09
22	b	610	CLA	CMB-C2B-C3B	2.50	129.98	125.09
22	h	101	CLA	C4A-NA-C1A	2.50	109.59	106.36
22	c	509	CLA	CMB-C2B-C3B	2.50	129.98	125.09
22	C	520	CLA	CMB-C2B-C3B	2.50	129.98	125.09
22	C	505	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	503	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	a	405	CLA	CMB-C2B-C3B	2.51	129.99	125.09
22	A	405	CLA	C4A-NA-C1A	2.51	109.60	106.36
22	c	507	CLA	C4A-NA-C1A	2.51	109.60	106.36
22	b	606	CLA	O2D-CGD-CBD	2.51	114.75	111.30
22	a	404	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	B	614	CLA	CMB-C2B-C3B	2.52	130.01	125.09
22	b	611	CLA	O1D-CGD-CBD	2.52	128.23	124.62
22	c	504	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	C	508	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	613	CLA	O2D-CGD-CBD	2.52	114.75	111.30
23	D	406	PL9	C20-C19-C21	2.52	119.25	115.41
22	b	619	CLA	C4A-NA-C1A	2.52	109.62	106.36
22	B	609	CLA	C4A-NA-C1A	2.52	109.62	106.36
22	B	604	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	c	520	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	C	512	CLA	C4A-NA-C1A	2.53	109.62	106.36
22	B	612	CLA	C4A-NA-C1A	2.53	109.62	106.36
22	B	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	h	101	CLA	CMB-C2B-C3B	2.53	130.04	125.09
22	c	510	CLA	C4A-NA-C1A	2.53	109.63	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	601	CLA	CMB-C2B-C3B	2.53	130.04	125.09
24	c	514	BCR	C29-C30-C25	2.53	114.37	110.36
22	C	501	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	b	618	CLA	CMB-C2B-C3B	2.53	130.04	125.09
22	C	512	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	c	508	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	a	408	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	C	504	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	H	101	CLA	C4A-NA-C1A	2.55	109.65	106.36
22	B	608	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	H	101	CLA	O1D-CGD-CBD	2.55	128.28	124.62
22	c	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	c	505	CLA	C4A-NA-C1A	2.55	109.66	106.36
30	B	622	SQD	C44-O6-C1	2.56	119.19	113.82
24	C	514	BCR	C29-C30-C25	2.56	114.41	110.36
22	B	607	CLA	C4A-NA-C1A	2.56	109.67	106.36
24	b	620	BCR	C27-C26-C25	2.56	126.05	122.78
22	b	617	CLA	C4A-NA-C1A	2.56	109.67	106.36
22	C	507	CLA	C4A-NA-C1A	2.57	109.67	106.36
22	B	614	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	B	604	CLA	CMB-C2B-C3B	2.57	130.11	125.09
22	C	506	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	b	608	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	c	512	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	c	512	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	c	512	CLA	O1D-CGD-CBD	2.57	128.31	124.62
22	a	408	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	c	506	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	b	615	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	c	505	CLA	CHB-C4A-NA	2.58	128.09	124.51
22	B	605	CLA	CMB-C2B-C3B	2.59	130.15	125.09
22	b	616	CLA	C4A-NA-C1A	2.59	109.70	106.36
22	d	404	CLA	CMB-C2B-C3B	2.59	130.15	125.09
24	B	616	BCR	C27-C26-C25	2.59	126.08	122.78
22	B	604	CLA	C4A-NA-C1A	2.59	109.70	106.36
22	C	511	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	D	405	CLA	CMB-C2B-C3B	2.59	130.16	125.09
22	C	520	CLA	CHB-C4A-NA	2.59	128.10	124.51
30	d	402	SQD	C44-O6-C1	2.60	119.27	113.82
22	b	618	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	c	501	CLA	C4A-NA-C1A	2.60	109.72	106.36
22	C	503	CLA	CHB-C4A-NA	2.60	128.11	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	520	CLA	C4A-NA-C1A	2.60	109.72	106.36
22	c	511	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	C	519	LHG	O8-C23-C24	2.61	119.84	111.90
30	b	602	SQD	C4-C3-C2	2.61	115.66	110.79
22	d	405	CLA	CMB-C2B-C3B	2.61	130.19	125.09
22	b	608	CLA	CMB-C2B-C3B	2.61	130.19	125.09
22	B	615	CLA	C4A-NA-C1A	2.61	109.74	106.36
22	C	511	CLA	C4A-NA-C1A	2.62	109.74	106.36
22	a	405	CLA	C4A-NA-C1A	2.62	109.74	106.36
22	c	511	CLA	C4A-NA-C1A	2.62	109.74	106.36
22	c	506	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	c	511	CLA	CMB-C2B-C3B	2.62	130.22	125.09
22	C	520	CLA	C4A-NA-C1A	2.62	109.75	106.36
22	B	605	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	C	511	CLA	CMB-C2B-C3B	2.63	130.23	125.09
24	b	622	BCR	C29-C30-C25	2.63	114.52	110.36
22	a	405	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	b	608	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	B	618	BCR	C29-C30-C25	2.63	114.53	110.36
22	b	609	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	B	607	CLA	O1D-CGD-CBD	2.63	128.40	124.62
22	C	501	CLA	C4A-NA-C1A	2.63	109.76	106.36
22	c	502	CLA	CMB-C2B-C3B	2.64	130.24	125.09
24	a	410	BCR	C27-C26-C25	2.65	126.15	122.78
22	c	503	CLA	C4A-NA-C1A	2.65	109.78	106.36
24	A	407	BCR	C27-C26-C25	2.65	126.15	122.78
22	C	510	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	A	405	CLA	CMB-C2B-C3B	2.65	130.27	125.09
22	D	404	CLA	CMB-C2B-C3B	2.65	130.27	125.09
22	b	618	CLA	C4A-NA-C1A	2.65	109.79	106.36
22	C	506	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	B	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	c	519	LHG	O8-C23-C24	2.66	120.00	111.90
24	B	619	BCR	C27-C26-C25	2.67	126.18	122.78
22	b	607	CLA	CHB-C4A-NA	2.67	128.20	124.51
22	B	605	CLA	C4A-NA-C1A	2.67	109.81	106.36
22	B	611	CLA	CMB-C2B-C3B	2.67	130.31	125.09
22	c	503	CLA	CMB-C2B-C3B	2.67	130.32	125.09
22	B	609	CLA	CMB-C2B-C3B	2.68	130.33	125.09
22	C	502	CLA	CMB-C2B-C3B	2.68	130.33	125.09
22	C	503	CLA	C4A-NA-C1A	2.68	109.83	106.36
22	C	510	CLA	C4A-NA-C1A	2.68	109.83	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	403	CLA	C4A-NA-C1A	2.68	109.83	106.36
22	B	610	CLA	O1D-CGD-CBD	2.69	128.48	124.62
22	c	505	CLA	CMB-C2B-C3B	2.69	130.35	125.09
22	C	510	CLA	CMB-C2B-C3B	2.69	130.35	125.09
22	b	609	CLA	C4A-NA-C1A	2.69	109.84	106.36
22	a	408	CLA	CMB-C2B-C3B	2.70	130.36	125.09
23	a	409	PL9	C20-C19-C21	2.70	119.53	115.41
22	C	503	CLA	O2D-CGD-CBD	2.70	115.00	111.30
22	c	512	CLA	CMB-C2B-C3B	2.71	130.38	125.09
22	b	614	CLA	O1D-CGD-CBD	2.71	128.51	124.62
22	C	512	CLA	O1D-CGD-CBD	2.71	128.51	124.62
22	A	403	CLA	CHB-C4A-NA	2.72	128.28	124.51
24	b	623	BCR	C27-C26-C25	2.73	126.25	122.78
22	C	512	CLA	CMB-C2B-C3B	2.73	130.42	125.09
22	b	607	CLA	C4A-NA-C1A	2.73	109.89	106.36
22	C	505	CLA	CMB-C2B-C3B	2.74	130.45	125.09
22	B	603	CLA	C4A-NA-C1A	2.74	109.91	106.36
24	K	102	BCR	C27-C26-C25	2.74	126.28	122.78
24	c	521	BCR	C27-C26-C25	2.75	126.28	122.78
22	b	613	CLA	CMB-C2B-C3B	2.75	130.47	125.09
22	c	510	CLA	CMB-C2B-C3B	2.75	130.47	125.09
22	b	615	CLA	CMB-C2B-C3B	2.76	130.48	125.09
22	b	615	CLA	C4A-NA-C1A	2.76	109.93	106.36
22	a	404	CLA	O1D-CGD-CBD	2.76	128.58	124.62
22	b	617	CLA	CMB-C2B-C3B	2.77	130.50	125.09
24	K	102	BCR	C2-C1-C6	2.77	114.75	110.36
22	A	402	CLA	O1D-CGD-CBD	2.77	128.60	124.62
22	c	506	CLA	CMB-C2B-C3B	2.78	130.52	125.09
22	B	607	CLA	CMB-C2B-C3B	2.78	130.52	125.09
22	C	503	CLA	CMB-C2B-C3B	2.78	130.53	125.09
22	c	507	CLA	O2D-CGD-CBD	2.78	115.11	111.30
22	c	504	CLA	C4A-NA-C1A	2.79	109.97	106.36
22	B	611	CLA	C4A-NA-C1A	2.79	109.97	106.36
24	F	102	BCR	C29-C30-C25	2.79	114.79	110.36
22	B	602	CLA	CMB-C2B-C3B	2.81	130.58	125.09
22	C	504	CLA	C4A-NA-C1A	2.81	109.99	106.36
22	c	503	CLA	O2D-CGD-CBD	2.82	115.16	111.30
24	f	102	BCR	C29-C30-C25	2.82	114.83	110.36
22	b	606	CLA	CMB-C2B-C3B	2.83	130.61	125.09
22	C	506	CLA	CMB-C2B-C3B	2.83	130.62	125.09
24	B	619	BCR	C2-C1-C6	2.85	114.88	110.36
22	B	613	CLA	CMB-C2B-C3B	2.85	130.67	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	409	LHG	O8-C23-C24	2.88	120.68	111.90
24	b	623	BCR	C2-C1-C6	2.88	114.93	110.36
24	c	521	BCR	C2-C1-C6	2.88	114.93	110.36
22	b	611	CLA	CMB-C2B-C3B	2.89	130.74	125.09
22	C	504	CLA	O1D-CGD-CBD	2.90	128.78	124.62
22	B	610	CLA	CMB-C2B-C3B	2.90	130.76	125.09
34	F	101	HEM	CMD-C2D-C3D	2.91	127.20	114.35
22	c	504	CLA	O1D-CGD-CBD	2.91	128.79	124.62
22	C	507	CLA	CMB-C2B-C3B	2.92	130.79	125.09
34	f	101	HEM	CMD-C2D-C3D	2.92	127.27	114.35
22	b	614	CLA	CMB-C2B-C3B	2.93	130.82	125.09
26	a	412	LHG	O8-C23-C24	2.94	120.86	111.90
22	b	609	CLA	O1D-CGD-CBD	2.95	128.85	124.62
24	b	622	BCR	C2-C1-C6	2.98	115.09	110.36
23	D	406	PL9	C40-C39-C41	2.99	119.98	115.41
30	A	414	SQD	C44-O6-C1	3.02	120.15	113.82
30	a	415	SQD	C3-C4-C5	3.02	115.45	110.20
22	b	616	CLA	CMB-C2B-C3B	3.02	131.00	125.09
22	c	507	CLA	CMB-C2B-C3B	3.02	131.00	125.09
24	B	618	BCR	C2-C1-C6	3.05	115.20	110.36
30	A	413	SQD	C3-C4-C5	3.06	115.54	110.20
22	d	404	CLA	O1D-CGD-CBD	3.07	129.02	124.62
23	d	406	PL9	C40-C39-C41	3.07	120.09	115.41
24	g	101	BCR	C27-C26-C25	3.07	126.69	122.78
22	B	605	CLA	O1D-CGD-CBD	3.07	129.02	124.62
22	B	612	CLA	CMB-C2B-C3B	3.07	131.10	125.09
24	y	101	BCR	C27-C26-C25	3.09	126.72	122.78
22	b	607	CLA	O1D-CGD-CBD	3.10	129.06	124.62
34	v	201	HEM	CMD-C2D-C3D	3.11	128.12	114.35
30	B	622	SQD	C3-C4-C5	3.12	115.64	110.20
22	D	404	CLA	O1D-CGD-CBD	3.15	129.13	124.62
24	j	102	BCR	C27-C26-C25	3.15	126.79	122.78
24	J	102	BCR	C27-C26-C25	3.19	126.84	122.78
24	a	410	BCR	C2-C1-C6	3.19	115.42	110.36
30	a	401	SQD	O47-C7-C8	3.20	118.47	111.53
30	a	401	SQD	C44-O6-C1	3.20	120.54	113.82
22	B	603	CLA	O1D-CGD-CBD	3.22	129.24	124.62
34	V	201	HEM	CMD-C2D-C3D	3.22	128.60	114.35
30	d	402	SQD	C3-C4-C5	3.23	115.83	110.20
30	b	602	SQD	C3-C4-C5	3.23	115.83	110.20
30	B	626	SQD	C3-C4-C5	3.24	115.84	110.20
32	D	401	PHO	O1D-CGD-CBD	3.24	129.27	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	103	SQD	O47-C7-C8	3.26	118.60	111.53
24	A	407	BCR	C2-C1-C6	3.26	115.53	110.36
32	d	401	PHO	O1D-CGD-CBD	3.28	129.32	124.62
34	F	101	HEM	C3B-C4B-CHC	3.30	127.81	123.16
30	B	622	SQD	O47-C7-C8	3.33	118.77	111.53
30	d	402	SQD	O47-C7-C8	3.35	118.80	111.53
34	f	101	HEM	C3B-C4B-CHC	3.35	127.88	123.16
32	D	402	PHO	O1D-CGD-CBD	3.37	129.45	124.62
32	a	407	PHO	O1D-CGD-CBD	3.37	129.46	124.62
30	F	103	SQD	O47-C7-C8	3.39	118.89	111.53
30	A	414	SQD	O47-C7-C8	3.43	118.98	111.53
24	J	102	BCR	C2-C1-C6	3.45	115.82	110.36
30	A	413	SQD	O5-C5-C4	3.47	116.19	109.68
24	j	102	BCR	C2-C1-C6	3.47	115.86	110.36
30	F	103	SQD	O5-C5-C4	3.50	116.25	109.68
30	B	626	SQD	O47-C7-C8	3.56	119.27	111.53
30	b	602	SQD	O47-C7-C8	3.57	119.29	111.53
30	a	415	SQD	O5-C5-C4	3.59	116.43	109.68
34	v	201	HEM	CMC-C2C-C3C	3.61	125.56	116.53
30	f	103	SQD	O5-C5-C4	3.62	116.47	109.68
34	F	101	HEM	CMB-C2B-C3B	3.67	125.69	116.53
30	a	415	SQD	O47-C7-C8	3.67	119.51	111.53
30	a	401	SQD	O5-C5-C4	3.67	116.57	109.68
34	f	101	HEM	CMB-C2B-C3B	3.67	125.70	116.53
25	b	601	DGD	O5D-C1E-C2E	3.68	112.68	108.04
31	i	102	LMT	O1'-C1'-C2'	3.69	112.69	108.04
34	V	201	HEM	CMC-C2C-C3C	3.73	125.83	116.53
30	B	626	SQD	O5-C5-C4	3.74	116.71	109.68
26	A	409	LHG	O4-P-O5	3.75	132.87	112.53
31	I	102	LMT	O1'-C1'-C2'	3.75	112.78	108.04
26	c	519	LHG	O4-P-O5	3.75	132.88	112.53
25	B	625	DGD	O5D-C1E-C2E	3.76	112.78	108.04
26	a	412	LHG	O4-P-O5	3.76	132.92	112.53
26	C	519	LHG	O4-P-O5	3.77	132.97	112.53
30	b	602	SQD	O5-C5-C4	3.78	116.78	109.68
24	c	513	BCR	C2-C1-C6	3.78	116.35	110.36
30	A	413	SQD	O47-C7-C8	3.78	119.75	111.53
34	v	201	HEM	CAD-C3D-C4D	3.79	125.84	112.47
34	V	201	HEM	CAD-C3D-C4D	3.80	125.88	112.47
24	C	513	BCR	C2-C1-C6	3.81	116.39	110.36
30	A	414	SQD	O5-C5-C4	3.81	116.84	109.68
34	F	101	HEM	CAD-C3D-C4D	3.98	126.52	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	f	101	HEM	CAD-C3D-C4D	4.03	126.67	112.47
30	f	103	SQD	O6-C1-C2	4.20	113.34	108.04
30	d	402	SQD	O5-C5-C4	4.26	117.68	109.68
30	B	622	SQD	O5-C5-C4	4.32	117.79	109.68
30	F	103	SQD	O6-C1-C2	4.47	113.68	108.04
30	F	103	SQD	O9-S-C6	4.62	110.83	106.94
30	f	103	SQD	O9-S-C6	4.73	110.93	106.94
34	f	101	HEM	CMC-C2C-C3C	4.74	128.36	116.53
34	F	101	HEM	CMC-C2C-C3C	4.77	128.43	116.53
30	A	414	SQD	O9-S-C6	4.84	111.02	106.94
34	V	201	HEM	CMB-C2B-C3B	4.88	128.71	116.53
34	v	201	HEM	CMB-C2B-C3B	4.94	128.86	116.53
30	a	401	SQD	O9-S-C6	5.03	111.18	106.94
34	f	101	HEM	CAD-C3D-C2D	5.12	127.94	113.22
30	B	622	SQD	O9-S-C6	5.12	111.26	106.94
30	d	402	SQD	O9-S-C6	5.15	111.28	106.94
34	F	101	HEM	CAD-C3D-C2D	5.17	128.09	113.22
30	a	415	SQD	O7-S-C6	5.21	111.34	106.94
30	d	402	SQD	O7-S-C6	5.27	111.38	106.94
30	B	626	SQD	O7-S-C6	5.29	111.40	106.94
30	A	413	SQD	O7-S-C6	5.34	111.44	106.94
30	B	622	SQD	O7-S-C6	5.44	111.52	106.94
34	V	201	HEM	CAD-C3D-C2D	5.45	128.88	113.22
34	v	201	HEM	CAD-C3D-C2D	5.45	128.90	113.22
30	B	622	SQD	O6-C1-C2	5.48	114.96	108.04
30	d	402	SQD	O6-C1-C2	5.55	115.05	108.04
30	b	602	SQD	O9-S-C6	5.61	111.67	106.94
30	b	602	SQD	O7-S-C6	5.65	111.70	106.94
30	A	414	SQD	O7-S-C6	5.78	111.81	106.94
30	B	626	SQD	O9-S-C6	5.86	111.88	106.94
30	F	103	SQD	O7-S-C6	5.91	111.92	106.94
30	a	401	SQD	O7-S-C6	5.97	111.97	106.94
30	f	103	SQD	O7-S-C6	6.06	112.05	106.94
30	B	626	SQD	O6-C1-C2	6.92	116.78	108.04
30	b	602	SQD	O6-C1-C2	6.98	116.86	108.04
30	A	413	SQD	O6-C1-C2	7.05	116.95	108.04
30	a	415	SQD	O6-C1-C2	7.18	117.11	108.04
30	a	415	SQD	O9-S-C6	7.30	113.10	106.94
30	A	413	SQD	O9-S-C6	7.36	113.15	106.94

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	a	408	CLA	NC
22	a	408	CLA	ND
22	a	408	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	h	101	CLA	NC

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Mol	Chain	Res	Type	Atom
22	h	101	CLA	ND
22	h	101	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND
22	b	619	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	B	608	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	608	CLA	ND
22	B	608	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND
22	a	404	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	C	520	CLA	NC
22	C	520	CLA	ND
22	C	520	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	B	607	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	607	CLA	ND
22	B	607	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	NA
22	c	520	CLA	NC
22	c	520	CLA	ND
22	c	520	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	608	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	D	404	CLA	NC
22	D	404	CLA	ND
22	D	404	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	d	404	CLA	NC
22	d	404	CLA	ND
22	d	404	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C8-O7-C10-C11
25	c	516	DGD	C2G-O2G-C1B-C2B
25	C	516	DGD	C2G-O2G-C1B-C2B
30	B	622	SQD	C45-O47-C7-C8
30	d	402	SQD	C45-O47-C7-C8

There are no ring outliers.

79 monomers are involved in 311 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	11	0
22	A	403	CLA	12	0
22	A	404	CLA	14	0
22	A	405	CLA	12	0
23	A	406	PL9	5	0
24	A	407	BCR	2	0
25	A	408	DGD	1	0
26	A	409	LHG	3	0
27	A	410	LMG	2	0
30	A	413	SQD	3	0
30	A	414	SQD	5	0
27	A	415	LMG	1	0
22	B	601	CLA	1	0
22	B	602	CLA	11	0
22	B	603	CLA	4	0
22	B	604	CLA	9	0
22	B	605	CLA	7	0
22	B	606	CLA	16	0
22	B	607	CLA	11	0
22	B	608	CLA	15	0
22	B	609	CLA	3	0
22	B	610	CLA	5	0
22	B	611	CLA	10	0
22	B	612	CLA	9	0
22	B	613	CLA	5	0
22	B	614	CLA	4	0
22	B	615	CLA	6	0
24	B	616	BCR	6	0
24	B	617	BCR	2	0
24	B	618	BCR	4	0
24	B	619	BCR	1	0
25	B	620	DGD	2	0
27	B	621	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	622	SQD	3	0
31	B	623	LMT	2	0
25	B	625	DGD	2	0
30	B	626	SQD	2	0
31	B	627	LMT	2	0
31	B	628	LMT	2	0
22	C	501	CLA	7	0
22	C	503	CLA	5	0
22	C	504	CLA	4	0
22	C	505	CLA	3	0
22	C	506	CLA	6	0
22	C	507	CLA	4	0
22	C	508	CLA	3	0
22	C	509	CLA	6	0
22	C	510	CLA	9	0
22	C	511	CLA	1	0
22	C	512	CLA	3	0
24	C	513	BCR	7	0
24	C	514	BCR	7	0
25	C	515	DGD	3	0
25	C	516	DGD	4	0
25	C	517	DGD	5	0
27	C	518	LMG	3	0
26	C	519	LHG	3	0
22	C	520	CLA	5	0
32	D	401	PHO	8	0
32	D	402	PHO	5	0
22	D	404	CLA	10	0
22	D	405	CLA	4	0
23	D	406	PL9	12	0
27	D	407	LMG	4	0
27	D	408	LMG	6	0
25	D	409	DGD	1	0
27	D	411	LMG	1	0
27	E	101	LMG	2	0
34	F	101	HEM	4	0
24	F	102	BCR	3	0
30	F	103	SQD	3	0
22	H	101	CLA	11	0
24	H	102	BCR	1	0
27	I	101	LMG	1	0
31	I	102	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	J	102	BCR	2	0
24	K	102	BCR	3	0
27	M	101	LMG	2	0
34	V	201	HEM	3	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	335/344 (97%)	0.59	31 (9%) 11 10	205, 207, 208, 208	0
1	a	335/344 (97%)	0.61	44 (13%) 5 6	204, 207, 208, 209	0
2	B	490/510 (96%)	0.37	40 (8%) 14 12	205, 207, 208, 208	0
2	b	490/510 (96%)	0.48	47 (9%) 10 9	205, 207, 208, 209	0
3	C	447/461 (96%)	0.41	37 (8%) 14 12	205, 207, 208, 209	0
3	c	447/461 (96%)	0.25	27 (6%) 25 20	206, 207, 208, 209	0
4	D	340/352 (96%)	0.44	18 (5%) 30 25	204, 207, 208, 209	0
4	d	340/352 (96%)	0.40	16 (4%) 35 29	204, 207, 208, 208	0
5	E	82/84 (97%)	0.26	3 (3%) 45 37	205, 207, 208, 208	0
5	e	82/84 (97%)	0.15	2 (2%) 62 54	206, 207, 208, 208	0
6	F	35/45 (77%)	0.03	1 (2%) 55 45	206, 207, 208, 208	0
6	f	35/45 (77%)	-0.37	1 (2%) 55 45	206, 207, 208, 208	0
7	H	65/66 (98%)	0.53	9 (13%) 4 5	206, 207, 208, 209	0
7	h	65/66 (98%)	0.90	14 (21%) 1 3	206, 207, 208, 208	0
8	I	35/38 (92%)	0.62	4 (11%) 7 7	206, 207, 208, 208	0
8	i	35/38 (92%)	-0.04	0 100 100	206, 207, 208, 208	0
9	J	34/40 (85%)	0.11	1 (2%) 55 45	205, 207, 207, 208	0
9	j	34/40 (85%)	-0.42	0 100 100	206, 207, 208, 209	0
10	K	37/46 (80%)	-0.05	0 100 100	206, 207, 208, 208	0
10	k	37/46 (80%)	0.46	5 (13%) 4 6	206, 207, 208, 209	0
11	L	37/37 (100%)	0.68	3 (8%) 15 13	205, 207, 208, 208	0
11	l	37/37 (100%)	0.26	1 (2%) 58 49	206, 207, 208, 209	0
12	M	34/36 (94%)	0.67	4 (11%) 6 7	205, 206, 207, 208	0
12	m	34/36 (94%)	0.32	1 (2%) 55 45	205, 207, 207, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.70	28 (11%) 6 7	205, 207, 208, 209	0
13	o	243/272 (89%)	0.68	21 (8%) 13 12	205, 207, 208, 209	0
14	T	32/32 (100%)	0.24	3 (9%) 11 10	206, 207, 208, 209	0
14	t	32/32 (100%)	0.62	3 (9%) 11 10	205, 206, 208, 208	0
15	U	97/134 (72%)	0.92	11 (11%) 7 7	205, 207, 208, 208	0
15	u	97/134 (72%)	0.78	10 (10%) 9 9	205, 207, 208, 208	0
16	V	137/163 (84%)	0.29	4 (2%) 55 45	205, 207, 208, 208	0
16	v	137/163 (84%)	0.78	17 (12%) 5 7	206, 207, 208, 208	0
17	g	28/46 (60%)	0.27	1 (3%) 46 39	206, 207, 208, 209	0
17	y	28/46 (60%)	-0.01	0 100 100	206, 207, 208, 208	0
18	X	37/41 (90%)	0.73	6 (16%) 3 4	205, 207, 208, 209	0
18	x	37/41 (90%)	1.03	5 (13%) 4 6	206, 207, 208, 208	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.28	3 (4%) 34 28	205, 207, 208, 209	0
20	z	62/62 (100%)	0.87	9 (14%) 3 5	206, 207, 208, 209	0
All	All	5214/5674 (91%)	0.47	430 (8%) 14 12	204, 207, 208, 209	0

All (430) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	7.6
18	x	11	THR	7.2
13	o	169	LYS	6.5
1	a	239	PHE	6.1
7	H	64	ALA	5.7
3	C	149	TYR	5.4
5	e	84	LYS	5.1
18	x	42	GLN	5.0
1	a	299	GLY	5.0
15	U	38	GLU	4.9
15	U	39	LEU	4.9
3	C	332	GLN	4.9
18	x	12	ILE	4.8
1	A	299	GLY	4.8
4	D	24	ARG	4.7
5	e	82	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	11	ALA	4.7
4	d	295	SER	4.6
14	t	31	LYS	4.4
1	A	138	GLY	4.3
13	o	84	ASN	4.3
2	B	347	ARG	4.3
3	C	147	PHE	4.3
18	X	46	VAL	4.3
18	X	45	LYS	4.2
1	A	179	THR	4.2
13	O	84	ASN	4.2
2	b	490	GLN	4.2
2	b	483	ASP	4.2
3	c	372	PRO	4.1
16	v	47	LEU	4.1
14	t	32	LYS	4.0
1	A	165	GLN	4.0
7	H	2	ALA	4.0
2	b	482	ILE	4.0
7	h	4	ARG	3.9
2	b	228	ALA	3.9
1	A	177	SER	3.9
7	H	63	LYS	3.9
2	b	229	LEU	3.8
4	d	95	PRO	3.8
3	C	44	ASN	3.8
14	T	28	ARG	3.8
18	X	47	GLN	3.8
3	C	148	GLY	3.8
12	M	2	GLU	3.8
3	C	212	TYR	3.8
3	C	151	TRP	3.8
15	U	40	VAL	3.8
3	C	266	TRP	3.7
1	A	14	TRP	3.7
2	b	302	TRP	3.7
2	b	133	LEU	3.7
1	A	12	ASN	3.7
1	a	165	GLN	3.7
16	v	133	LEU	3.7
1	a	282	GLY	3.6
1	A	175	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	10	SER	3.6
2	B	354	LEU	3.6
2	b	305	ILE	3.6
2	B	309	LEU	3.6
1	A	190	HIS	3.6
16	V	47	LEU	3.6
3	c	202	PRO	3.6
16	v	132	ASN	3.6
2	B	353	GLU	3.5
3	c	78	GLU	3.5
2	B	183	PRO	3.5
2	b	393	GLU	3.5
16	v	130	MET	3.5
1	a	191	ASN	3.5
3	C	142	GLU	3.4
15	u	50	ALA	3.4
3	C	46	SER	3.4
3	c	260	ALA	3.4
7	h	66	GLY	3.4
13	O	222	GLN	3.4
2	b	127	ARG	3.4
1	a	201	GLY	3.4
2	B	411	PHE	3.4
16	v	117	VAL	3.4
1	a	240	GLY	3.4
14	t	30	THR	3.4
2	B	120	LEU	3.4
4	D	295	SER	3.3
4	d	236	ASN	3.3
3	C	265	ILE	3.3
3	C	145	SER	3.3
10	k	14	ALA	3.3
12	M	4	ASN	3.3
7	h	14	LEU	3.3
2	B	477	ASP	3.2
7	H	4	ARG	3.2
11	L	33	SER	3.2
13	O	262	GLN	3.2
13	o	168	PHE	3.2
8	I	25	SER	3.2
16	v	51	GLN	3.2
4	D	192	THR	3.2

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Mol	Chain	Res	Type	RSRZ
13	O	234	THR	3.2
3	C	144	SER	3.2
3	c	200	THR	3.2
3	C	261	ARG	3.2
2	b	304	ALA	3.2
1	A	13	LEU	3.2
18	X	42	GLN	3.1
1	a	175	GLY	3.1
3	C	402	GLY	3.1
1	A	294	ALA	3.1
1	a	301	ASN	3.1
4	D	190	ASN	3.1
13	O	50	ASP	3.1
1	A	262	TYR	3.1
4	d	191	TRP	3.1
3	C	267	SER	3.1
1	a	178	GLY	3.1
1	a	190	HIS	3.1
4	d	176	ALA	3.1
13	O	170	GLY	3.1
2	B	185	TRP	3.1
13	O	126	GLY	3.1
4	d	195	PRO	3.1
2	b	398	THR	3.1
3	c	201	ASN	3.0
7	H	3	ARG	3.0
2	B	162	PHE	3.0
1	a	325	ASN	3.0
4	d	255	GLN	3.0
2	B	293	ALA	3.0
7	h	11	LEU	3.0
2	B	84	THR	3.0
7	h	27	THR	3.0
13	O	269	ILE	3.0
13	o	220	LYS	3.0
3	C	45	LEU	3.0
15	u	72	TYR	3.0
2	B	123	PHE	3.0
13	O	223	ILE	3.0
4	D	197	HIS	3.0
16	v	46	THR	3.0
1	A	178	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	127	ARG	2.9
2	B	351	GLY	2.9
13	o	89	ALA	2.9
2	b	120	LEU	2.9
9	J	8	ILE	2.9
4	D	170	ALA	2.9
2	b	491	VAL	2.9
4	d	262	SER	2.9
4	D	297	ASP	2.9
16	v	113	GLU	2.9
7	H	65	LEU	2.9
1	a	179	THR	2.9
13	o	238	ALA	2.9
3	C	139	THR	2.9
13	O	169	LYS	2.8
1	A	15	GLU	2.8
1	A	195	HIS	2.8
12	M	5	GLN	2.8
13	O	47	THR	2.8
2	b	70	GLY	2.8
2	B	70	GLY	2.8
6	F	11	VAL	2.8
7	H	27	THR	2.8
1	a	10	SER	2.8
16	v	44	THR	2.8
2	b	431	GLU	2.8
3	C	140	LEU	2.8
1	a	198	HIS	2.8
12	m	1	MET	2.8
15	u	57	LEU	2.8
7	H	6	TRP	2.8
1	a	171	GLY	2.7
2	b	194	ASN	2.7
2	b	298	LEU	2.7
4	D	171	PRO	2.7
4	D	198	MET	2.7
13	O	58	ILE	2.7
3	C	143	TYR	2.7
1	A	137	LEU	2.7
15	u	58	ASN	2.7
1	a	137	LEU	2.7
2	B	164	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	c	261	ARG	2.7
2	B	295	GLY	2.7
2	B	121	GLU	2.7
2	B	410	THR	2.7
2	b	412	THR	2.7
4	d	197	HIS	2.7
4	d	239	GLN	2.7
2	B	402	TYR	2.7
2	b	411	PHE	2.7
2	B	352	GLU	2.7
13	O	79	LYS	2.7
7	h	64	ALA	2.7
3	C	262	ARG	2.7
2	b	303	SER	2.6
2	b	297	THR	2.6
1	a	16	ARG	2.6
3	C	137	PRO	2.6
4	D	191	TRP	2.6
15	U	45	GLU	2.6
18	X	13	THR	2.6
10	k	17	ILE	2.6
20	z	1	MET	2.6
15	u	70	GLY	2.6
3	C	263	ALA	2.6
1	a	200	LEU	2.6
4	d	199	MET	2.6
2	b	125	ASP	2.6
1	a	170	ASP	2.6
13	o	170	GLY	2.6
2	B	294	SER	2.6
3	C	184	GLY	2.6
3	c	389	GLU	2.6
15	u	51	TYR	2.6
13	o	225	LEU	2.6
2	b	301	ALA	2.6
1	a	172	MET	2.5
2	B	83	GLU	2.5
18	x	16	LEU	2.5
2	b	349	LYS	2.5
7	h	9	ASP	2.5
10	k	15	TYR	2.5
2	b	484	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
7	h	23	PRO	2.5
10	k	13	GLU	2.5
1	a	138	GLY	2.5
20	z	4	LEU	2.5
13	O	261	ILE	2.5
2	B	122	LEU	2.5
7	h	16	SER	2.5
15	U	65	PHE	2.5
8	I	35	LYS	2.5
15	U	122	VAL	2.5
3	C	155	ASN	2.5
13	o	111	LEU	2.5
7	h	26	GLY	2.5
2	b	217	ILE	2.5
3	C	268	GLY	2.5
20	z	29	SER	2.5
2	b	394	GLN	2.5
16	V	43	LYS	2.5
13	o	31	LEU	2.5
3	c	264	PHE	2.5
13	o	112	LYS	2.5
1	A	196	PRO	2.5
4	d	221	THR	2.5
16	v	131	ARG	2.5
3	c	373	ASN	2.5
13	O	220	LYS	2.5
16	v	92	ARG	2.5
1	a	25	ASP	2.4
2	B	326	ARG	2.4
2	b	409	GLN	2.4
2	B	69	LEU	2.4
1	a	286	THR	2.4
13	O	76	PHE	2.4
1	a	224	ILE	2.4
1	A	298	ASN	2.4
7	h	13	PRO	2.4
4	d	201	VAL	2.4
20	z	7	LEU	2.4
1	A	181	ASN	2.4
11	L	37	ASN	2.4
16	v	78	LEU	2.4
20	Z	62	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
14	T	27	PRO	2.4
14	T	3	THR	2.4
15	U	117	VAL	2.4
8	I	34	ARG	2.4
4	D	199	MET	2.4
16	v	114	ILE	2.4
1	a	298	ASN	2.4
3	c	457	LYS	2.4
13	O	219	THR	2.4
12	M	34	LYS	2.4
2	b	185	TRP	2.4
7	h	53	LEU	2.4
13	o	237	ILE	2.4
1	a	19	ASN	2.4
3	c	388	GLN	2.4
2	B	345	VAL	2.4
2	B	132	ALA	2.4
2	B	133	LEU	2.4
4	d	194	ASN	2.4
15	u	102	LYS	2.3
1	A	76	ASN	2.3
2	b	421	ALA	2.3
1	A	201	GLY	2.3
13	O	162	ILE	2.3
13	o	258	GLU	2.3
1	a	296	ASN	2.3
15	u	65	PHE	2.3
11	l	1	MET	2.3
15	U	121	LEU	2.3
20	Z	1	MET	2.3
4	D	195	PRO	2.3
13	o	229	LYS	2.3
2	B	161	LEU	2.3
1	a	225	ARG	2.3
2	b	69	LEU	2.3
20	z	28	ALA	2.3
15	u	114	VAL	2.3
2	B	166	MET	2.3
8	I	3	THR	2.3
2	b	219	VAL	2.3
1	A	286	THR	2.3
3	c	402	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	c	403	SER	2.3
3	C	258	GLY	2.3
3	C	146	PHE	2.3
13	O	243	SER	2.3
5	E	21	VAL	2.3
1	A	266	ASN	2.3
13	o	164	THR	2.3
3	c	430	HIS	2.3
2	B	475	PHE	2.3
3	c	199	ILE	2.3
15	u	38	GLU	2.3
2	b	188	ASP	2.3
2	B	301	ALA	2.3
13	O	46	PRO	2.3
13	O	235	GLY	2.3
3	c	204	LEU	2.3
11	L	1	MET	2.3
4	d	297	ASP	2.3
1	a	287	ALA	2.3
3	c	180	MET	2.2
18	X	12	ILE	2.2
1	a	236	GLY	2.2
2	b	402	TYR	2.2
2	b	232	GLY	2.2
1	a	150	PRO	2.2
2	B	292	LEU	2.2
3	c	263	ALA	2.2
2	B	476	ARG	2.2
7	h	18	TYR	2.2
3	C	183	GLY	2.2
2	b	489	GLU	2.2
2	b	379	ALA	2.2
20	z	3	ILE	2.2
2	B	179	GLN	2.2
3	C	403	SER	2.2
20	Z	57	LEU	2.2
2	b	396	GLY	2.2
20	z	2	THR	2.2
13	O	242	GLU	2.2
4	D	282	SER	2.2
1	a	278	TRP	2.2
5	E	17	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	465	PRO	2.2
3	c	405	ASN	2.2
10	k	12	PRO	2.2
3	c	472	LEU	2.2
4	D	177	ALA	2.2
4	D	307	GLU	2.2
13	o	64	TYR	2.2
1	a	11	ALA	2.2
15	U	44	ASP	2.2
1	A	230	THR	2.2
7	h	5	THR	2.2
4	D	194	ASN	2.2
2	B	399	VAL	2.2
20	z	60	PHE	2.2
13	O	224	SER	2.1
17	g	27	MET	2.1
2	b	410	THR	2.1
7	H	62	TRP	2.1
3	c	203	THR	2.1
1	a	322	ASN	2.1
3	C	415	ASN	2.1
15	U	74	THR	2.1
1	A	171	GLY	2.1
20	z	6	GLN	2.1
2	b	119	ASP	2.1
3	c	340	TYR	2.1
15	U	55	ILE	2.1
13	o	120	THR	2.1
1	a	285	PHE	2.1
13	O	225	LEU	2.1
13	o	91	PHE	2.1
13	o	61	SER	2.1
3	c	149	TYR	2.1
3	C	201	ASN	2.1
13	O	91	PHE	2.1
16	v	45	ILE	2.1
16	v	36	VAL	2.1
13	o	110	GLU	2.1
1	a	24	THR	2.1
13	O	51	THR	2.1
3	C	203	THR	2.1
6	f	11	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	303	ASN	2.1
2	b	166	MET	2.1
1	A	166	GLY	2.1
13	o	154	SER	2.1
1	a	153	SER	2.1
2	b	126	PRO	2.1
13	O	119	LEU	2.1
3	C	200	THR	2.1
2	b	178	VAL	2.1
3	c	259	TRP	2.1
3	c	411	ALA	2.1
2	b	395	GLN	2.1
1	a	100	ALA	2.1
3	C	197	ARG	2.1
1	A	192	ILE	2.0
3	C	269	GLU	2.0
1	a	139	MET	2.0
2	B	184	GLU	2.0
3	c	329	GLY	2.0
2	b	218	LEU	2.0
13	O	168	PHE	2.0
1	A	75	ASN	2.0
16	V	39	ASN	2.0
2	b	338	GLN	2.0
1	a	173	PRO	2.0
4	D	95	PRO	2.0
18	x	13	THR	2.0
1	a	181	ASN	2.0
16	V	49	GLU	2.0
4	d	136	VAL	2.0
4	D	174	GLY	2.0
16	v	103	LYS	2.0
1	a	187	GLN	2.0
16	v	138	LEU	2.0
1	A	156	ALA	2.0
2	B	155	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
31	LMT	i	102	35/35	0.31	1.62	13.57	206,208,209,210	0
27	LMG	C	518	45/55	0.61	0.98	6.09	205,206,208,208	0
23	PL9	J	101	35/55	0.24	0.59	5.85	204,207,208,209	0
24	BCR	C	513	40/40	0.89	0.83	5.85	205,206,207,208	0
23	PL9	j	101	35/55	0.26	0.49	5.81	205,208,209,209	0
24	BCR	a	410	40/40	0.81	0.70	5.59	205,206,207,207	0
24	BCR	c	521	40/40	0.79	1.36	5.43	205,207,208,209	0
24	BCR	b	623	40/40	0.69	0.82	5.26	204,206,207,207	0
24	BCR	B	619	40/40	0.73	0.94	4.84	205,206,207,207	0
33	BCT	d	403	4/4	0.77	1.00	4.36	207,207,207,208	0
24	BCR	y	101	40/40	0.73	0.81	4.08	205,206,207,207	0
27	LMG	c	518	45/55	0.66	0.96	3.91	206,207,208,208	0
22	CLA	a	408	65/65	0.78	0.76	3.85	205,206,207,209	0
24	BCR	c	513	40/40	0.78	1.04	3.83	204,206,207,208	0
25	DGD	D	409	63/66	0.68	0.82	3.61	205,208,209,211	0
22	CLA	b	605	65/65	0.50	1.07	3.60	205,208,209,209	0
31	LMT	I	102	35/35	0.38	0.89	3.50	205,207,209,210	0
22	CLA	B	601	65/65	0.61	1.07	3.47	206,207,208,209	0
31	LMT	b	627	35/35	0.69	1.25	3.32	205,208,210,210	0
24	BCR	g	101	40/40	0.51	0.74	3.29	204,206,207,207	0
22	CLA	B	609	65/65	0.90	0.68	3.09	205,206,208,208	0
22	CLA	D	405	65/65	0.86	0.62	3.09	205,206,207,207	0
24	BCR	H	102	40/40	0.69	1.01	3.02	206,207,208,208	0
31	LMT	D	410	31/35	0.74	0.76	2.76	206,208,208,209	0
25	DGD	B	625	52/66	0.71	0.65	2.75	205,208,210,210	0
24	BCR	f	102	40/40	0.60	0.47	2.74	206,206,207,208	0
31	LMT	B	624	35/35	0.79	0.56	2.72	205,207,210,210	0
30	SQD	B	626	47/54	0.66	0.68	2.64	204,207,209,211	0
22	CLA	b	607	65/65	0.80	0.56	2.63	205,206,207,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	B	603	65/65	0.74	0.55	2.56	204,206,207,208	0
25	DGD	d	409	63/66	0.70	0.77	2.52	205,208,210,211	0
22	CLA	b	606	65/65	0.83	0.77	2.51	205,206,207,207	0
24	BCR	F	102	40/40	0.58	0.52	2.44	205,206,207,208	0
22	CLA	B	611	65/65	0.88	0.51	2.34	204,206,207,208	0
22	CLA	B	604	65/65	0.86	0.66	2.33	205,207,208,208	0
22	CLA	c	501	65/65	0.84	0.63	2.31	205,207,208,209	0
22	CLA	c	512	65/65	0.75	0.72	2.28	205,207,208,208	0
24	BCR	K	102	40/40	0.77	0.95	2.26	204,207,208,209	0
22	CLA	A	405	65/65	0.79	0.65	2.24	204,206,208,208	0
30	SQD	d	402	43/54	0.65	1.13	2.19	205,207,209,211	0
27	LMG	e	101	44/55	0.74	0.42	2.17	204,207,208,209	0
27	LMG	M	101	42/55	0.74	0.49	2.04	205,207,209,210	0
24	BCR	A	407	40/40	0.78	0.56	2.01	205,206,207,208	0
27	LMG	D	411	46/55	0.75	0.42	1.99	205,206,207,208	0
24	BCR	c	514	40/40	0.72	0.86	1.98	205,206,207,208	0
27	LMG	E	101	44/55	0.39	0.77	1.97	204,207,209,210	0
22	CLA	b	613	65/65	0.77	0.87	1.95	205,207,208,209	0
22	CLA	c	511	65/65	0.86	0.75	1.90	205,207,208,209	0
30	SQD	a	401	54/54	0.85	0.50	1.88	205,207,209,211	0
22	CLA	B	608	65/65	0.88	0.62	1.84	205,207,208,209	0
22	CLA	c	506	65/65	0.86	0.73	1.79	206,207,208,208	0
22	CLA	B	614	65/65	0.86	0.89	1.77	205,206,207,208	0
22	CLA	C	506	65/65	0.74	0.86	1.77	204,207,207,208	0
22	CLA	b	608	65/65	0.86	0.61	1.76	205,206,207,208	0
22	CLA	c	510	65/65	0.71	0.61	1.75	206,207,208,209	0
22	CLA	c	508	65/65	0.80	0.55	1.70	205,207,208,208	0
22	CLA	C	511	65/65	0.84	1.13	1.69	205,207,208,208	0
24	BCR	C	514	40/40	0.70	0.86	1.66	205,206,207,207	0
27	LMG	a	402	42/55	0.56	0.47	1.62	204,207,209,209	0
27	LMG	m	101	42/55	0.74	0.58	1.55	203,207,208,209	0
22	CLA	c	503	65/65	0.77	0.59	1.55	205,207,208,208	0
25	DGD	b	601	52/66	0.79	0.46	1.49	204,207,208,209	0
31	LMT	d	410	31/35	0.52	0.72	1.45	206,208,209,210	0
30	SQD	F	103	45/54	0.70	0.85	1.41	205,207,209,210	0
34	HEM	F	101	43/43	0.90	0.54	1.41	205,207,208,209	0
31	LMT	B	627	35/35	0.76	0.60	1.37	205,207,209,209	0
22	CLA	C	512	65/65	0.77	0.93	1.34	205,207,208,209	0
22	CLA	d	405	65/65	0.81	0.51	1.33	204,206,207,208	0
31	LMT	b	603	35/35	0.67	0.56	1.33	205,207,208,209	0
22	CLA	B	605	65/65	0.83	0.80	1.33	205,206,207,208	0
22	CLA	c	502	65/65	0.54	0.65	1.33	205,207,208,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	BCR	B	616	40/40	0.60	0.54	1.32	205,206,207,207	0
22	CLA	b	609	65/65	0.86	0.64	1.30	205,207,208,209	0
24	BCR	B	617	40/40	0.71	0.43	1.28	204,206,207,208	0
22	CLA	C	503	65/65	0.84	0.45	1.28	205,207,207,208	0
22	CLA	C	501	65/65	0.90	0.46	1.25	205,206,207,208	0
30	SQD	f	103	45/54	0.86	0.60	1.24	205,207,208,210	0
22	CLA	h	101	65/65	0.87	0.52	1.23	204,207,208,209	0
27	LMG	A	415	42/55	0.60	0.45	1.22	204,207,208,209	0
22	CLA	b	615	65/65	0.89	0.37	1.21	205,206,207,208	0
23	PL9	A	406	45/55	0.52	0.53	1.14	205,206,207,208	0
22	CLA	C	508	65/65	0.79	0.85	1.13	205,206,207,208	0
31	LMT	b	604	35/35	0.69	0.48	1.08	205,207,209,209	0
22	CLA	C	502	65/65	0.73	0.50	1.04	205,206,207,208	0
31	LMT	B	628	35/35	0.65	0.51	1.01	204,207,209,209	0
24	BCR	J	102	40/40	0.52	0.37	0.97	205,207,208,209	0
22	CLA	B	615	65/65	0.86	0.80	0.97	205,206,208,208	0
34	HEM	V	201	43/43	0.88	0.50	0.95	203,206,207,208	0
25	DGD	A	408	56/66	0.63	0.50	0.93	206,207,209,210	0
27	LMG	d	411	46/55	0.88	0.30	0.91	204,206,207,208	0
22	CLA	B	613	65/65	0.72	0.50	0.90	205,206,207,208	0
22	CLA	b	616	65/65	0.95	0.34	0.90	204,206,208,209	0
22	CLA	B	602	65/65	0.92	0.52	0.86	204,206,208,209	0
34	HEM	v	201	43/43	0.87	0.71	0.84	205,207,207,208	0
22	CLA	B	607	65/65	0.86	0.43	0.83	205,206,207,209	0
22	CLA	b	619	65/65	0.69	0.78	0.82	205,207,208,209	0
27	LMG	l	101	51/55	0.70	0.40	0.81	205,206,208,208	0
22	CLA	c	505	65/65	0.85	0.56	0.78	204,206,208,208	0
24	BCR	x	101	40/40	0.62	0.88	0.78	205,207,208,208	0
22	CLA	b	618	65/65	0.83	0.77	0.76	205,207,208,208	0
26	LHG	c	519	37/49	0.66	0.36	0.69	205,207,211,214	0
30	SQD	B	622	43/54	0.80	0.46	0.68	205,207,209,212	0
22	CLA	b	611	65/65	0.86	0.43	0.68	205,206,207,208	0
23	PL9	a	409	45/55	0.73	0.36	0.67	204,206,207,208	0
30	SQD	b	602	47/54	0.77	0.39	0.67	205,207,209,212	0
22	CLA	C	505	65/65	0.79	0.56	0.65	205,206,207,208	0
30	SQD	A	414	54/54	0.83	0.40	0.64	204,207,208,210	0
22	CLA	b	612	65/65	0.87	0.60	0.63	205,206,207,209	0
22	CLA	b	617	65/65	0.81	0.41	0.59	205,206,208,209	0
22	CLA	C	510	65/65	0.83	0.49	0.56	205,206,207,208	0
34	HEM	f	101	43/43	0.92	0.30	0.40	206,207,207,208	0
24	BCR	b	621	40/40	0.78	0.34	0.40	204,206,207,207	0
24	BCR	b	622	40/40	0.83	0.31	0.38	204,206,207,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	BCR	B	618	40/40	0.87	0.29	0.38	204,205,207,207	0
27	LMG	C	521	48/55	0.73	0.34	0.36	204,206,207,208	0
24	BCR	j	102	40/40	0.68	0.29	0.34	206,207,209,209	0
22	CLA	H	101	65/65	0.84	0.41	0.29	205,206,207,208	0
22	CLA	b	614	65/65	0.91	0.30	0.29	205,206,207,208	0
22	CLA	a	404	65/65	0.83	0.58	0.26	205,206,207,208	0
27	LMG	d	408	48/55	0.75	0.40	0.25	204,206,207,208	0
22	CLA	A	403	65/65	0.89	0.58	0.24	204,206,207,207	0
22	CLA	a	405	65/65	0.81	0.58	0.20	202,206,207,208	0
25	DGD	a	411	56/66	0.74	0.36	0.14	205,207,209,209	0
22	CLA	c	509	65/65	0.86	0.37	0.14	204,206,208,209	0
30	SQD	A	413	51/54	0.76	0.33	0.12	205,207,208,208	0
22	CLA	C	504	65/65	0.83	0.39	0.10	205,206,207,207	0
24	BCR	b	620	40/40	0.92	0.34	0.09	205,206,207,208	0
22	CLA	c	504	65/65	0.85	0.33	0.08	205,207,208,208	0
25	DGD	b	624	58/66	0.85	0.34	0.06	205,206,207,208	0
27	LMG	c	522	48/55	0.81	0.29	0.02	205,206,207,208	0
23	PL9	D	406	55/55	0.57	0.43	-0.05	204,206,207,207	0
32	PHO	d	401	64/64	0.70	0.43	-0.06	204,206,207,207	0
22	CLA	A	402	65/65	0.90	0.45	-0.06	205,206,207,208	0
22	CLA	c	507	65/65	0.89	0.31	-0.10	205,207,208,208	0
25	DGD	c	515	53/66	0.88	0.37	-0.16	205,207,208,209	0
22	CLA	C	509	65/65	0.87	0.35	-0.17	205,206,207,208	0
30	SQD	a	415	51/54	0.81	0.30	-0.18	205,206,208,208	0
22	CLA	C	507	65/65	0.88	0.30	-0.26	205,206,208,210	0
33	BCT	D	403	4/4	0.93	0.38	-0.31	206,206,206,206	0
25	DGD	C	517	66/66	0.67	0.36	-0.33	205,206,207,208	0
23	PL9	d	406	55/55	0.68	0.37	-0.36	204,206,207,208	0
32	PHO	D	402	64/64	0.77	0.34	-0.37	205,206,207,208	0
27	LMG	A	410	51/55	0.80	0.32	-0.41	204,206,207,208	0
25	DGD	B	620	58/66	0.87	0.31	-0.45	203,206,208,209	0
26	LHG	A	409	39/49	0.90	0.28	-0.46	205,206,208,209	0
29	OEX	A	412	10/10	0.96	0.44	-0.46	198,204,206,206	0
29	OEX	a	414	10/10	0.95	0.48	-0.46	198,203,205,207	0
26	LHG	C	519	37/49	0.73	0.38	-0.50	204,207,210,212	0
27	LMG	D	408	48/55	0.90	0.26	-0.50	202,206,208,208	0
32	PHO	a	407	64/64	0.82	0.28	-0.55	205,207,207,208	0
22	CLA	d	404	65/65	0.82	0.40	-0.55	204,206,207,207	0
32	PHO	D	401	64/64	0.82	0.32	-0.56	203,206,207,208	0
22	CLA	B	610	65/65	0.86	0.33	-0.59	205,206,207,207	0
25	DGD	c	517	66/66	0.77	0.31	-0.63	204,206,207,208	0
22	CLA	B	612	65/65	0.91	0.28	-0.63	204,206,207,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	c	520	65/65	0.90	0.27	-0.66	205,207,207,208	0
22	CLA	a	406	65/65	0.79	0.35	-0.67	205,207,208,209	0
26	LHG	a	412	39/49	0.81	0.28	-0.69	205,207,208,210	0
22	CLA	D	404	65/65	0.90	0.38	-0.69	203,206,207,208	0
22	CLA	A	404	65/65	0.86	0.35	-0.71	204,206,207,208	0
25	DGD	C	515	53/66	0.89	0.27	-0.76	204,206,207,208	0
22	CLA	C	520	65/65	0.81	0.30	-0.77	205,207,208,209	0
31	LMT	M	103	35/35	0.79	0.40	-0.81	205,206,208,210	0
31	LMT	M	102	35/35	0.68	0.39	-0.82	205,207,208,209	0
22	CLA	b	610	65/65	0.86	0.30	-0.91	205,206,207,208	0
27	LMG	b	625	49/55	0.78	0.29	-1.02	205,206,207,208	0
25	DGD	C	516	62/66	0.84	0.26	-1.13	204,206,208,208	0
22	CLA	B	606	65/65	0.90	0.28	-1.14	205,206,207,208	0
25	DGD	c	516	62/66	0.88	0.25	-1.16	205,207,208,209	0
27	LMG	D	407	49/55	0.78	0.27	-1.17	205,206,207,208	0
27	LMG	d	407	49/55	0.92	0.24	-1.22	205,206,207,207	0
28	CL	A	411	1/1	0.85	0.27	-1.26	207,207,207,207	0
21	FE2	a	403	1/1	0.78	0.28	-1.31	211,211,211,211	0
27	LMG	B	621	49/55	0.85	0.26	-1.46	204,206,207,208	0
28	CL	a	413	1/1	0.81	0.20	-3.00	204,204,204,204	0
21	FE2	A	401	1/1	0.88	0.17	-3.33	206,206,206,206	0
27	LMG	i	101	43/55	0.77	0.79	-	205,207,209,209	0
31	LMT	b	626	35/35	0.62	0.61	-	205,208,210,210	0
31	LMT	B	623	35/35	0.64	0.79	-	205,208,209,210	0
35	CA	k	101	1/1	0.55	0.23	-	204,204,204,204	0
35	CA	K	101	1/1	0.51	0.36	-	210,210,210,210	0
35	CA	o	301	1/1	0.55	1.07	-	209,209,209,209	0
35	CA	O	301	1/1	0.44	0.28	-	207,207,207,207	0
27	LMG	I	101	43/55	0.68	0.94	-	204,207,209,210	0

6.5 Other polymers (i)

There are no such residues in this entry.