Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:46 PM GMT

PDB ID	:	4TNI
Title	:	RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 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	:	4.60 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 (i)) were used in the production of this report:

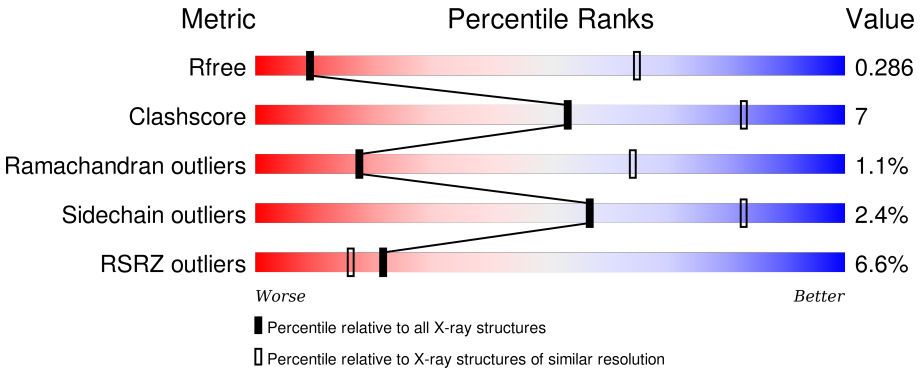
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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 4.60 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	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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% 70% 25%
1	a	344	10% 95%
2	B	510	5% 76% 19%
2	b	510	7% 94%

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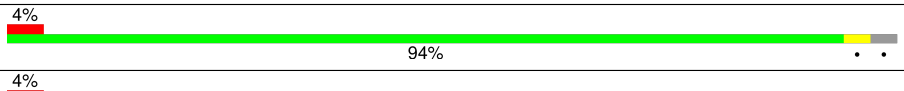
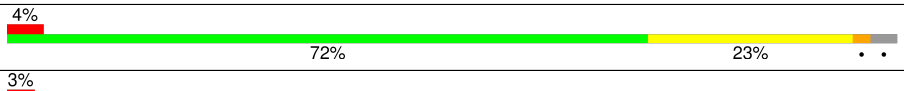
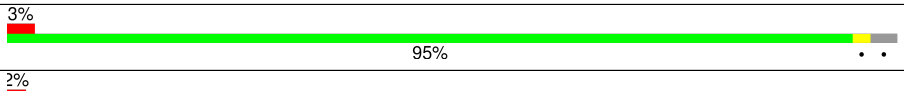
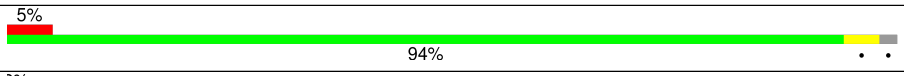
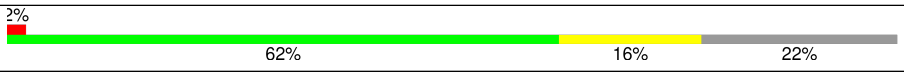
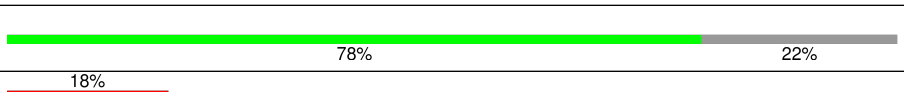
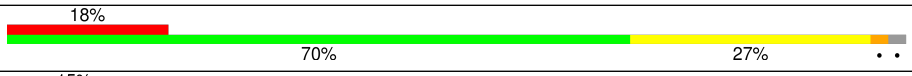
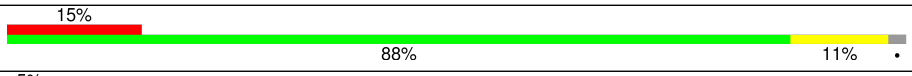
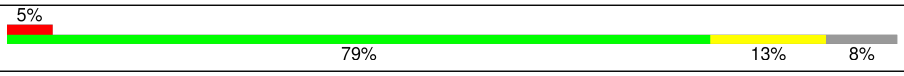
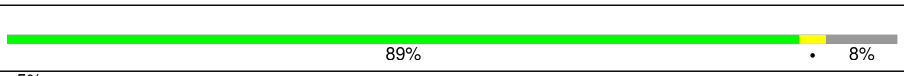
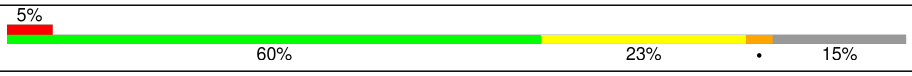
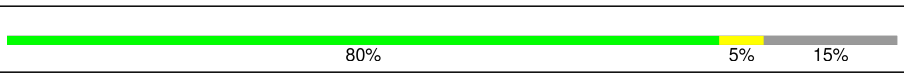
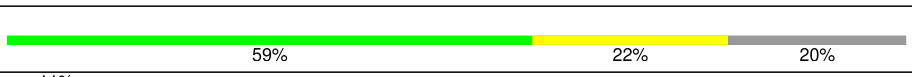
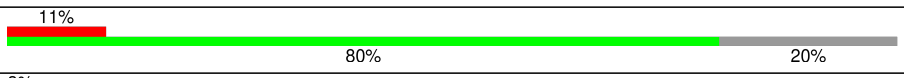
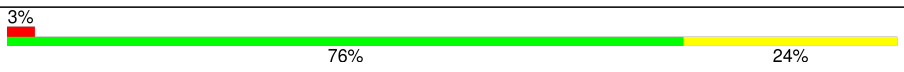
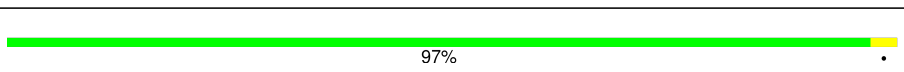
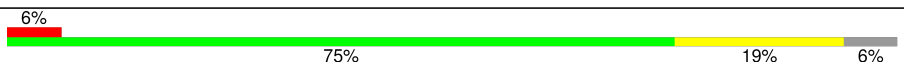
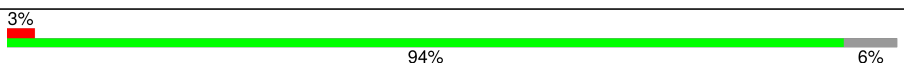
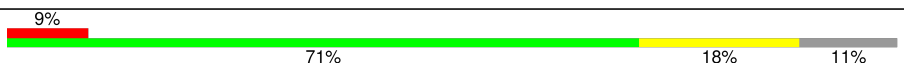
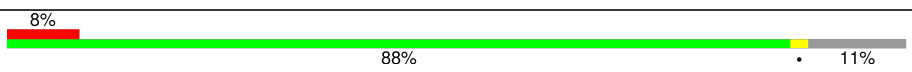
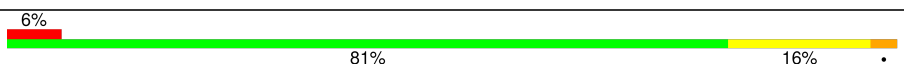
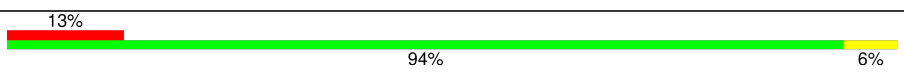
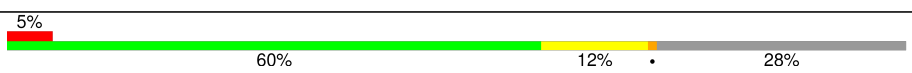
Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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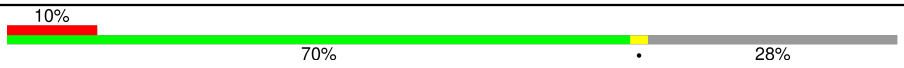
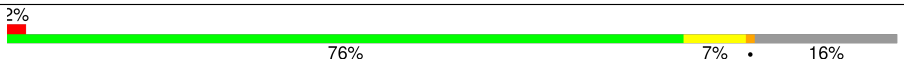
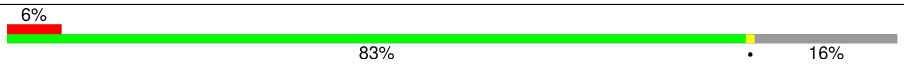
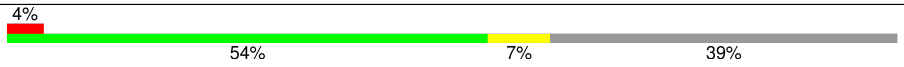
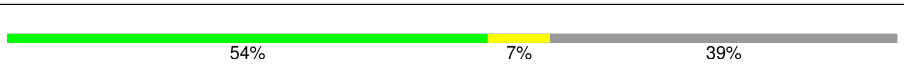
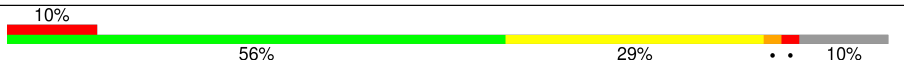
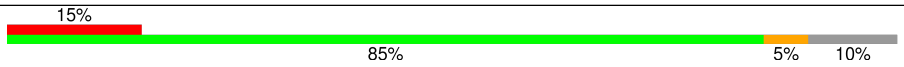
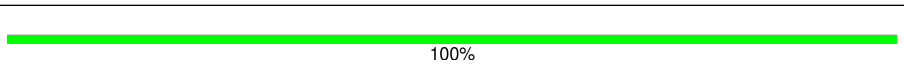
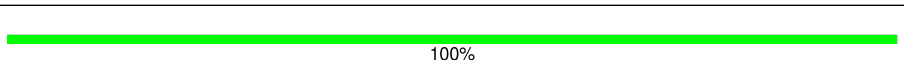
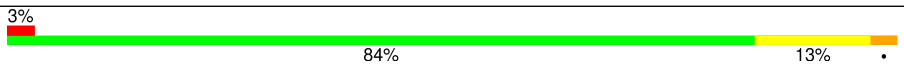
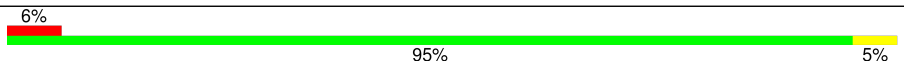
Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

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	-	-	-
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	405	X	-	-	-
22	CLA	D	406	X	-	-	X
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	X	-	-	-
22	CLA	a	407	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	-	-	-
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	405	X	-	-	X
22	CLA	d	406	X	-	-	X
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	d	407	-	-	-	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	J	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	409	-	-	-	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	C	517	-	-	-	X
25	DGD	D	410	-	-	-	X
25	DGD	a	410	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	410	-	-	-	X
27	LMG	A	414	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	m	101	-	-	-	X
28	OEX	A	411	-	-	-	X
28	OEX	a	414	-	-	-	X
29	SQD	B	622	-	-	-	X
29	SQD	B	626	-	-	-	X
29	SQD	F	103	-	-	-	X
29	SQD	a	401	-	-	-	X
29	SQD	b	602	-	-	-	X
29	SQD	d	403	-	-	-	X
29	SQD	f	103	-	-	-	X
30	LMT	B	624	-	-	-	X
30	LMT	B	627	-	-	-	X
30	LMT	B	628	-	-	-	X
30	LMT	D	411	-	-	-	X
30	LMT	I	102	-	-	-	X
30	LMT	M	103	-	-	-	X
30	LMT	b	603	-	-	-	X
30	LMT	b	604	-	-	-	X
30	LMT	b	627	-	-	-	X
30	LMT	d	411	-	-	-	X
30	LMT	i	102	-	-	-	X
31	PHO	d	401	-	-	-	X
32	CL	a	413	-	-	-	X
34	HEM	F	101	-	-	-	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 666	C 434	N 108	O 124	0	0	0
5	e	82	Total 666	C 434	N 108	O 124	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	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			

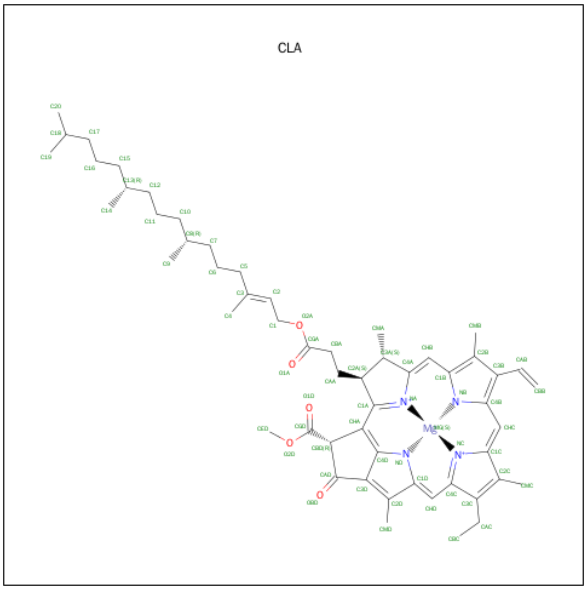
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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
			Total	C	Mg	N	O		
22	C	1	65	55	1	4	5	0	0
22	D	1	65	55	1	4	5	0	0
22	D	1	65	55	1	4	5	0	0
22	H	1	65	55	1	4	5	0	0
22	a	1	65	55	1	4	5	0	0
22	a	1	65	55	1	4	5	0	0
22	a	1	65	55	1	4	5	0	0
22	a	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0
22	b	1	65	55	1	4	5	0	0

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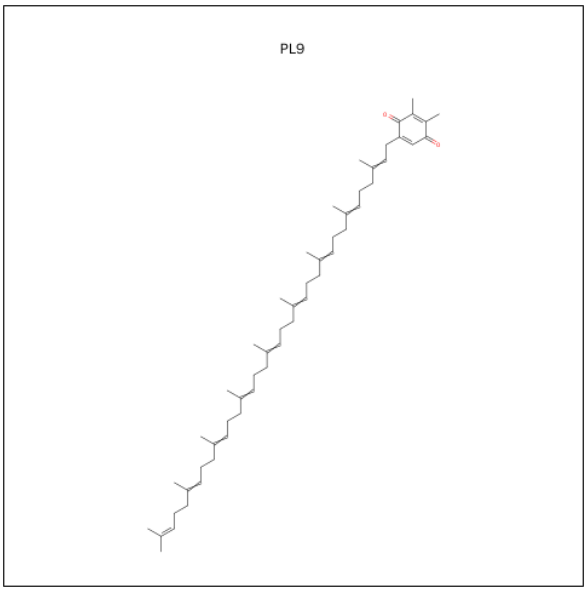
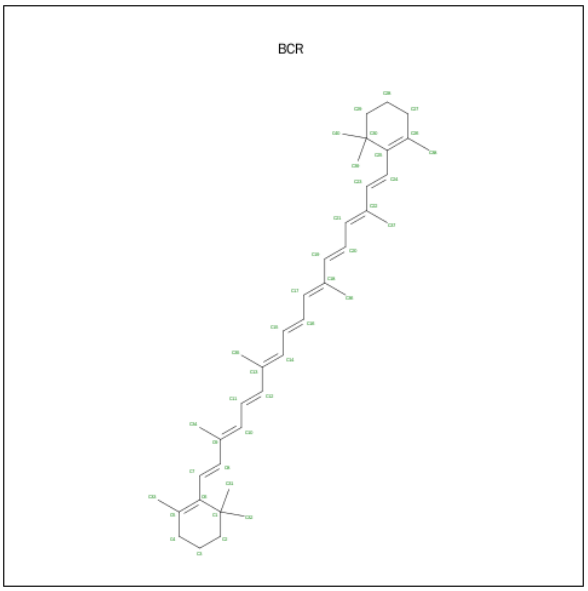
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	b	1	Total C Mg N O 65 55 1 4 5	0	0
22	b	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 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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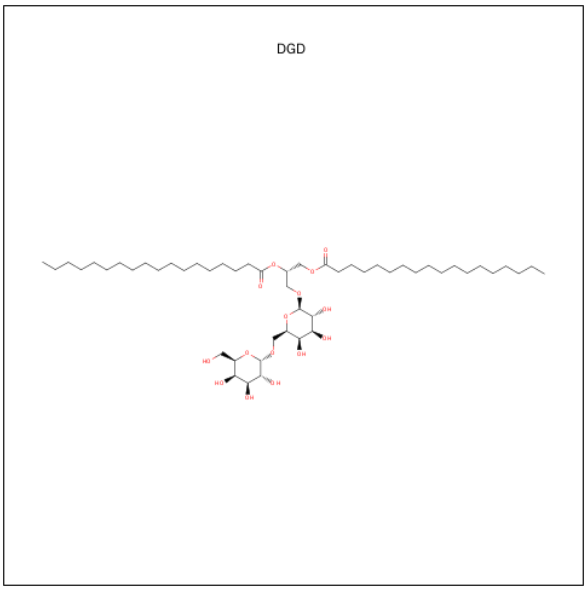
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- 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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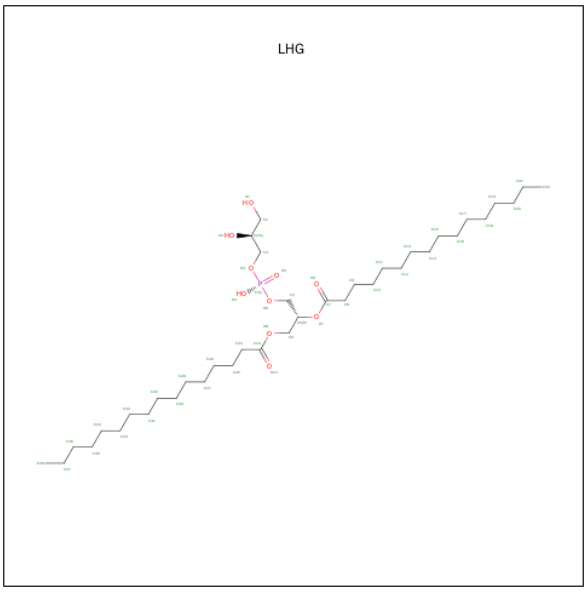
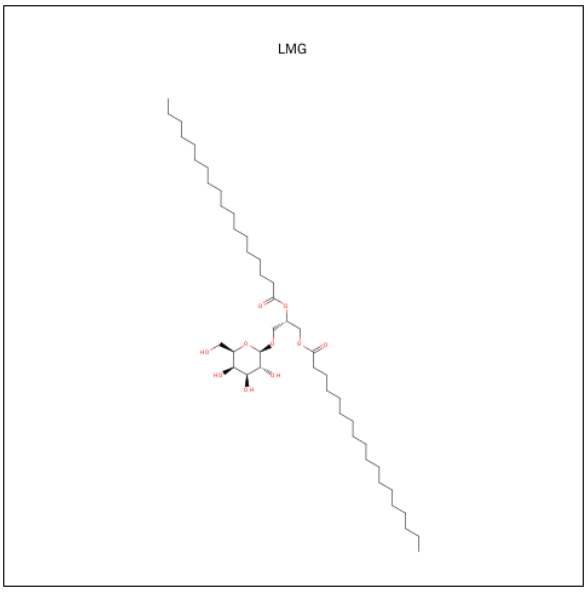
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 58 43 15	0	0
25	B	1	Total C O 52 37 15	0	0
25	C	1	Total C O 53 38 15	0	0
25	C	1	Total C O 62 47 15	0	0
25	C	1	Total C O 66 51 15	0	0
25	D	1	Total C O 63 48 15	0	0
25	a	1	Total C O 56 41 15	0	0
25	b	1	Total C O 52 37 15	0	0
25	b	1	Total C O 58 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: $C_{38}H_{75}O_{10}P$).



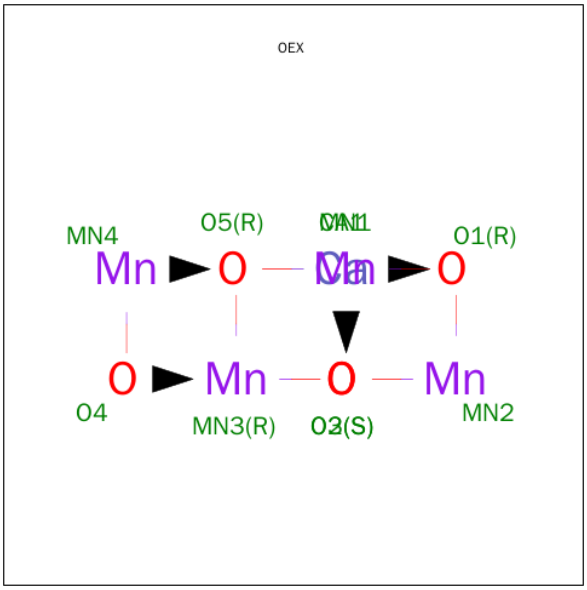
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

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



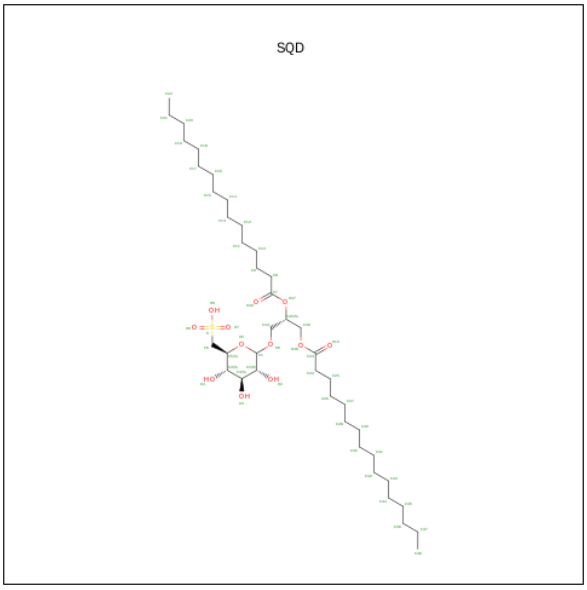
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 51 41 10	0	0
27	A	1	Total C O 42 32 10	0	0
27	B	1	Total C O 49 39 10	0	0
27	C	1	Total C O 45 35 10	0	0
27	C	1	Total C O 48 38 10	0	0
27	D	1	Total C O 49 39 10	0	0
27	D	1	Total C O 48 38 10	0	0
27	D	1	Total C O 46 36 10	0	0
27	E	1	Total C O 44 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	a	1	Total C O 51 41 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

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



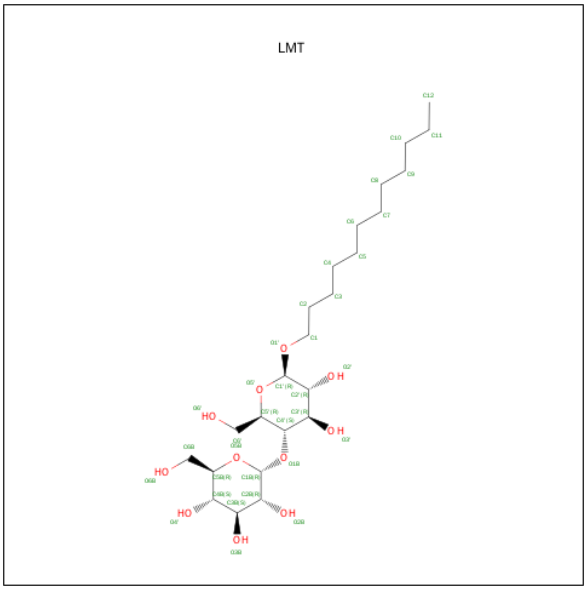
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 29 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
29	A	1	Total	C	O	S	0	0
			51	38	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			43	30	12	1		
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	F	1	Total	C	O	S	0	0
			45	32	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O	S	0	0
			51	38	12	1		
29	b	1	Total	C	O	S	0	0
			47	34	12	1		
29	d	1	Total	C	O	S	0	0
			43	30	12	1		
29	f	1	Total	C	O	S	0	0
			45	32	12	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		

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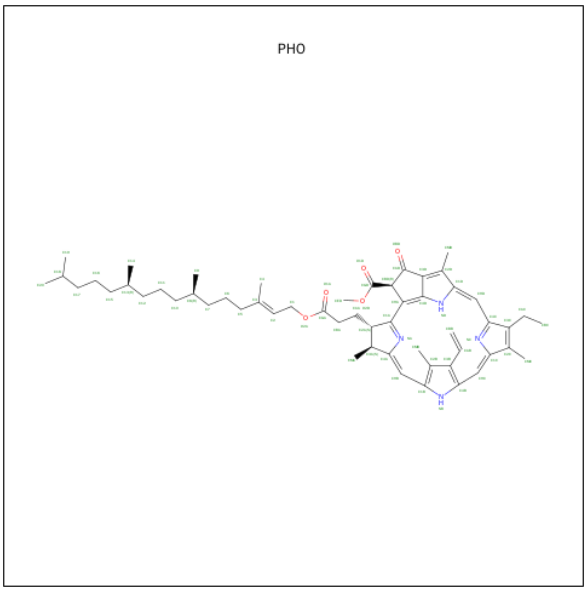
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total C O 35 24 11	0	0
30	B	1	Total C O 35 24 11	0	0
30	B	1	Total C O 35 24 11	0	0
30	D	1	Total C O 31 20 11	0	0
30	I	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	b	1	Total C O 35 24 11	0	0
30	b	1	Total C O 35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

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).

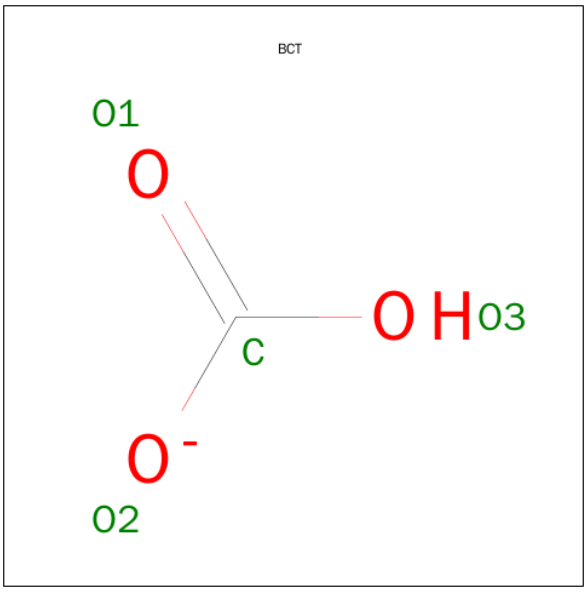


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	D	1	Total C N O 64 55 4 5	0	0
31	D	1	Total C N O 64 55 4 5	0	0
31	d	1	Total C N O 64 55 4 5	0	0
31	d	1	Total C N O 64 55 4 5	0	0

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

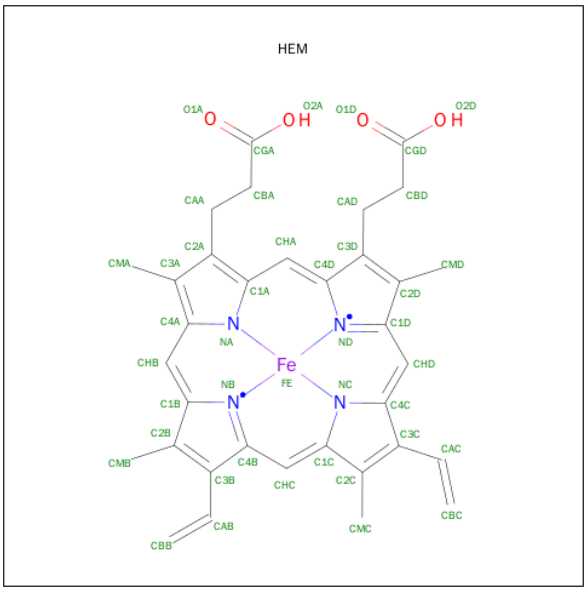
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total Cl 1 1	0	0
32	D	1	Total Cl 1 1	0	0

- 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

Continued on next page...

Continued from previous page...

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

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

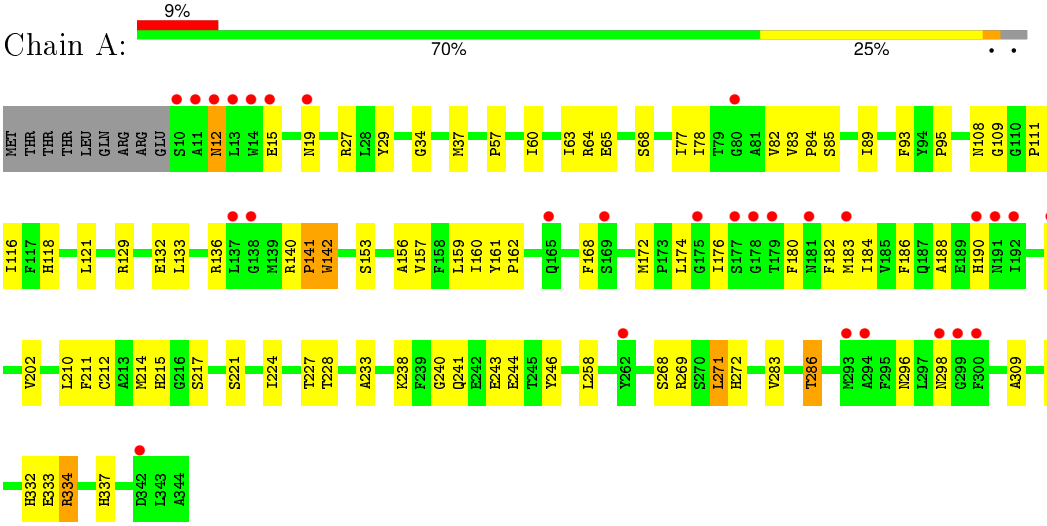
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	K	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		

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.

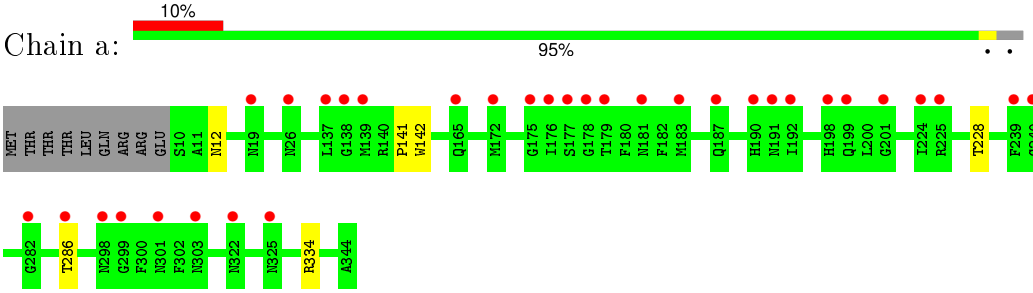
- Molecule 1: Photosystem Q(B) protein 1

Chain A:



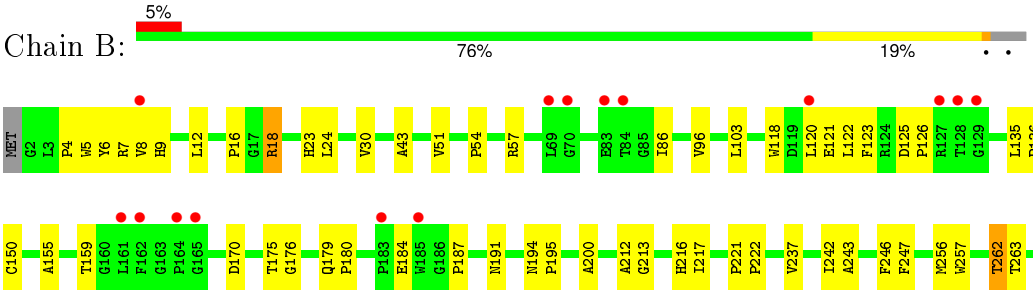
- Molecule 1: Photosystem Q(B) protein 1

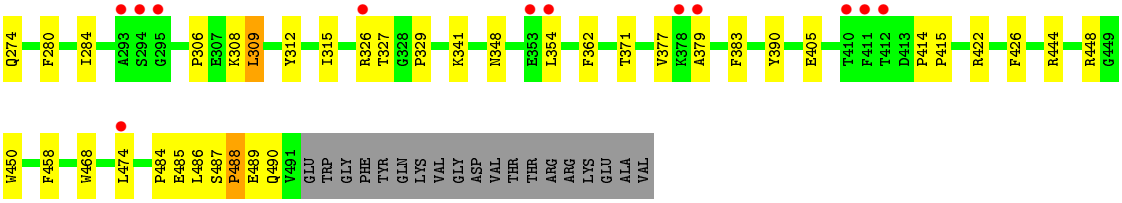
Chain a:



- Molecule 2: Photosystem II core light harvesting protein

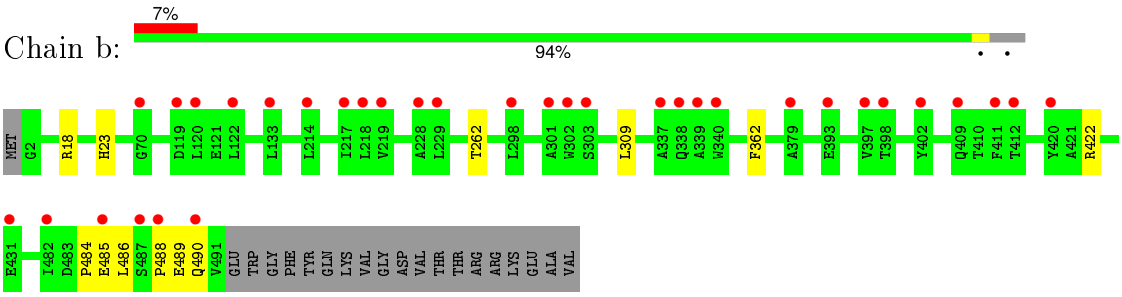
Chain B:





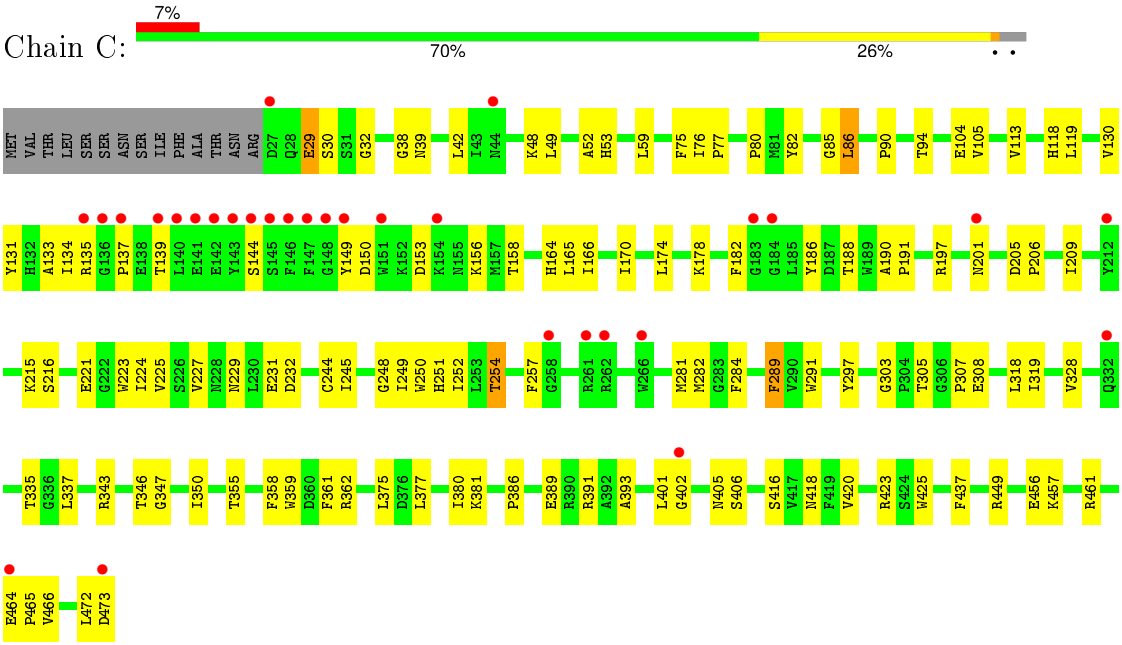
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



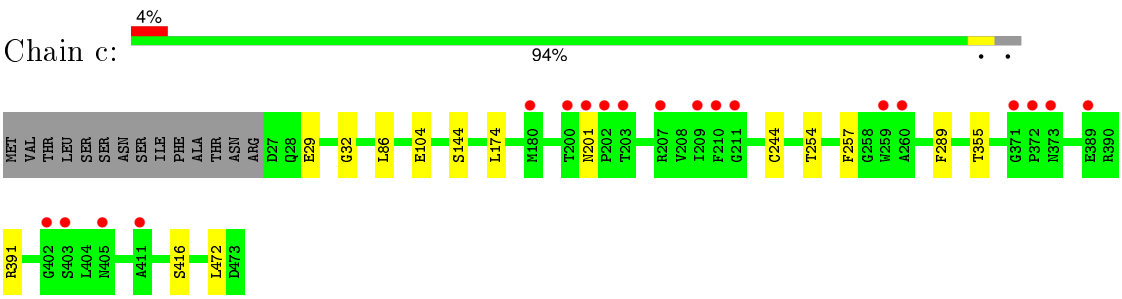
• Molecule 3: Photosystem II CP43 protein

Chain C:



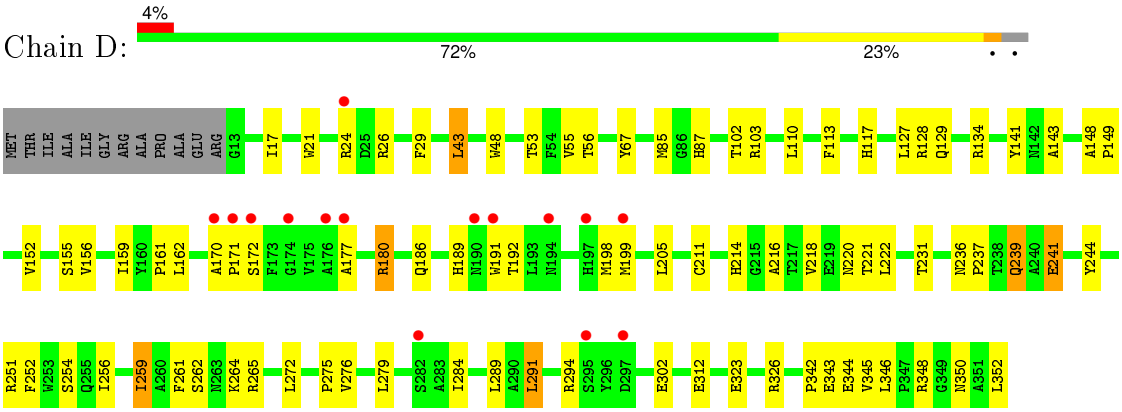
• Molecule 3: Photosystem II CP43 protein

Chain c:



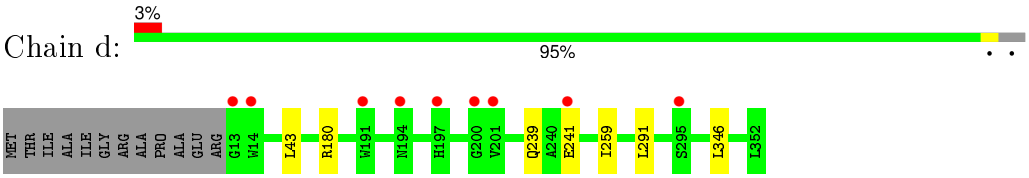
• Molecule 4: Photosystem II D2 protein

Chain D:



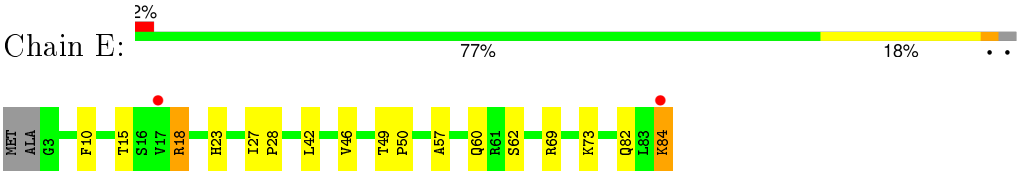
- Molecule 4: Photosystem II D2 protein

Chain d:



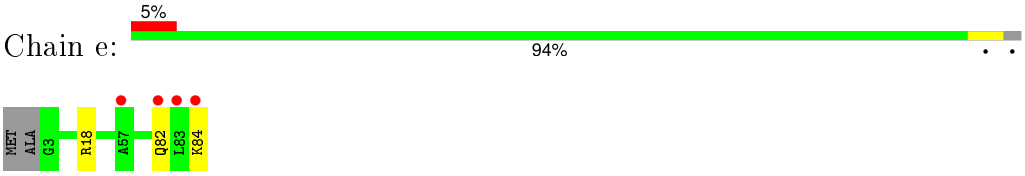
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:



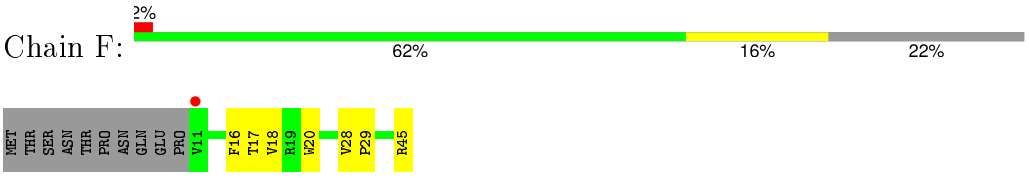
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:



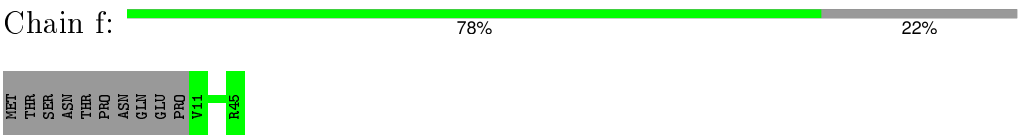
- Molecule 6: Cytochrome b559 subunit beta

Chain F:



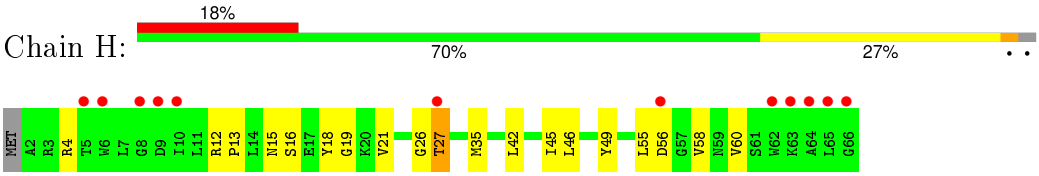
- Molecule 6: Cytochrome b559 subunit beta

Chain f:



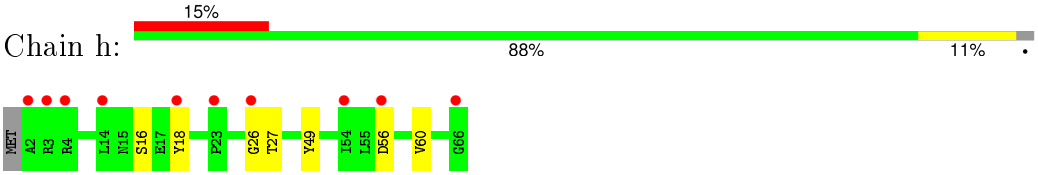
- Molecule 7: Photosystem II reaction center protein H

Chain H:



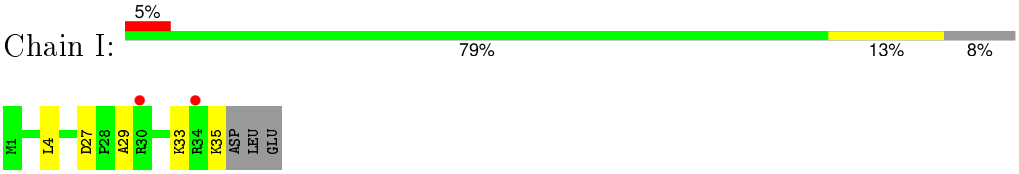
• Molecule 7: Photosystem II reaction center protein H

Chain h:



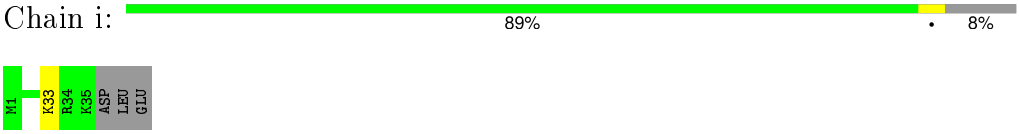
• Molecule 8: Photosystem II reaction center protein I

Chain I:



• Molecule 8: Photosystem II reaction center protein I

Chain i:

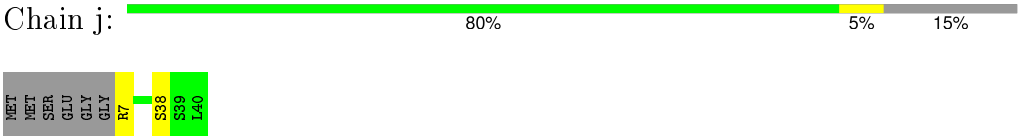


• Molecule 9: Photosystem II reaction center protein J

Chain J:

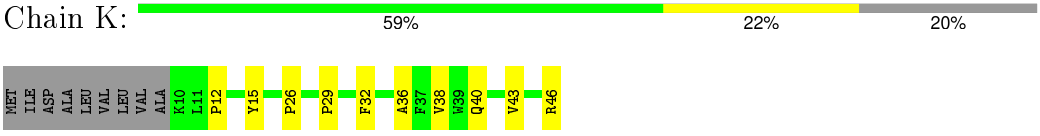
• Molecule 9: Photosystem II reaction center protein J

Chain j:



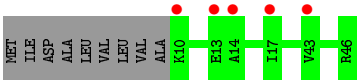
• Molecule 10: Photosystem II reaction center protein K

Chain K:



• Molecule 10: Photosystem II reaction center protein K

Chain k:

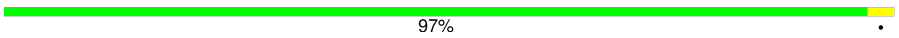


• Molecule 11: Photosystem II reaction center protein L

Chain L:

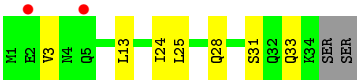
• Molecule 11: Photosystem II reaction center protein L

Chain l:



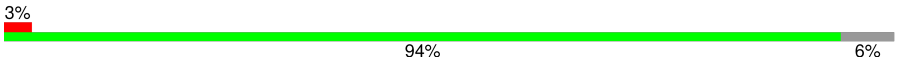
• Molecule 12: Photosystem II reaction center protein M

Chain M:



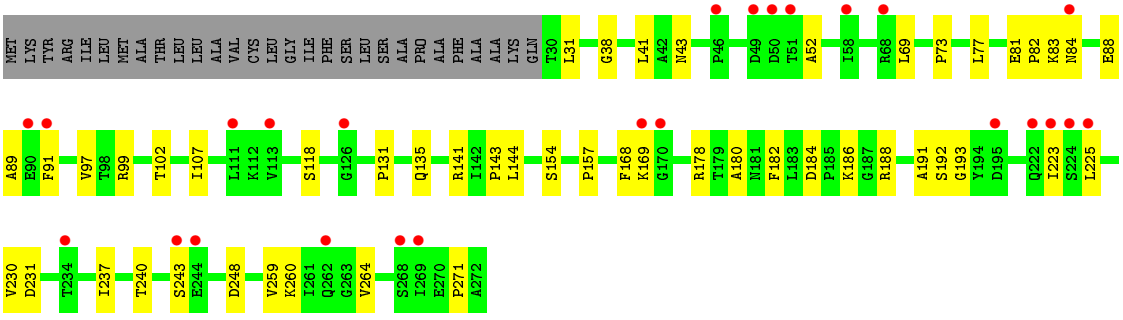
• Molecule 12: Photosystem II reaction center protein M

Chain m:



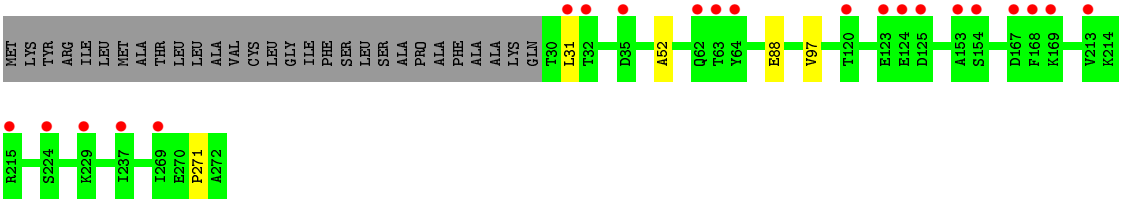
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

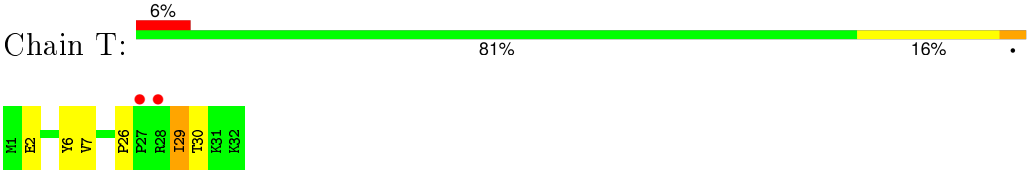


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

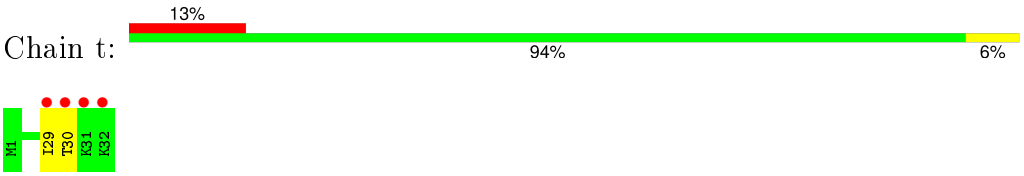
Chain o:



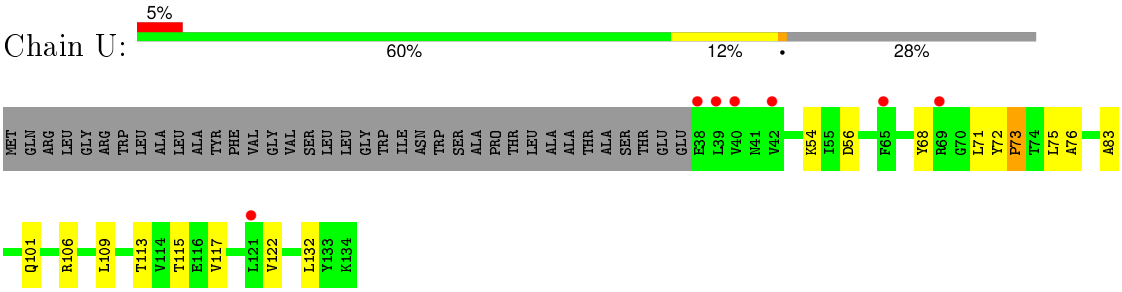
• Molecule 14: Photosystem II reaction center protein T



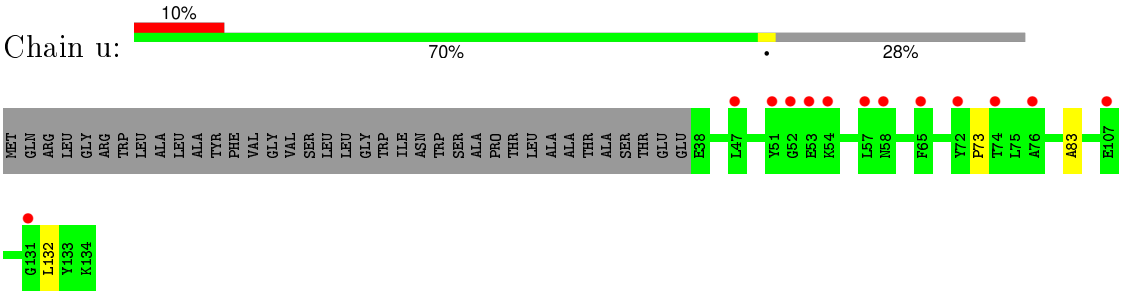
• Molecule 14: Photosystem II reaction center protein T



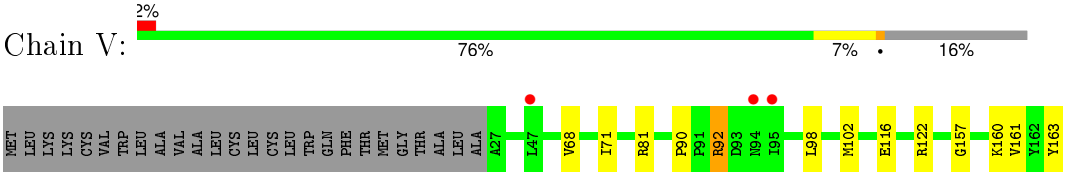
• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

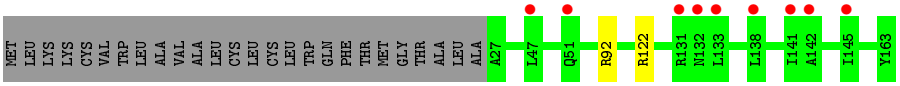


• Molecule 16: Cytochrome c-550



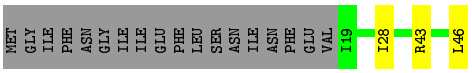
• Molecule 16: Cytochrome c-550

Chain v:



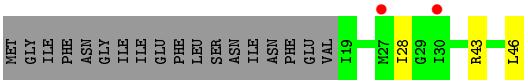
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



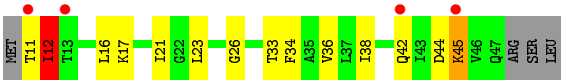
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



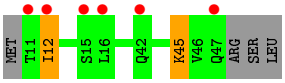
• Molecule 18: Photosystem II reaction center X protein

Chain X:



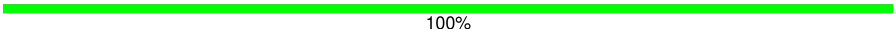
• Molecule 18: Photosystem II reaction center X protein

Chain x:



• Molecule 19: Photosystem II reaction center protein Y

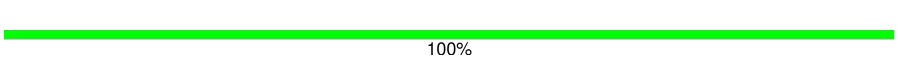
Chain Y:



There are no outlier residues recorded for this chain.

• Molecule 19: Photosystem II reaction center protein Y

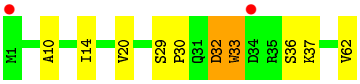
Chain G:



There are no outlier residues recorded for this chain.

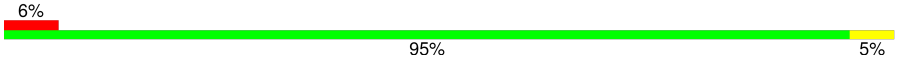
• Molecule 20: Photosystem II reaction center protein Z

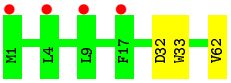
Chain Z:



• Molecule 20: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.7 (72.96-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.278 , 0.284 0.295 , 0.286	Depositor DCC
R_{free} test set	2522 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 126.1	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 51515 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å^2)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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	0.22	0/3556	0.41	0/4842
3	c	0.22	0/3556	0.41	0/4842
4	D	0.23	0/2801	0.40	0/3818
4	d	0.24	0/2801	0.40	0/3818
5	E	0.23	0/685	0.42	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	0.45	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.21	0/255	0.39	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.48	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	0.43	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	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.42	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	0.40	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	g	0.21	0/202	0.45	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.25	0/273	0.43	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	78	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	83	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	74	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	17	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	8	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	7	0
11	l	304	0	316	0	0
12	M	267	0	289	7	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	5	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	8	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	44	0
22	B	975	0	1080	90	0
22	C	845	0	936	47	0
22	D	130	0	144	11	0
22	H	65	0	72	9	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	4	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	3	0
24	B	160	0	224	10	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	4	0
24	H	40	0	56	2	0
24	J	40	0	56	1	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	11	0
25	D	63	0	87	2	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	2	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	4	0
27	D	143	0	196	11	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	93	0	126	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	m	42	0	54	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	105	0	147	6	0
29	B	90	0	111	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	45	0	54	3	0
29	a	105	0	147	0	0
29	b	47	0	61	0	0
29	d	43	0	50	0	0
29	f	45	0	54	0	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	1	0
30	M	70	0	91	0	0
30	b	140	0	183	0	0
30	d	31	0	35	0	0
30	i	35	0	46	0	0
31	D	128	0	148	15	0
31	d	128	0	148	0	0
32	D	1	0	0	0	0
32	a	1	0	0	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	51372	579	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 (579) 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	1.55	0.87
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.51	0.81
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.61	0.80
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.66	0.77
4:D:199:MET:HG2	23:D:407:PL9:H322	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.72	0.74
22:B:605:CLA:H72	24:B:619:BCR:H311	1.70	0.73
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.70	0.72
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.72	0.71
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.74	0.70
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.56	0.70
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.73	0.70
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.74	0.70
4:D:29:PHE:O	4:D:128:ARG:NH2	2.25	0.70
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.73	0.70
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.69
3:C:250:TRP:O	3:C:254:THR:OG1	2.10	0.69
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.68
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.28	0.68
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.76	0.67
4:D:259:ILE:HG12	27:D:409:LMG:H292	1.78	0.67
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.67
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.76	0.67
1:A:63:ILE:HB	3:C:335:THR:HG21	1.77	0.67
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.76	0.67
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.76	0.66
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.77	0.66
12:M:31:SER:HA	27:M:101:LMG:HC1	1.83	0.66
22:B:611:CLA:H42	4:D:127:LEU:HD11	29.95	0.66
22:C:506:CLA:H112	24:C:514:BCR:H362	1.77	0.66
4:D:236:ASN:ND2	4:D:239:GLN:O	2.30	0.66
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.66
1:A:15:GLU:O	1:A:19:ASN:ND2	2.27	0.66
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.69	0.65
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.65
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.79	0.65
1:A:174:LEU:HD22	31:D:401:PHO:H151	1.82	0.64
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.78	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.81	0.64
22:A:404:CLA:H142	22:D:405:CLA:H151	1.79	0.64
22:B:607:CLA:HBA2	29:B:622:SQD:H101	1.80	0.64
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.79	0.64
1:A:183:MET:HB3	22:A:404:CLA:HBC2	14.89	0.63
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.63
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:406:SER:O	3:C:418:ASN:ND2	2.32	0.63
31:D:402:PHO:H151	22:D:405:CLA:H172	1.89	0.63
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.80	0.63
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.63
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
27:D:409:LMG:HO5	27:D:409:LMG:HO4	1.52	0.62
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.87	0.62
1:A:183:MET:HA	22:A:404:CLA:HMD2	12.59	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.32	0.62
2:B:149:LEU:HG	22:B:606:CLA:HBC1	27.91	0.62
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.62
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.81	0.62
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.82	0.61
1:A:329:GLU:O	1:A:332:HIS:ND1	2.36	0.61
22:H:101:CLA:HBD	22:H:101:CLA:H2	1.87	0.61
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.61
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.82	0.61
22:A:404:CLA:H122	31:D:401:PHO:H3A	32.56	0.61
22:A:404:CLA:HHC	22:A:404:CLA:HBB1	3.83	0.61
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.82	0.61
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.85	0.61
29:A:412:SQD:H172	26:C:519:LHG:H172	1.84	0.60
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.60
22:A:404:CLA:H71	22:A:405:CLA:HAB	46.99	0.60
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.67	0.60
2:B:327:THR:HG21	27:B:621:LMG:H111	1.83	0.60
22:B:612:CLA:HMD1	7:H:27:THR:HB	39.61	0.60
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.84	0.59
4:D:216:ALA:O	4:D:220:ASN:ND2	2.34	0.59
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.67	0.59
2:B:262:THR:OG1	22:B:606:CLA:O1D	22.24	0.59
4:D:24:ARG:NH2	18:X:44:ASP:O	2.36	0.59
22:B:606:CLA:H193	7:H:42:LEU:HD12	33.90	0.59
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.84	0.59
2:B:12:LEU:HB2	22:B:615:CLA:HMC2	13.41	0.59
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.59
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.84	0.58
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.86	0.58
29:B:622:SQD:H171	29:B:622:SQD:H301	1.86	0.58
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.88	0.58
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:HIS:CE1	27:C:518:LMG:H192	2.39	0.57
27:D:409:LMG:O6	11:L:15:THR:HG21	2.05	0.57
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.69	0.57
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.88	0.57
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.78	0.57
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.87	0.57
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.86	0.57
13:O:83:LYS:HG2	13:O:84:ASN:H	1.69	0.57
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.34	0.57
1:A:268:SER:O	1:A:272:HIS:ND1	2.35	0.57
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.57
1:A:64:ARG:O	13:O:178:ARG:NH2	2.41	0.56
22:A:402:CLA:H122	31:D:401:PHO:H3A	1.87	0.56
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.56
22:A:404:CLA:H93	22:D:405:CLA:H152	1.87	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.23	0.56
27:D:412:LMG:H171	24:F:102:BCR:H383	1.95	0.56
1:A:217:SER:HA	4:D:272:LEU:HD12	1.91	0.56
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.88	0.56
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.45	0.56
22:C:501:CLA:HMB3	24:C:514:BCR:H403	1.88	0.56
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
4:D:214:HIS:ND1	23:D:407:PL9:O2	2.27	0.55
22:B:607:CLA:HBD	22:B:608:CLA:H43	4.18	0.55
22:A:403:CLA:H203	31:D:401:PHO:H71	1.87	0.55
22:B:606:CLA:C2D	22:B:608:CLA:H2	40.02	0.55
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.40	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.88	0.55
27:A:410:LMG:H231	23:D:407:PL9:H352	1.89	0.55
22:D:406:CLA:H43	18:X:23:LEU:HA	1.89	0.55
22:D:406:CLA:H42	18:X:26:GLY:HA3	1.92	0.55
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.88	0.55
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.39	0.55
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.41	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.88	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.55
1:A:29:TYR:O	1:A:129:ARG:NH1	2.55	0.55
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.92	0.55
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.55
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.25	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.55
22:B:611:CLA:H151	22:B:612:CLA:H203	19.95	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.35	0.54
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.37	0.54
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.54
2:B:458:PHE:HB3	22:B:607:CLA:HBC2	12.96	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.91	0.54
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.89	0.54
2:B:262:THR:HG22	2:B:263:THR:HG23	1.89	0.54
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.38	0.54
22:A:405:CLA:HED1	23:D:407:PL9:H372	28.93	0.54
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.90	0.54
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.90	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
24:A:407:BCR:H342	29:A:413:SQD:H311	1.90	0.54
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.89	0.54
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.85	0.54
25:B:625:DGD:O2D	25:B:625:DGD:O1B	2.25	0.54
26:C:519:LHG:H271	26:C:519:LHG:H101	1.90	0.54
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.54
13:O:73:PRO:HG2	13:O:102:THR:HB	1.90	0.54
22:A:403:CLA:HED1	23:D:407:PL9:H372	1.90	0.53
22:A:405:CLA:H203	31:D:401:PHO:H71	33.12	0.53
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.53
29:F:103:SQD:H131	18:X:36:VAL:HG11	1.96	0.53
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.94	0.53
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.91	0.53
29:B:626:SQD:H1	29:B:626:SQD:H462	1.90	0.53
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.90	0.53
2:B:474:LEU:O	4:D:134:ARG:NH1	2.50	0.53
22:B:607:CLA:H151	22:B:608:CLA:H203	1.90	0.53
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.91	0.53
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.47	0.53
2:B:103:LEU:HD21	22:B:608:CLA:HMC3	26.63	0.53
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.93	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.91	0.53
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.44	0.53
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.91	0.53
22:C:510:CLA:HMB2	24:C:513:BCR:H382	1.90	0.53
22:B:605:CLA:OBD	30:B:623:LMT:O6'	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:407:BCR:H321	29:A:413:SQD:H321	1.91	0.52
2:B:271:THR:HB	2:B:274:GLN:HG3	1.91	0.52
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.91	0.52
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
22:B:606:CLA:C3D	22:B:608:CLA:H2	40.25	0.52
1:A:244:GLU:HG3	1:A:246:TYR:H	1.76	0.52
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.74	0.52
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.93	0.52
1:A:211:PHE:HA	1:A:214:MET:HB2	1.91	0.52
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.91	0.52
1:A:153:SER:HB3	22:A:404:CLA:HED1	19.17	0.51
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.92	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.91	0.51
2:B:150:CYS:HB2	22:B:606:CLA:HMC3	24.92	0.51
2:B:212:ALA:HB2	22:B:612:CLA:HMC3	27.35	0.51
4:D:275:PRO:O	4:D:279:LEU:HD23	2.14	0.51
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.93	0.51
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.91	0.51
22:A:405:CLA:H42	23:D:407:PL9:H162	36.95	0.51
29:A:412:SQD:H311	22:C:507:CLA:H71	1.93	0.51
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.51
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.94	0.51
22:C:504:CLA:HBD	22:C:504:CLA:HBA1	1.94	0.51
3:C:85:GLY:N	25:C:516:DGD:HE4	2.26	0.51
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.54	0.51
1:A:132:GLU:O	1:A:136:ARG:HG2	2.11	0.51
2:B:135:LEU:HA	2:B:138:MET:HE3	2.02	0.51
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	2.05	0.50
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.94	0.50
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.79	0.50
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.94	0.50
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.92	0.50
22:B:608:CLA:H202	22:B:612:CLA:HBB2	21.88	0.50
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.97	0.50
22:A:403:CLA:HMA2	23:D:407:PL9:H411	1.93	0.50
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.50
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.42	0.50
2:B:150:CYS:HA	22:B:606:CLA:HBC2	29.83	0.50
4:D:85:MET:HA	5:E:69:ARG:HB3	2.03	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.44	0.50
29:A:412:SQD:H223	25:C:517:DGD:HAE1	1.93	0.50
4:D:279:LEU:HG	31:D:402:PHO:HBC3	1.96	0.50
25:D:410:DGD:O5E	25:D:410:DGD:O4E	2.25	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.50
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.83	0.50
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.27	0.49
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.93	0.49
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.94	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.49
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.49
4:D:348:ARG:NH2	4:D:352:LEU:O	2.39	0.49
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.51	0.49
2:B:327:THR:HG22	22:B:606:CLA:H12	1.94	0.49
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.77	0.49
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.00	0.49
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.75	0.49
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.42	0.49
27:D:409:LMG:H111	11:L:19:LEU:HD21	1.97	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.49
1:A:210:LEU:HG	31:D:402:PHO:NC	2.28	0.49
29:F:103:SQD:H162	18:X:33:THR:HA	1.94	0.49
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.94	0.49
22:B:611:CLA:H51	22:B:612:CLA:H101	18.01	0.49
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.95	0.49
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.49
2:B:222:PRO:HG3	7:H:27:THR:H	1.78	0.48
29:B:622:SQD:H111	29:B:622:SQD:H241	1.96	0.48
22:B:612:CLA:H51	27:D:408:LMG:H231	1.95	0.48
30:B:627:LMT:H62	8:I:4:LEU:HD22	82.08	0.48
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.95	0.48
1:A:78:ILE:O	1:A:176:ILE:HB	2.13	0.48
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.48	0.48
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.48
2:B:327:THR:HG22	22:B:610:CLA:H12	26.92	0.48
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.94	0.48
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.95	0.48
25:B:625:DGD:HD1	30:B:627:LMT:H32	1.95	0.48
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.94	0.48
27:A:414:LMG:H112	2:B:43:ALA:HA	42.29	0.48
4:D:102:THR:OG1	25:D:410:DGD:HD62	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.48
13:O:118:SER:HB3	13:O:157:PRO:HA	1.99	0.48
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.95	0.48
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.48
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.70	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
27:C:518:LMG:H292	27:C:518:LMG:H111	1.95	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
22:A:405:CLA:HMA2	23:D:407:PL9:H411	24.71	0.47
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.96	0.47
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.52	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.47
3:C:158:THR:O	3:C:251:HIS:HB3	2.14	0.47
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.63	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	1.99	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.80	0.47
22:B:615:CLA:H12	22:B:615:CLA:H72	1.97	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.97	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.98	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.47
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.97	0.47
22:C:501:CLA:H193	22:C:506:CLA:H111	2.04	0.47
4:D:262:SER:N	27:D:409:LMG:O3	2.46	0.47
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.47
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.97	0.47
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.47	0.47
22:A:405:CLA:H162	22:A:405:CLA:H141	1.71	0.46
22:B:607:CLA:H18	22:B:608:CLA:H192	1.97	0.46
27:I:101:LMG:H181	30:I:102:LMT:H42	2.04	0.46
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.46
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.98	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
1:A:202:VAL:HB	22:A:404:CLA:HMB3	12.99	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.01	0.46
4:D:48:TRP:CE2	31:D:402:PHO:H161	2.50	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.99	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.98	0.46
22:H:101:CLA:H62	22:H:101:CLA:H41	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.05	0.46
22:H:101:CLA:H162	22:H:101:CLA:H122	1.50	0.46
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.52	0.46
22:A:404:CLA:H161	23:A:406:PL9:H253	1.96	0.46
4:D:261:PHE:HB2	23:D:407:PL9:H522	1.98	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.51	0.46
31:D:401:PHO:H41	31:D:401:PHO:H62	1.47	0.46
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.46
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.18	0.46
2:B:170:ASP:OD1	2:B:175:THR:N	2.50	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
24:B:616:BCR:H361	24:B:616:BCR:H20C	1.76	0.46
22:C:510:CLA:H61	22:C:510:CLA:H93	1.81	0.46
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.79	0.46
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.51	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.98	0.46
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.01	0.46
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.46
27:D:409:LMG:O9	27:D:409:LMG:HC1	2.18	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.52	0.45
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.82	0.45
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.45
12:M:24:ILE:HG21	27:M:101:LMG:H322	9.39	0.45
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.45
22:B:607:CLA:H51	22:B:608:CLA:H101	1.98	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.48	0.45
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.99	0.45
22:B:603:CLA:HMD2	22:B:611:CLA:H193	1.99	0.45
24:B:618:BCR:H361	24:B:618:BCR:H20C	1.82	0.45
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.45
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.77	0.45
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.45
22:A:402:CLA:HBA1	22:A:402:CLA:H3A	1.53	0.45
2:B:212:ALA:O	2:B:216:HIS:ND1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.19	0.45
1:A:114:LEU:O	1:A:118:HIS:ND1	2.46	0.45
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.45
22:B:614:CLA:H172	22:B:614:CLA:H111	1.99	0.45
24:C:514:BCR:H20C	24:C:514:BCR:H361	1.83	0.45
13:O:143:PRO:HG2	13:O:248:ASP:HB3	1.98	0.45
22:A:402:CLA:H51	31:D:401:PHO:C3B	2.47	0.45
22:B:611:CLA:H162	22:B:611:CLA:H122	1.76	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
30:B:628:LMT:H122	14:T:7:VAL:HG12	34.40	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.18	0.45
16:V:98:LEU:O	16:V:102:MET:HG3	2.22	0.45
22:A:405:CLA:H162	22:A:405:CLA:H202	3.78	0.45
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.17	0.45
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.04	0.45
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.03	0.45
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.31	0.45
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.45
1:A:224:ILE:O	4:D:265:ARG:NH2	2.49	0.45
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.45
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.57	0.44
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.27	0.44
22:B:605:CLA:HBA2	22:B:605:CLA:H3A	1.26	0.44
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.00	0.44
22:C:508:CLA:H11	22:C:508:CLA:H51	1.82	0.44
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.42	0.44
22:C:504:CLA:H11	24:C:514:BCR:H312	2.01	0.44
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.44
22:B:613:CLA:H51	24:B:616:BCR:H372	1.98	0.44
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.44
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.78	0.44
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.44
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.18	0.44
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.99	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
22:C:501:CLA:H141	22:C:501:CLA:H162	1.78	0.44
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.71	0.44
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.99	0.44
3:C:224:ILE:O	3:C:227:VAL:HG23	2.18	0.44
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.01	0.44
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.00	0.44
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.44
1:A:202:VAL:HB	22:A:402:CLA:HMB3	2.00	0.44
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.53	0.44
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.00	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.92	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.18	0.44
22:C:512:CLA:HBA2	22:C:512:CLA:H3A	1.72	0.43
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.81	0.43
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.06	0.43
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.43
3:C:245:ILE:O	3:C:249:ILE:HG12	2.17	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
22:B:605:CLA:C3D	30:B:623:LMT:H11	2.49	0.43
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
1:A:271:LEU:HD21	23:A:406:PL9:HC71	1.99	0.43
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.43
22:C:503:CLA:HMD2	22:C:503:CLA:H201	2.02	0.43
31:D:401:PHO:H102	31:D:401:PHO:H13	1.82	0.43
22:D:405:CLA:H62	22:D:405:CLA:H92	1.79	0.43
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.58	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.18	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
22:B:606:CLA:H2	22:B:608:CLA:H93	34.06	0.43
24:C:513:BCR:H371	24:C:513:BCR:H24C	1.78	0.43
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.54	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.43
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.43
22:A:404:CLA:H143	22:A:404:CLA:H161	1.86	0.43
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.06	0.43
30:B:628:LMT:H1B	30:B:628:LMT:H3'	1.53	0.43
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.58	0.43
11:L:4:ASN:OD1	11:L:6:ASN:ND2	2.49	0.43
2:B:468:TRP:HH2	27:D:408:LMG:HO2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:615:CLA:H162	22:B:615:CLA:H122	5.18	0.43
6:F:16:PHE:HB3	29:F:103:SQD:H241	2.07	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
3:C:29:GLU:HB2	3:C:30:SER:H	1.64	0.43
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.06	0.43
22:B:611:CLA:H171	22:B:612:CLA:HBB2	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.84	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.35	0.43
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.03	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
26:A:409:LHG:H382	22:C:509:CLA:H93	2.01	0.43
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.01	0.43
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.76	0.43
22:D:405:CLA:H3A	22:D:405:CLA:HBA1	1.82	0.43
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.67	0.43
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.01	0.43
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.12	0.43
22:B:606:CLA:H41	22:B:606:CLA:H61	2.89	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.78	0.42
7:H:12:ARG:HD3	7:H:12:ARG:O	2.19	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
23:D:407:PL9:H421	23:D:407:PL9:H401	1.86	0.42
24:F:102:BCR:H15C	24:F:102:BCR:H351	1.91	0.42
15:U:72:TYR:O	15:U:76:ALA:HB3	2.19	0.42
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.04	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42
25:B:620:DGD:HAW2	22:H:101:CLA:H152	2.02	0.42
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.88	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.74	0.42
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.32	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.01	0.42
22:C:511:CLA:H61	22:C:511:CLA:H13	2.05	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.53	0.42
1:A:140:ARG:HH22	26:A:409:LHG:P	2.41	0.42
22:A:404:CLA:H51	31:D:401:PHO:C3B	21.31	0.42
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.02	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.91	0.42
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.95	0.42
3:C:377:LEU:O	3:C:381:LYS:HB2	2.20	0.42
22:B:612:CLA:H171	27:D:408:LMG:H401	2.01	0.42
22:C:511:CLA:H143	22:C:512:CLA:H162	2.02	0.42
22:B:613:CLA:H12	22:B:613:CLA:H51	4.48	0.42
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.84	0.42
22:A:403:CLA:H42	23:D:407:PL9:H162	2.01	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.04	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.42
22:C:520:CLA:H112	22:C:520:CLA:H142	1.77	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.42
3:C:456:GLU:N	3:C:456:GLU:OE1	2.52	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.02	0.42
22:A:405:CLA:H51	22:A:405:CLA:H11	4.35	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.88	0.42
31:D:401:PHO:H202	31:D:401:PHO:H162	1.87	0.42
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.42
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.42
13:O:192:SER:OG	13:O:193:GLY:N	2.52	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.42
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.02	0.42
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
1:A:182:PHE:O	1:A:186:PHE:HB2	2.21	0.42
4:D:155:SER:HA	4:D:159:ILE:HB	2.05	0.42
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.63	0.41
22:D:406:CLA:H41	22:D:406:CLA:H61	1.86	0.41
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.83	0.41
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.50	0.41
4:D:252:PHE:O	4:D:256:ILE:HG22	2.21	0.41
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.02	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.48	0.41
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.02	0.41
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.41
22:A:403:CLA:H202	22:A:403:CLA:H162	1.76	0.41
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:611:CLA:H18	22:B:612:CLA:H192	22.27	0.41
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.03	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.41
22:A:403:CLA:H41	22:A:403:CLA:H62	1.76	0.41
22:A:403:CLA:HED2	4:D:198:MET:SD	2.60	0.41
22:B:602:CLA:H92	22:B:602:CLA:HBB2	2.03	0.41
24:F:102:BCR:H341	24:F:102:BCR:H11C	1.94	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.84	0.41
1:A:238:LYS:O	1:A:241:GLN:HG3	2.21	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.79	0.41
3:C:282:MET:HG2	22:C:501:CLA:H61	2.09	0.41
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.54	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.41
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.54	0.41
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.41
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.37	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
1:A:269:ARG:NH1	4:D:231:THR:HB	2.38	0.41
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.04	0.41
1:A:153:SER:HB2	22:A:404:CLA:H43	19.16	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.88	0.41
31:D:402:PHO:CHB	22:D:405:CLA:H101	2.51	0.41
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.97	0.41
24:A:407:BCR:H341	24:A:407:BCR:H11C	1.94	0.41
22:B:611:CLA:H143	22:B:611:CLA:H161	4.42	0.41
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.02	0.41
22:B:602:CLA:H162	22:B:602:CLA:H192	1.77	0.41
1:A:258:LEU:O	4:D:128:ARG:NH1	2.54	0.41
3:C:303:GLY:O	3:C:423:ARG:NE	2.41	0.41
3:C:119:LEU:HG	24:C:513:BCR:H10C	2.15	0.41
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.26	0.41
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.02	0.41
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.21	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.21	0.41
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.10	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:342:PRO:O	4:D:345:VAL:HG12	2.22	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.07	0.41
7:H:35:MET:HE3	7:H:35:MET:HB2	1.87	0.41
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.92	0.41
22:A:404:CLA:H62	22:A:404:CLA:H102	4.12	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.94	0.41
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.21	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.04	0.41
24:H:102:BCR:HC31	24:H:102:BCR:H323	1.89	0.41
22:B:605:CLA:H41	22:B:605:CLA:H62	1.86	0.40
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.03	0.40
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.40
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.40
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
3:C:375:LEU:HB3	3:C:380:ILE:HD11	2.04	0.40
24:K:102:BCR:H361	24:K:102:BCR:H20C	1.81	0.40
2:B:179:GLN:HA	2:B:180:PRO:HD3	1.97	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.40
22:B:602:CLA:H61	22:B:602:CLA:H41	1.67	0.40
22:B:606:CLA:H41	22:B:606:CLA:H62	1.90	0.40
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.08	0.40
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.04	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.61	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.04	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.52	0.40
22:B:606:CLA:H161	22:B:606:CLA:H141	2.05	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.51	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.96	0.40
1:A:180:PHE:O	1:A:184:ILE:HG13	2.26	0.40
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.86	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.40
11:L:11:GLU:HG2	11:L:12:LEU:N	2.35	0.40
29:A:413:SQD:H332	22:B:609:CLA:H203	66.25	0.40
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.40
2:B:6:TYR:OH	27:D:408:LMG:HC5	2.26	0.40
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.59	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%)	311 (93%)	18 (5%)	4 (1%)	16 62
1	a	333/344 (97%)	309 (93%)	20 (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%)	36 (8%)	4 (1%)	21 67
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	46 83
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%)	26 (79%)	7 (21%)	0	100 100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 44
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 44
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	52
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9	52
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	38
17	y	26/46 (56%)	19 (73%)	6 (23%)	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
All	All	5138/5618 (92%)	4675 (91%)	408 (8%)	55 (1%)	17	64

All (55) 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
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
7	H	26	GLY
9	J	38	SER
13	O	52	ALA
14	T	30	THR
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO

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Mol	Chain	Res	Type
3	c	257	PHE
3	c	416	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
2	B	489	GLU
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
18	X	12	ILE
2	b	489	GLU
3	c	32	GLY
4	d	239	GLN
7	h	26	GLY
9	j	38	SER
13	o	88	GLU
1	A	142	TRP
3	C	32	GLY
5	E	82	GLN
1	a	142	TRP
1	a	334	ARG
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
7	H	16	SER
15	U	73	PRO
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

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%)	269 (98%)	6 (2%)	60	84
5	E	72/73 (99%)	70 (97%)	2 (3%)	51	79
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	56
7	h	53/55 (96%)	49 (92%)	4 (8%)	17	56
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	72
9	j	24/28 (86%)	23 (96%)	1 (4%)	36	72
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	77
14	t	29/29 (100%)	28 (97%)	1 (3%)	44	77
15	U	84/112 (75%)	83 (99%)	1 (1%)	78	90
15	u	84/112 (75%)	83 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	4142 (98%)	102 (2%)	57 83

All (102) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
3	C	118	HIS
4	D	117	HIS
4	d	117	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	1.19	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	1.19	6 (9%)
22	CLA	A	405	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
23	PL9	A	406	-	45,45,55	1.12	3 (6%)	56,57,69	1.59	12 (21%)
24	BCR	A	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	6 (10%)
25	DGD	A	408	-	57,57,67	0.91	0	71,71,81	1.44	8 (11%)
26	LHG	A	409	-	38,38,48	0.67	0	39,44,54	1.19	3 (7%)
27	LMG	A	410	-	51,51,55	0.74	1 (1%)	59,59,63	1.36	6 (10%)
28	OEX	A	411	1,3	0,15,15	0.00	-	0,32,32	0.00	-
29	SQD	A	412	-	50,51,54	0.95	3 (6%)	58,62,65	1.96	9 (15%)
29	SQD	A	413	-	53,54,54	0.93	3 (5%)	61,65,65	1.64	9 (14%)
27	LMG	A	414	-	42,42,55	0.82	0	50,50,63	1.25	4 (8%)
22	CLA	B	601	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	1.20	7 (11%)
22	CLA	B	605	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	B	606	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	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	0.97	3 (5%)	61,113,113	1.19	8 (13%)
22	CLA	B	609	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	B	610	-	55,73,73	1.03	4 (7%)	61,113,113	1.33	7 (11%)
22	CLA	B	611	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	8 (13%)
22	CLA	B	612	-	55,73,73	0.92	3 (5%)	61,113,113	1.22	8 (13%)
22	CLA	B	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	B	614	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	8 (13%)
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	1.08	2 (4%)	56,56,56	1.24	7 (12%)
24	BCR	B	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.34	9 (16%)
24	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	11 (19%)
24	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	8 (14%)
25	DGD	B	620	-	59,59,67	0.89	1 (1%)	73,73,81	1.35	7 (9%)
27	LMG	B	621	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	6 (10%)
29	SQD	B	622	-	42,43,54	1.03	2 (4%)	50,54,65	1.89	10 (20%)
30	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	0.99	2 (4%)
30	LMT	B	624	-	36,36,36	1.07	4 (11%)	47,47,47	1.04	3 (6%)
25	DGD	B	625	-	53,53,67	1.05	3 (5%)	67,67,81	1.35	7 (10%)
29	SQD	B	626	-	46,47,54	1.00	4 (8%)	54,58,65	1.94	9 (16%)
30	LMT	B	627	-	36,36,36	1.09	4 (11%)	47,47,47	0.98	2 (4%)
30	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	1.17	8 (13%)
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	1.22	8 (13%)
22	CLA	C	504	-	55,73,73	0.96	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	C	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	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	1.25	7 (11%)
22	CLA	C	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	6 (9%)
22	CLA	C	510	3	55,73,73	0.94	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	C	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	C	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
24	BCR	C	513	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	10 (17%)
24	BCR	C	514	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	9 (16%)
25	DGD	C	515	-	54,54,67	0.95	2 (3%)	68,68,81	1.27	8 (11%)
25	DGD	C	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.45	14 (18%)
25	DGD	C	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.43	10 (12%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.28	4 (7%)
26	LHG	C	519	-	36,36,48	0.70	0	37,42,54	1.28	4 (10%)
22	CLA	C	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	8 (13%)
27	LMG	C	521	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
31	PHO	D	401	-	67,69,69	1.21	9 (13%)	84,99,99	1.02	5 (5%)
31	PHO	D	402	-	67,69,69	1.23	10 (14%)	84,99,99	1.02	4 (4%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.17	8 (13%)
22	CLA	D	406	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	D	407	-	55,55,55	1.16	3 (5%)	68,69,69	1.58	15 (22%)
27	LMG	D	408	-	49,49,55	0.75	1 (2%)	57,57,63	1.31	5 (8%)
27	LMG	D	409	-	48,48,55	0.76	0	56,56,63	1.38	5 (8%)
25	DGD	D	410	-	64,64,67	0.90	0	78,78,81	1.34	10 (12%)
30	LMT	D	411	-	32,32,36	1.15	4 (12%)	43,43,47	1.05	2 (4%)
27	LMG	D	412	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	5 (9%)
27	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.29	5 (9%)
34	HEM	F	101	5,6	30,50,50	2.11	10 (33%)	24,82,82	2.31	9 (37%)
24	BCR	F	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
29	SQD	F	103	-	44,45,54	1.02	4 (9%)	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	1.09	2 (4%)	56,56,56	1.22	3 (5%)
27	LMG	I	101	-	43,43,55	0.79	0	51,51,63	1.27	5 (9%)
30	LMT	I	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.08	2 (4%)
23	PL9	J	101	-	35,35,55	1.15	1 (2%)	44,45,69	1.54	6 (13%)
24	BCR	J	102	-	41,41,41	1.05	3 (7%)	56,56,56	1.61	13 (23%)
24	BCR	K	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LMG	M	101	-	42,42,55	0.84	1 (2%)	50,50,63	1.24	4 (8%)
30	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.03	3 (6%)
30	LMT	M	103	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	3 (6%)
34	HEM	V	201	16	30,50,50	2.23	11 (36%)	24,82,82	2.25	6 (25%)
29	SQD	a	401	-	53,54,54	0.94	3 (5%)	61,65,65	1.64	8 (13%)
27	LMG	a	402	-	42,42,55	0.82	0	50,50,63	1.26	4 (8%)
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	1.20	6 (9%)
22	CLA	a	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	a	407	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
23	PL9	a	408	-	45,45,55	1.18	3 (6%)	56,57,69	1.59	13 (23%)
24	BCR	a	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	7 (12%)
25	DGD	a	410	-	57,57,67	0.91	1 (1%)	71,71,81	1.42	8 (11%)
26	LHG	a	411	-	38,38,48	0.67	1 (2%)	39,44,54	1.19	3 (7%)
27	LMG	a	412	-	51,51,55	0.75	1 (1%)	59,59,63	1.34	7 (11%)
28	OEX	a	414	1,3	0,15,15	0.00	-	0,32,32	0.00	-
29	SQD	a	415	-	50,51,54	0.95	3 (6%)	58,62,65	1.97	9 (15%)
25	DGD	b	601	-	53,53,67	1.03	4 (7%)	67,67,81	1.35	7 (10%)
29	SQD	b	602	-	46,47,54	1.01	4 (8%)	54,58,65	1.97	9 (16%)
30	LMT	b	603	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
30	LMT	b	604	-	36,36,36	1.10	4 (11%)	47,47,47	1.07	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	1.20	8 (13%)
22	CLA	b	607	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	8 (13%)
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	1.21	6 (9%)
22	CLA	b	610	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
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	0.96	3 (5%)	61,113,113	1.17	7 (11%)
22	CLA	b	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	b	614	-	55,73,73	1.03	4 (7%)	61,113,113	1.33	7 (11%)
22	CLA	b	615	-	55,73,73	0.94	4 (7%)	61,113,113	1.21	8 (13%)
22	CLA	b	616	-	55,73,73	0.93	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	617	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	b	618	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	619	-	55,73,73	0.94	4 (7%)	61,113,113	1.17	6 (9%)
24	BCR	b	620	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
24	BCR	b	621	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	9 (16%)
24	BCR	b	622	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	10 (17%)
24	BCR	b	623	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	8 (14%)
25	DGD	b	624	-	59,59,67	0.89	0	73,73,81	1.34	6 (8%)
27	LMG	b	625	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	6 (10%)
30	LMT	b	626	-	36,36,36	1.10	4 (11%)	47,47,47	0.98	2 (4%)
30	LMT	b	627	-	36,36,36	1.07	4 (11%)	47,47,47	1.02	3 (6%)
22	CLA	c	501	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	c	502	-	55,73,73	0.96	4 (7%)	61,113,113	1.21	7 (11%)
22	CLA	c	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	c	504	-	55,73,73	0.96	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	c	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	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	1.27	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	0.94	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	c	511	-	55,73,73	0.93	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	c	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
24	BCR	c	513	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	10 (17%)
24	BCR	c	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	8 (14%)
25	DGD	c	515	-	54,54,67	0.94	1 (1%)	68,68,81	1.28	7 (10%)
25	DGD	c	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.45	12 (15%)
25	DGD	c	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.42	9 (11%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.28	5 (9%)
26	LHG	c	519	-	36,36,48	0.71	0	37,42,54	1.27	4 (10%)
22	CLA	c	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	8 (13%)
24	BCR	c	521	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	8 (14%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
31	PHO	d	401	-	67,69,69	1.21	10 (14%)	84,99,99	1.02	5 (5%)
31	PHO	d	402	-	67,69,69	1.23	8 (11%)	84,99,99	1.00	4 (4%)
29	SQD	d	403	-	42,43,54	1.04	3 (7%)	50,54,65	1.90	10 (20%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	d	405	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	d	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	d	407	-	55,55,55	1.18	3 (5%)	68,69,69	1.59	14 (20%)
27	LMG	d	408	-	49,49,55	0.75	0	57,57,63	1.31	5 (8%)
27	LMG	d	409	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
25	DGD	d	410	-	64,64,67	0.90	1 (1%)	78,78,81	1.35	10 (12%)
30	LMT	d	411	-	32,32,36	1.15	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	d	412	-	46,46,55	0.77	1 (2%)	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	2.11	12 (40%)	24,82,82	2.32	10 (41%)
24	BCR	f	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
29	SQD	f	103	-	44,45,54	1.02	4 (9%)	52,56,65	1.77	9 (17%)
24	BCR	g	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	6 (10%)
22	CLA	h	101	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
27	LMG	i	101	-	43,43,55	0.80	0	51,51,63	1.28	5 (9%)
30	LMT	i	102	-	36,36,36	1.07	4 (11%)	47,47,47	1.06	2 (4%)
23	PL9	j	101	-	35,35,55	1.13	2 (5%)	44,45,69	1.54	6 (13%)
24	BCR	j	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.59	13 (23%)
27	LMG	m	101	-	42,42,55	0.84	1 (2%)	50,50,63	1.23	4 (8%)
34	HEM	v	201	16	30,50,50	2.22	11 (36%)	24,82,82	2.24	6 (25%)
24	BCR	x	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)
24	BCR	y	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.27	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	A	410	-	-	0/46/66/70	0/1/1/1
28	OEX	A	411	1,3	-	0/0/68/68	0/0/6/6
29	SQD	A	412	-	-	0/46/66/69	0/1/1/1
29	SQD	A	413	-	-	0/49/69/69	0/1/1/1
27	LMG	A	414	-	-	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
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
29	SQD	B	622	-	-	1/38/58/69	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
30	LMT	B	624	-	-	0/21/61/61	0/2/2/2
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
29	SQD	B	626	-	-	0/42/62/69	0/1/1/1
30	LMT	B	627	-	-	0/21/61/61	0/2/2/2
30	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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
31	PHO	D	401	-	-	0/53/103/103	0/1/6/6
31	PHO	D	402	-	-	0/53/103/103	0/1/6/6
33	BCT	D	404	21	-	0/0/0/0	0/0/0/0
22	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	D	406	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PL9	D	407	-	-	0/53/73/73	0/1/1/1
27	LMG	D	408	-	-	0/44/64/70	0/1/1/1
27	LMG	D	409	-	-	0/43/63/70	0/1/1/1
25	DGD	D	410	-	-	0/52/92/95	0/2/2/2
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
27	LMG	D	412	-	-	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
29	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
30	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	-	-	0/37/57/70	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/10/54/54	0/0/8/8
29	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
22	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	a	408	-	-	0/41/61/73	0/1/1/1
24	BCR	a	409	-	-	0/29/63/63	0/2/2/2
25	DGD	a	410	-	-	0/45/85/95	0/2/2/2
26	LHG	a	411	-	-	0/43/43/53	0/0/0/0
27	LMG	a	412	-	-	0/46/66/70	0/1/1/1
28	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
29	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2
29	SQD	b	602	-	-	0/42/62/69	0/1/1/1
30	LMT	b	603	-	-	0/21/61/61	0/2/2/2
30	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	b	624	-	-	0/47/87/95	0/2/2/2
27	LMG	b	625	-	-	0/44/64/70	0/1/1/1
30	LMT	b	626	-	-	0/21/61/61	0/2/2/2
30	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
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
31	PHO	d	401	-	-	0/53/103/103	0/1/6/6
31	PHO	d	402	-	-	0/53/103/103	0/1/6/6
29	SQD	d	403	-	-	1/38/58/69	0/1/1/1
33	BCT	d	404	21	-	0/0/0/0	0/0/0/0
22	CLA	d	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	406	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	d	407	-	-	0/53/73/73	0/1/1/1
27	LMG	d	408	-	-	0/44/64/70	0/1/1/1
27	LMG	d	409	-	-	0/43/63/70	0/1/1/1
25	DGD	d	410	-	-	0/52/92/95	0/2/2/2
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
27	LMG	d	412	-	-	0/41/61/70	0/1/1/1
27	LMG	e	101	-	-	0/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
29	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
30	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	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 (492) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-7.27	1.45	1.51
34	v	201	HEM	C3B-C4B	-7.10	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.17	1.46	1.51
34	f	101	HEM	C3B-C4B	-6.11	1.46	1.51
34	f	101	HEM	C3D-C4D	-5.28	1.44	1.51
23	d	407	PL9	C7-C3	-5.25	1.47	1.51
34	F	101	HEM	C3D-C4D	-5.24	1.44	1.51
34	V	201	HEM	C3D-C4D	-4.94	1.45	1.51
23	D	407	PL9	C7-C3	-4.85	1.47	1.51
34	v	201	HEM	C3D-C4D	-4.83	1.45	1.51
23	a	408	PL9	C7-C3	-4.77	1.47	1.51
23	J	101	PL9	C7-C3	-4.30	1.48	1.51
23	A	406	PL9	C7-C3	-4.28	1.48	1.51
23	j	101	PL9	C7-C3	-4.15	1.48	1.51
34	V	201	HEM	C2C-C1C	-3.93	1.45	1.52
34	v	201	HEM	C2C-C1C	-3.83	1.45	1.52
22	b	614	CLA	CMB-C2B	-3.75	1.44	1.51
22	B	610	CLA	CMB-C2B	-3.65	1.44	1.51
24	y	101	BCR	C1-C6	-3.64	1.48	1.53
34	F	101	HEM	C2C-C1C	-3.59	1.45	1.52
24	H	102	BCR	C1-C6	-3.58	1.48	1.53
24	g	101	BCR	C1-C6	-3.55	1.48	1.53
34	f	101	HEM	C2C-C1C	-3.54	1.45	1.52
24	F	102	BCR	C1-C6	-3.52	1.48	1.53
24	f	102	BCR	C1-C6	-3.47	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	x	101	BCR	C1-C6	-3.47	1.48	1.53
24	B	616	BCR	C1-C6	-3.27	1.49	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	-3.22	1.49	1.53
24	b	621	BCR	C1-C6	-3.19	1.49	1.53
24	y	101	BCR	C30-C25	-3.18	1.49	1.53
24	b	622	BCR	C30-C25	-3.17	1.49	1.53
24	B	617	BCR	C1-C6	-3.12	1.49	1.53
24	J	102	BCR	C30-C25	-3.12	1.49	1.53
24	g	101	BCR	C30-C25	-3.12	1.49	1.53
24	C	513	BCR	C1-C6	-3.12	1.49	1.53
24	j	102	BCR	C30-C25	-3.10	1.49	1.53
24	c	513	BCR	C1-C6	-3.08	1.49	1.53
24	B	618	BCR	C30-C25	-3.07	1.49	1.53
24	K	102	BCR	C30-C25	-3.06	1.49	1.53
24	F	102	BCR	C30-C25	-3.03	1.49	1.53
24	c	521	BCR	C30-C25	-3.01	1.49	1.53
24	A	407	BCR	C30-C25	-3.00	1.49	1.53
24	B	618	BCR	C1-C6	-2.99	1.49	1.53
24	a	409	BCR	C30-C25	-2.98	1.49	1.53
24	f	102	BCR	C30-C25	-2.98	1.49	1.53
24	B	619	BCR	C30-C25	-2.98	1.49	1.53
24	b	623	BCR	C1-C6	-2.97	1.49	1.53
24	B	616	BCR	C30-C25	-2.97	1.49	1.53
24	b	620	BCR	C30-C25	-2.97	1.49	1.53
24	b	623	BCR	C30-C25	-2.95	1.49	1.53
24	B	619	BCR	C1-C6	-2.95	1.49	1.53
24	b	622	BCR	C1-C6	-2.95	1.49	1.53
24	A	407	BCR	C1-C6	-2.95	1.49	1.53
24	a	409	BCR	C1-C6	-2.94	1.49	1.53
24	C	514	BCR	C30-C25	-2.90	1.49	1.53
24	K	102	BCR	C1-C6	-2.89	1.49	1.53
24	C	513	BCR	C30-C25	-2.87	1.49	1.53
24	c	514	BCR	C30-C25	-2.86	1.49	1.53
24	x	101	BCR	C30-C25	-2.82	1.49	1.53
24	c	521	BCR	C1-C6	-2.80	1.49	1.53
24	H	102	BCR	C30-C25	-2.77	1.49	1.53
24	J	102	BCR	C1-C6	-2.70	1.50	1.53
24	j	102	BCR	C1-C6	-2.70	1.50	1.53
24	c	513	BCR	C30-C25	-2.69	1.50	1.53
22	C	507	CLA	CMB-C2B	-2.66	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	CMB-C2B	-2.65	1.46	1.51
24	b	621	BCR	C30-C25	-2.64	1.50	1.53
24	B	617	BCR	C30-C25	-2.63	1.50	1.53
22	B	611	CLA	CMD-C2D	-2.58	1.46	1.51
30	d	411	LMT	O3'-C3'	-2.58	1.36	1.43
30	b	627	LMT	O3'-C3'	-2.58	1.36	1.43
23	a	408	PL9	C3-C4	-2.56	1.45	1.49
30	D	411	LMT	O3'-C3'	-2.56	1.36	1.43
30	M	102	LMT	O3'-C3'	-2.55	1.36	1.43
30	I	102	LMT	O3'-C3'	-2.55	1.36	1.43
22	a	404	CLA	CMB-C2B	-2.55	1.46	1.51
30	M	103	LMT	O3'-C3'	-2.55	1.36	1.43
22	C	509	CLA	CMB-C2B	-2.55	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.54	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.54	1.46	1.51
30	b	626	LMT	O3'-C3'	-2.54	1.36	1.43
22	b	611	CLA	CMB-C2B	-2.53	1.46	1.51
22	A	403	CLA	CMB-C2B	-2.53	1.46	1.51
22	b	615	CLA	CMD-C2D	-2.53	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	603	CLA	CMB-C2B	-2.52	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.52	1.46	1.51
30	b	603	LMT	O3'-C3'	-2.52	1.36	1.43
30	b	604	LMT	O3'-C3'	-2.52	1.36	1.43
22	C	501	CLA	CMB-C2B	-2.51	1.46	1.51
23	D	407	PL9	C3-C4	-2.51	1.45	1.49
22	A	404	CLA	CMB-C2B	-2.51	1.46	1.51
30	B	627	LMT	O3'-C3'	-2.51	1.37	1.43
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	a	407	CLA	CMB-C2B	-2.51	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.50	1.46	1.51
30	B	624	LMT	O3'-C3'	-2.50	1.37	1.43
22	C	505	CLA	CMB-C2B	-2.50	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.50	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.50	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.50	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.49	1.46	1.51
30	i	102	LMT	O3'-C3'	-2.49	1.37	1.43
22	C	508	CLA	CMB-C2B	-2.49	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.49	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	623	LMT	O3'-C3'	-2.48	1.37	1.43
22	B	601	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.48	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.47	1.46	1.51
23	d	407	PL9	C3-C4	-2.47	1.45	1.49
22	b	609	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	504	CLA	CMD-C2D	-2.47	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.47	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.46	1.46	1.51
22	h	101	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.46	1.46	1.51
22	D	406	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	515	DGD	O2G-C2G	-2.45	1.40	1.46
22	C	504	CLA	CMD-C2D	-2.45	1.46	1.51
22	d	406	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	619	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	-2.43	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.43	1.46	1.51
30	B	628	LMT	O3'-C3'	-2.43	1.37	1.43
22	b	612	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	618	CLA	CMB-C2B	-2.43	1.46	1.51
22	D	405	CLA	CMD-C2D	-2.42	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.42	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.39	1.46	1.51
23	A	406	PL9	C3-C4	-2.39	1.45	1.49
22	b	611	CLA	CMD-C2D	-2.39	1.46	1.51
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	D	405	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	614	CLA	C3B-C2B	-2.36	1.37	1.40
22	A	402	CLA	CMD-C2D	-2.36	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.36	1.46	1.51
22	A	404	CLA	CMD-C2D	-2.35	1.46	1.51
22	a	406	CLA	CMD-C2D	-2.35	1.46	1.51
22	a	404	CLA	CMD-C2D	-2.34	1.46	1.51
22	b	607	CLA	CMD-C2D	-2.33	1.46	1.51
22	b	619	CLA	CMD-C2D	-2.33	1.46	1.51
22	B	615	CLA	CMD-C2D	-2.33	1.46	1.51
23	a	408	PL9	C53-C6	-2.32	1.46	1.50
22	d	405	CLA	CMD-C2D	-2.32	1.46	1.51
22	a	405	CLA	CMD-C2D	-2.32	1.46	1.51
22	A	403	CLA	CMD-C2D	-2.31	1.46	1.51
30	I	102	LMT	O2'-C2'	-2.31	1.37	1.43
22	B	602	CLA	CMD-C2D	-2.31	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	610	CLA	C3B-C2B	-2.30	1.37	1.40
22	B	604	CLA	CMD-C2D	-2.30	1.46	1.51
22	H	101	CLA	CMD-C2D	-2.30	1.46	1.51
22	b	608	CLA	CMD-C2D	-2.30	1.46	1.51
30	I	102	LMT	O2B-C2B	-2.30	1.37	1.43
22	C	502	CLA	CMD-C2D	-2.29	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.29	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.29	1.46	1.51
22	h	101	CLA	CMD-C2D	-2.29	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.28	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.28	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.28	1.46	1.51
30	i	102	LMT	O2'-C2'	-2.28	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	CMD-C2D	-2.28	1.46	1.51
30	i	102	LMT	O2B-C2B	-2.28	1.37	1.43
30	b	626	LMT	O2'-C2'	-2.28	1.37	1.43
22	B	614	CLA	CMD-C2D	-2.28	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.28	1.46	1.51
22	c	520	CLA	CMD-C2D	-2.28	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.28	1.46	1.51
23	A	406	PL9	C53-C6	-2.27	1.46	1.50
22	b	606	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
22	b	617	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	507	CLA	CMD-C2D	-2.27	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.27	1.46	1.51
22	b	616	CLA	CMD-C2D	-2.27	1.46	1.51
22	c	503	CLA	CMD-C2D	-2.27	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.27	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.27	1.46	1.51
22	c	505	CLA	CMD-C2D	-2.26	1.46	1.51
22	B	601	CLA	CMD-C2D	-2.26	1.46	1.51
22	b	618	CLA	CMD-C2D	-2.26	1.46	1.51
22	c	511	CLA	CMD-C2D	-2.26	1.46	1.51
22	C	520	CLA	CMD-C2D	-2.26	1.46	1.51
31	D	401	PHO	C1C-NC	-2.26	1.33	1.38
22	B	605	CLA	CMD-C2D	-2.25	1.46	1.51
31	d	402	PHO	C1C-NC	-2.25	1.33	1.38
22	a	407	CLA	CMD-C2D	-2.24	1.46	1.51
22	c	510	CLA	CMD-C2D	-2.24	1.46	1.51
22	d	406	CLA	CMD-C2D	-2.24	1.46	1.51
22	c	506	CLA	CMD-C2D	-2.24	1.46	1.51
22	B	612	CLA	CMD-C2D	-2.24	1.46	1.51
22	c	501	CLA	CMD-C2D	-2.24	1.46	1.51
31	D	402	PHO	C1C-NC	-2.24	1.33	1.38
22	C	506	CLA	CMD-C2D	-2.24	1.46	1.51
22	b	613	CLA	CMD-C2D	-2.23	1.46	1.51
31	d	401	PHO	C1C-NC	-2.23	1.33	1.38
30	M	103	LMT	O2'-C2'	-2.23	1.37	1.43
22	C	510	CLA	CMD-C2D	-2.23	1.46	1.51
30	B	623	LMT	O2'-C2'	-2.23	1.37	1.43
22	D	406	CLA	CMD-C2D	-2.23	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	103	LMT	O3B-C3B	-2.22	1.37	1.43
30	b	627	LMT	O2'-C2'	-2.22	1.37	1.43
30	B	627	LMT	O2'-C2'	-2.22	1.37	1.43
30	B	628	LMT	O3B-C3B	-2.21	1.37	1.43
22	B	610	CLA	CMD-C2D	-2.21	1.46	1.51
30	M	102	LMT	O3B-C3B	-2.21	1.37	1.43
30	b	627	LMT	O3B-C3B	-2.21	1.37	1.43
22	c	512	CLA	CMD-C2D	-2.21	1.46	1.51
30	M	103	LMT	O2B-C2B	-2.21	1.37	1.43
30	M	102	LMT	O2'-C2'	-2.21	1.37	1.43
22	C	501	CLA	CMD-C2D	-2.21	1.46	1.51
30	b	603	LMT	O2B-C2B	-2.20	1.37	1.43
30	D	411	LMT	O3B-C3B	-2.20	1.37	1.43
30	b	603	LMT	O3B-C3B	-2.20	1.37	1.43
25	C	515	DGD	O1G-C1G	-2.20	1.40	1.45
30	B	623	LMT	O3B-C3B	-2.20	1.37	1.43
30	M	102	LMT	O2B-C2B	-2.19	1.37	1.43
30	b	626	LMT	O2B-C2B	-2.19	1.37	1.43
22	b	614	CLA	CMD-C2D	-2.19	1.46	1.51
30	b	604	LMT	O3B-C3B	-2.19	1.37	1.43
30	B	624	LMT	O3B-C3B	-2.18	1.37	1.43
24	g	101	BCR	C33-C5	-2.18	1.47	1.51
30	I	102	LMT	O3B-C3B	-2.18	1.37	1.43
22	C	512	CLA	CMD-C2D	-2.18	1.46	1.51
30	D	411	LMT	O2'-C2'	-2.17	1.37	1.43
30	B	627	LMT	O2B-C2B	-2.17	1.37	1.43
30	d	411	LMT	O3B-C3B	-2.17	1.37	1.43
29	b	602	SQD	O2-C2	-2.17	1.37	1.43
30	b	603	LMT	O2'-C2'	-2.17	1.37	1.43
30	b	604	LMT	O2B-C2B	-2.16	1.37	1.43
30	d	411	LMT	O2'-C2'	-2.16	1.37	1.43
25	c	515	DGD	O2G-C2G	-2.16	1.41	1.46
30	D	411	LMT	O2B-C2B	-2.16	1.37	1.43
30	b	626	LMT	O3B-C3B	-2.16	1.37	1.43
30	B	624	LMT	O2'-C2'	-2.16	1.37	1.43
30	i	102	LMT	O3B-C3B	-2.16	1.37	1.43
34	F	101	HEM	C2B-C1B	-2.15	1.44	1.51
30	B	627	LMT	O3B-C3B	-2.15	1.37	1.43
30	B	628	LMT	O2'-C2'	-2.15	1.37	1.43
30	B	628	LMT	O2B-C2B	-2.15	1.37	1.43
29	B	626	SQD	O2-C2	-2.15	1.37	1.43
30	B	623	LMT	O2B-C2B	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	411	LMT	O2B-C2B	-2.14	1.37	1.43
34	f	101	HEM	C2B-C1B	-2.12	1.44	1.51
30	b	604	LMT	O2'-C2'	-2.12	1.37	1.43
22	b	619	CLA	CMC-C2C	-2.11	1.46	1.50
24	y	101	BCR	C33-C5	-2.11	1.47	1.51
25	c	516	DGD	O2G-C2G	-2.11	1.41	1.46
34	V	201	HEM	C2D-C1D	-2.10	1.45	1.51
26	a	411	LHG	O7-C5	-2.09	1.41	1.46
22	B	615	CLA	CMC-C2C	-2.09	1.46	1.50
31	D	402	PHO	CMC-C2C	-2.09	1.46	1.50
29	A	413	SQD	O3-C3	-2.08	1.38	1.43
25	a	410	DGD	O1G-C1G	-2.08	1.40	1.45
25	C	516	DGD	O2G-C2G	-2.08	1.41	1.46
30	b	627	LMT	O2B-C2B	-2.07	1.38	1.43
30	B	624	LMT	O2B-C2B	-2.07	1.38	1.43
23	D	407	PL9	C53-C6	-2.06	1.46	1.50
22	C	502	CLA	CMC-C2C	-2.06	1.46	1.50
27	D	412	LMG	O7-C8	-2.06	1.41	1.46
29	a	401	SQD	O3-C3	-2.06	1.38	1.43
30	M	103	LMT	O4'-C4B	-2.06	1.38	1.43
25	B	620	DGD	O2G-C2G	-2.05	1.41	1.46
31	d	402	PHO	CMC-C2C	-2.05	1.46	1.50
29	f	103	SQD	O3-C3	-2.04	1.38	1.43
34	v	201	HEM	C2D-C1D	-2.04	1.45	1.51
29	A	412	SQD	O2-C2	-2.04	1.38	1.43
22	b	615	CLA	CMC-C2C	-2.04	1.46	1.50
27	d	412	LMG	O7-C8	-2.04	1.41	1.46
24	C	514	BCR	C38-C26	-2.03	1.47	1.51
29	a	415	SQD	O2-C2	-2.03	1.38	1.43
34	f	101	HEM	C2D-C1D	-2.03	1.45	1.51
31	d	401	PHO	CMC-C2C	-2.03	1.46	1.50
29	b	602	SQD	O3-C3	-2.03	1.38	1.43
22	c	502	CLA	CMC-C2C	-2.02	1.46	1.50
34	F	101	HEM	C2D-C1D	-2.02	1.45	1.51
29	f	103	SQD	O2-C2	-2.02	1.38	1.43
30	B	628	LMT	O4'-C4B	-2.02	1.38	1.43
29	F	103	SQD	O3-C3	-2.02	1.38	1.43
31	D	401	PHO	CMC-C2C	-2.02	1.46	1.50
31	d	401	PHO	CMD-C2D	-2.02	1.46	1.50
22	B	601	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	605	CLA	CMC-C2C	-2.01	1.46	1.50
30	M	102	LMT	O4'-C4B	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	618	CLA	CMC-C2C	-2.01	1.46	1.50
31	D	402	PHO	CMD-C2D	-2.01	1.46	1.50
23	j	101	PL9	C53-C6	-2.01	1.46	1.50
27	D	408	LMG	O7-C8	-2.01	1.41	1.46
29	B	626	SQD	O3-C3	-2.01	1.38	1.43
29	d	403	SQD	O2-C2	-2.01	1.38	1.43
22	B	611	CLA	CMC-C2C	-2.01	1.46	1.50
31	D	401	PHO	CMD-C2D	-2.00	1.46	1.50
23	d	407	PL9	C53-C6	-2.00	1.46	1.50
29	F	103	SQD	O2-C2	-2.00	1.38	1.43
30	d	411	LMT	O4'-C4B	-2.00	1.38	1.43
24	J	102	BCR	C38-C26	-2.00	1.47	1.51
31	d	401	PHO	C1B-C2B	2.01	1.50	1.45
34	f	101	HEM	C4C-NC	2.01	1.38	1.36
25	d	410	DGD	C1D-C2D	2.02	1.58	1.52
34	V	201	HEM	FE-NB	2.03	2.08	1.97
34	F	101	HEM	C1C-NC	2.03	1.38	1.36
34	f	101	HEM	C3B-CAB	2.03	1.55	1.51
31	D	402	PHO	C1B-C2B	2.06	1.50	1.45
34	V	201	HEM	C1C-NC	2.07	1.38	1.36
34	F	101	HEM	C3B-CAB	2.07	1.55	1.51
25	c	517	DGD	C3G-C2G	2.07	1.56	1.50
25	b	601	DGD	C4D-C5D	2.08	1.57	1.53
34	f	101	HEM	C1C-NC	2.09	1.38	1.36
34	v	201	HEM	C1C-NC	2.10	1.38	1.36
25	C	517	DGD	C3G-C2G	2.12	1.56	1.50
27	b	625	LMG	C4-C5	2.13	1.57	1.53
27	A	410	LMG	C7-C8	2.14	1.56	1.50
27	m	101	LMG	C7-C8	2.16	1.56	1.50
34	f	101	HEM	FE-NB	2.17	2.09	1.97
27	M	101	LMG	C7-C8	2.19	1.56	1.50
27	a	412	LMG	C7-C8	2.19	1.56	1.50
34	V	201	HEM	C3C-CAC	2.19	1.55	1.51
25	c	517	DGD	C1G-C2G	2.20	1.56	1.50
27	B	621	LMG	C4-C5	2.20	1.57	1.53
25	C	517	DGD	C1G-C2G	2.20	1.57	1.50
31	d	401	PHO	CHD-C1D	2.21	1.43	1.38
34	v	201	HEM	C3C-CAC	2.21	1.55	1.51
34	v	201	HEM	FE-NB	2.21	2.09	1.97
31	D	401	PHO	CHD-C1D	2.22	1.43	1.38
22	b	614	CLA	CHC-C1C	2.23	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	401	PHO	C4C-C3C	2.23	1.49	1.45
22	B	610	CLA	CHC-C1C	2.23	1.42	1.35
31	D	402	PHO	C4C-C3C	2.24	1.49	1.45
25	b	601	DGD	C1G-C2G	2.25	1.57	1.50
34	V	201	HEM	C4C-NC	2.25	1.38	1.36
31	d	402	PHO	C1A-NA	2.25	1.42	1.37
31	D	401	PHO	C4C-C3C	2.26	1.49	1.45
31	D	401	PHO	C1A-NA	2.27	1.42	1.37
34	F	101	HEM	C3C-CAC	2.27	1.55	1.51
31	d	402	PHO	C4C-C3C	2.29	1.49	1.45
25	b	601	DGD	C3G-C2G	2.29	1.57	1.50
31	d	401	PHO	C1A-NA	2.30	1.42	1.37
34	v	201	HEM	C4C-NC	2.31	1.38	1.36
31	D	402	PHO	C1A-NA	2.31	1.42	1.37
34	f	101	HEM	C3C-CAC	2.32	1.55	1.51
34	v	201	HEM	C3B-CAB	2.33	1.55	1.51
25	B	625	DGD	C3G-C2G	2.33	1.57	1.50
34	V	201	HEM	C3B-CAB	2.35	1.55	1.51
31	D	402	PHO	CHD-C1D	2.36	1.43	1.38
34	f	101	HEM	FE-NC	2.37	2.05	1.95
22	a	405	CLA	CHC-C1C	2.38	1.42	1.35
34	V	201	HEM	FE-NC	2.38	2.05	1.95
22	c	501	CLA	CHC-C1C	2.39	1.42	1.35
31	d	402	PHO	CHD-C1D	2.39	1.43	1.38
34	F	101	HEM	FE-NC	2.39	2.05	1.95
25	B	625	DGD	C4D-C5D	2.40	1.58	1.53
22	B	615	CLA	CHC-C1C	2.40	1.42	1.35
22	A	405	CLA	CHC-C1C	2.41	1.42	1.35
22	B	611	CLA	CHC-C1C	2.41	1.42	1.35
22	b	619	CLA	CHC-C1C	2.41	1.42	1.35
22	D	406	CLA	CHC-C1C	2.41	1.42	1.35
22	C	503	CLA	CHC-C1C	2.41	1.42	1.35
22	C	501	CLA	CHC-C1C	2.41	1.42	1.35
22	b	615	CLA	CHC-C1C	2.42	1.42	1.35
22	c	506	CLA	CHC-C1C	2.42	1.42	1.35
22	C	507	CLA	CHC-C1C	2.42	1.42	1.35
22	b	605	CLA	CHC-C1C	2.43	1.42	1.35
22	B	601	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	c	520	CLA	CHC-C1C	2.44	1.42	1.35
22	b	610	CLA	CHC-C1C	2.44	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	CHC-C1C	2.44	1.42	1.35
22	B	612	CLA	CHC-C1C	2.44	1.42	1.35
22	c	503	CLA	CHC-C1C	2.44	1.42	1.35
22	C	510	CLA	CHC-C1C	2.44	1.42	1.35
22	b	608	CLA	CHC-C1C	2.44	1.42	1.35
22	B	606	CLA	CHC-C1C	2.44	1.42	1.35
22	B	605	CLA	CHC-C1C	2.45	1.43	1.35
34	V	201	HEM	FE-ND	2.45	2.10	1.97
22	A	403	CLA	CHC-C1C	2.45	1.43	1.35
22	b	613	CLA	CHC-C1C	2.45	1.43	1.35
22	C	520	CLA	CHC-C1C	2.45	1.43	1.35
22	A	404	CLA	CHC-C1C	2.46	1.43	1.35
22	c	510	CLA	CHC-C1C	2.46	1.43	1.35
22	C	508	CLA	CHC-C1C	2.46	1.43	1.35
34	v	201	HEM	FE-ND	2.47	2.10	1.97
22	c	508	CLA	CHC-C1C	2.47	1.43	1.35
22	B	604	CLA	CHC-C1C	2.47	1.43	1.35
22	B	614	CLA	CHC-C1C	2.47	1.43	1.35
22	C	504	CLA	CHC-C1C	2.47	1.43	1.35
22	b	618	CLA	CHC-C1C	2.47	1.43	1.35
22	B	602	CLA	CHC-C1C	2.47	1.43	1.35
22	b	607	CLA	CHC-C1C	2.47	1.43	1.35
22	b	616	CLA	CHC-C1C	2.47	1.43	1.35
22	B	603	CLA	CHC-C1C	2.48	1.43	1.35
22	B	609	CLA	CHC-C1C	2.48	1.43	1.35
22	a	407	CLA	CHC-C1C	2.48	1.43	1.35
22	D	405	CLA	CHC-C1C	2.48	1.43	1.35
22	c	505	CLA	CHC-C1C	2.48	1.43	1.35
22	C	509	CLA	CHC-C1C	2.48	1.43	1.35
22	c	504	CLA	CHC-C1C	2.48	1.43	1.35
22	a	406	CLA	CHC-C1C	2.48	1.43	1.35
22	C	502	CLA	CHC-C1C	2.48	1.43	1.35
22	d	405	CLA	CHC-C1C	2.49	1.43	1.35
22	c	509	CLA	CHC-C1C	2.49	1.43	1.35
22	C	511	CLA	CHC-C1C	2.49	1.43	1.35
22	c	512	CLA	CHC-C1C	2.49	1.43	1.35
22	c	511	CLA	CHC-C1C	2.49	1.43	1.35
22	C	512	CLA	CHC-C1C	2.49	1.43	1.35
22	c	507	CLA	CHC-C1C	2.49	1.43	1.35
22	C	505	CLA	CHC-C1C	2.50	1.43	1.35
22	d	406	CLA	CHC-C1C	2.51	1.43	1.35
22	c	502	CLA	CHC-C1C	2.51	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	CHC-C1C	2.51	1.43	1.35
22	B	607	CLA	CHC-C1C	2.51	1.43	1.35
22	b	617	CLA	CHC-C1C	2.52	1.43	1.35
22	b	606	CLA	CHC-C1C	2.52	1.43	1.35
31	d	401	PHO	C4C-NC	2.53	1.42	1.37
31	D	401	PHO	C4C-NC	2.53	1.42	1.37
22	b	611	CLA	CHC-C1C	2.54	1.43	1.35
22	b	612	CLA	CHC-C1C	2.54	1.43	1.35
22	H	101	CLA	CHC-C1C	2.54	1.43	1.35
22	h	101	CLA	CHC-C1C	2.56	1.43	1.35
31	D	402	PHO	C4C-NC	2.56	1.42	1.37
22	B	613	CLA	CHC-C1C	2.58	1.43	1.35
22	B	608	CLA	CHC-C1C	2.58	1.43	1.35
31	d	402	PHO	C4C-NC	2.59	1.42	1.37
34	f	101	HEM	FE-ND	2.59	2.11	1.97
29	f	103	SQD	O47-C7	2.66	1.42	1.34
29	B	626	SQD	O47-C7	2.66	1.42	1.34
29	b	602	SQD	O47-C7	2.67	1.42	1.34
29	F	103	SQD	O47-C7	2.71	1.42	1.34
29	A	412	SQD	O47-C7	2.73	1.42	1.34
29	A	413	SQD	O47-C7	2.73	1.42	1.34
29	a	401	SQD	O47-C7	2.74	1.42	1.34
29	a	415	SQD	O47-C7	2.74	1.42	1.34
25	B	625	DGD	C1E-C2E	2.75	1.60	1.52
29	B	622	SQD	O47-C7	2.75	1.42	1.34
29	d	403	SQD	O47-C7	2.78	1.42	1.34
34	v	201	HEM	FE-NC	2.80	2.06	1.95
34	F	101	HEM	FE-ND	2.80	2.12	1.97
31	d	401	PHO	CHC-C1C	2.81	1.44	1.38
25	b	601	DGD	C1E-C2E	2.82	1.61	1.52
31	D	401	PHO	CHC-C1C	2.85	1.44	1.38
31	d	401	PHO	C3B-C4B	2.88	1.49	1.43
31	d	402	PHO	CHC-C1C	2.94	1.44	1.38
31	D	402	PHO	CHC-C1C	2.95	1.44	1.38
31	D	401	PHO	C3B-C4B	2.96	1.50	1.43
29	A	412	SQD	O48-C23	2.97	1.42	1.33
29	a	415	SQD	O48-C23	3.01	1.42	1.33
29	B	626	SQD	O48-C23	3.03	1.42	1.33
29	B	622	SQD	O48-C23	3.03	1.42	1.33
29	A	413	SQD	O48-C23	3.04	1.42	1.33
29	F	103	SQD	O48-C23	3.05	1.42	1.33
31	d	402	PHO	C3B-C4B	3.06	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	f	103	SQD	O48-C23	3.06	1.42	1.33
29	d	403	SQD	O48-C23	3.07	1.42	1.33
31	D	402	PHO	C3B-C4B	3.07	1.50	1.43
29	b	602	SQD	O48-C23	3.08	1.42	1.33
29	a	401	SQD	O48-C23	3.10	1.42	1.33

All (1184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	j	101	PL9	C7-C3-C2	-6.10	118.36	123.42
23	J	101	PL9	C7-C3-C2	-6.03	118.42	123.42
23	d	407	PL9	C7-C3-C2	-5.87	118.55	123.42
23	D	407	PL9	C7-C3-C2	-5.74	118.66	123.42
23	A	406	PL9	C7-C3-C2	-5.73	118.66	123.42
23	a	408	PL9	C7-C3-C2	-5.59	118.78	123.42
25	A	408	DGD	O3G-C3G-C2G	-4.95	99.22	110.99
25	a	410	DGD	O3G-C3G-C2G	-4.85	99.46	110.99
22	B	610	CLA	CMB-C2B-C1B	-4.73	120.54	128.36
22	b	614	CLA	CMB-C2B-C1B	-4.65	120.67	128.36
25	C	517	DGD	O3G-C3G-C2G	-4.56	100.13	110.99
25	c	517	DGD	O3G-C3G-C2G	-4.36	100.61	110.99
27	D	409	LMG	C1-C2-C3	-4.07	101.95	109.97
27	d	409	LMG	C1-C2-C3	-4.04	102.01	109.97
22	c	507	CLA	CMB-C2B-C1B	-3.87	121.97	128.36
25	c	516	DGD	O5D-C6D-C5D	-3.84	102.11	109.08
24	J	102	BCR	C11-C10-C9	-3.80	121.71	127.20
22	C	507	CLA	CMB-C2B-C1B	-3.78	122.11	128.36
22	b	616	CLA	CMB-C2B-C1B	-3.76	122.14	128.36
22	B	612	CLA	CMB-C2B-C1B	-3.74	122.17	128.36
25	C	516	DGD	O5D-C6D-C5D	-3.68	102.40	109.08
25	C	516	DGD	O3G-C3G-C2G	-3.62	102.37	110.99
24	j	102	BCR	C11-C10-C9	-3.62	121.97	127.20
25	c	516	DGD	O3G-C3G-C2G	-3.62	102.39	110.99
22	b	611	CLA	CMB-C2B-C1B	-3.58	122.44	128.36
25	d	410	DGD	O6D-C1D-O3G	-3.57	101.46	110.05
25	D	410	DGD	O6D-C1D-O3G	-3.55	101.51	110.05
24	B	617	BCR	C33-C5-C6	-3.53	121.14	124.61
24	b	621	BCR	C33-C5-C6	-3.52	121.15	124.61
29	F	103	SQD	O9-S-O7	-3.50	100.74	113.48
29	f	103	SQD	O9-S-O7	-3.48	100.78	113.48
22	B	607	CLA	CMB-C2B-C1B	-3.47	122.62	128.36
29	A	412	SQD	O9-S-O7	-3.45	100.90	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	620	DGD	O3G-C3G-C2G	-3.45	102.78	110.99
29	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	H	102	BCR	C33-C5-C6	-3.44	121.23	124.61
29	d	403	SQD	O9-S-O7	-3.43	100.97	113.48
22	c	510	CLA	CMB-C2B-C1B	-3.41	122.71	128.36
29	B	622	SQD	O9-S-O7	-3.41	101.06	113.48
29	a	401	SQD	O9-S-O7	-3.41	101.07	113.48
25	C	515	DGD	O3G-C3G-C2G	-3.40	102.89	110.99
29	B	626	SQD	O9-S-O7	-3.40	101.08	113.48
24	x	101	BCR	C33-C5-C6	-3.40	121.27	124.61
24	f	102	BCR	C33-C5-C6	-3.40	121.27	124.61
29	b	602	SQD	O9-S-O7	-3.39	101.12	113.48
29	A	413	SQD	O9-S-O7	-3.39	101.13	113.48
25	c	515	DGD	O3G-C3G-C2G	-3.39	102.93	110.99
22	b	615	CLA	CMB-C2B-C1B	-3.38	122.77	128.36
25	b	624	DGD	O3G-C3G-C2G	-3.37	102.98	110.99
22	b	617	CLA	CMB-C2B-C1B	-3.37	122.80	128.36
22	B	602	CLA	CMB-C2B-C1B	-3.36	122.80	128.36
24	J	102	BCR	C3-C4-C5	-3.36	108.53	113.87
22	c	512	CLA	CMB-C2B-C1B	-3.35	122.82	128.36
22	C	505	CLA	CMB-C2B-C1B	-3.35	122.82	128.36
22	B	613	CLA	CMB-C2B-C1B	-3.34	122.84	128.36
22	B	611	CLA	CMB-C2B-C1B	-3.34	122.84	128.36
22	b	613	CLA	CMB-C2B-C1B	-3.33	122.86	128.36
22	C	503	CLA	CMB-C2B-C1B	-3.33	122.86	128.36
22	C	506	CLA	CMB-C2B-C1B	-3.32	122.86	128.36
22	c	505	CLA	CMB-C2B-C1B	-3.32	122.87	128.36
22	b	606	CLA	CMB-C2B-C1B	-3.32	122.88	128.36
22	c	503	CLA	CMB-C2B-C1B	-3.32	122.88	128.36
22	A	405	CLA	CMB-C2B-C1B	-3.31	122.88	128.36
22	C	510	CLA	CMB-C2B-C1B	-3.31	122.88	128.36
22	c	506	CLA	CMB-C2B-C1B	-3.31	122.89	128.36
22	B	609	CLA	CMB-C2B-C1B	-3.31	122.89	128.36
24	j	102	BCR	C3-C4-C5	-3.30	108.63	113.87
22	a	404	CLA	CMB-C2B-C1B	-3.28	122.94	128.36
22	C	512	CLA	CMB-C2B-C1B	-3.28	122.94	128.36
22	c	511	CLA	CMB-C2B-C1B	-3.27	122.96	128.36
22	a	407	CLA	CMB-C2B-C1B	-3.26	122.96	128.36
22	C	502	CLA	CMB-C2B-C1B	-3.26	122.97	128.36
22	A	402	CLA	CMB-C2B-C1B	-3.25	122.99	128.36
22	c	502	CLA	CMB-C2B-C1B	-3.24	123.00	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	410	DGD	O3G-C3G-C2G	-3.24	103.28	110.99
22	D	405	CLA	CMB-C2B-C1B	-3.22	123.03	128.36
22	C	511	CLA	CMB-C2B-C1B	-3.22	123.04	128.36
22	D	406	CLA	CMB-C2B-C1B	-3.19	123.08	128.36
22	B	614	CLA	CMB-C2B-C1B	-3.19	123.09	128.36
22	C	509	CLA	CMB-C2B-C1B	-3.19	123.09	128.36
22	B	604	CLA	CMB-C2B-C1B	-3.19	123.09	128.36
22	b	605	CLA	CMB-C2B-C1B	-3.18	123.10	128.36
24	b	622	BCR	C24-C23-C22	-3.17	121.38	126.22
25	D	410	DGD	O3G-C3G-C2G	-3.17	103.44	110.99
30	B	628	LMT	C1'-O5'-C5'	-3.17	107.59	113.75
24	j	102	BCR	C24-C23-C22	-3.17	121.38	126.22
22	d	405	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
22	c	520	CLA	CMB-C2B-C1B	-3.16	123.13	128.36
22	a	405	CLA	CMB-C2B-C1B	-3.16	123.13	128.36
22	c	509	CLA	CMB-C2B-C1B	-3.15	123.14	128.36
22	B	601	CLA	CMB-C2B-C1B	-3.14	123.16	128.36
24	y	101	BCR	C38-C26-C25	-3.14	121.52	124.61
22	B	605	CLA	CMB-C2B-C1B	-3.14	123.17	128.36
22	C	520	CLA	CMB-C2B-C1B	-3.14	123.17	128.36
24	J	102	BCR	C24-C23-C22	-3.13	121.44	126.22
22	b	618	CLA	CMB-C2B-C1B	-3.13	123.19	128.36
22	d	406	CLA	CMB-C2B-C1B	-3.13	123.19	128.36
24	g	101	BCR	C38-C26-C25	-3.12	121.54	124.61
25	b	624	DGD	O6D-C1D-O3G	-3.12	102.54	110.05
22	A	403	CLA	CMB-C2B-C1B	-3.11	123.21	128.36
22	b	607	CLA	CMB-C2B-C1B	-3.11	123.22	128.36
25	B	620	DGD	O6D-C1D-O3G	-3.10	102.58	110.05
30	b	604	LMT	C1'-O5'-C5'	-3.10	107.73	113.75
22	C	508	CLA	CMB-C2B-C1B	-3.10	123.24	128.36
22	A	404	CLA	CMB-C2B-C1B	-3.09	123.26	128.36
25	c	516	DGD	O6D-C1D-O3G	-3.09	102.62	110.05
22	b	608	CLA	CMB-C2B-C1B	-3.08	123.27	128.36
22	c	508	CLA	CMB-C2B-C1B	-3.08	123.27	128.36
23	A	406	PL9	C22-C23-C24	-3.08	121.07	127.76
24	b	620	BCR	C33-C5-C6	-3.08	121.58	124.61
24	B	616	BCR	C33-C5-C6	-3.07	121.59	124.61
22	H	101	CLA	CMB-C2B-C1B	-3.07	123.29	128.36
23	a	408	PL9	C22-C23-C24	-3.05	121.13	127.76
22	h	101	CLA	CMB-C2B-C1B	-3.04	123.33	128.36
22	b	609	CLA	CMB-C2B-C1B	-3.04	123.33	128.36
22	b	610	CLA	CMB-C2B-C1B	-3.04	123.33	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	CMB-C2B-C1B	-3.04	123.33	128.36
25	A	408	DGD	O6D-C1D-O3G	-3.03	102.75	110.05
22	B	605	CLA	O2D-CGD-O1D	-3.03	117.54	123.79
25	c	517	DGD	C1D-C2D-C3D	-3.02	104.01	109.97
24	g	101	BCR	C33-C5-C6	-3.02	121.64	124.61
22	B	615	CLA	CMB-C2B-C1B	-3.02	123.37	128.36
25	C	516	DGD	O6D-C1D-O3G	-3.02	102.79	110.05
22	b	619	CLA	CMB-C2B-C1B	-3.01	123.39	128.36
24	j	102	BCR	C7-C8-C9	-3.01	121.63	126.22
22	a	406	CLA	CMB-C2B-C1B	-3.00	123.40	128.36
22	B	603	CLA	O2D-CGD-O1D	-3.00	117.60	123.79
22	b	609	CLA	O2D-CGD-O1D	-3.00	117.60	123.79
24	J	102	BCR	C38-C26-C25	-3.00	121.66	124.61
23	D	407	PL9	C22-C23-C24	-2.99	121.27	127.76
24	J	102	BCR	C7-C8-C9	-2.98	121.67	126.22
22	B	613	CLA	O2D-CGD-O1D	-2.98	117.64	123.79
25	B	625	DGD	C1D-C2D-C3D	-2.97	104.12	109.97
25	C	517	DGD	C1D-C2D-C3D	-2.96	104.14	109.97
24	B	619	BCR	C3-C4-C5	-2.95	109.18	113.87
22	c	503	CLA	O2D-CGD-O1D	-2.95	117.70	123.79
24	j	102	BCR	C38-C26-C25	-2.94	121.72	124.61
24	y	101	BCR	C33-C5-C6	-2.94	121.72	124.61
24	b	623	BCR	C3-C4-C5	-2.94	109.21	113.87
22	b	617	CLA	O2D-CGD-O1D	-2.93	117.74	123.79
27	d	408	LMG	O6-C1-O1	-2.93	103.00	110.05
22	b	606	CLA	O2D-CGD-O1D	-2.93	117.75	123.79
24	B	617	BCR	C28-C27-C26	-2.92	109.23	113.87
24	C	514	BCR	C33-C5-C6	-2.92	121.74	124.61
25	c	515	DGD	O6D-C1D-O3G	-2.91	103.04	110.05
22	B	606	CLA	CMB-C2B-C1B	-2.91	123.54	128.36
25	b	601	DGD	C3G-C2G-C1G	-2.91	105.27	112.07
25	a	410	DGD	O6D-C1D-O3G	-2.90	103.06	110.05
25	C	517	DGD	O5D-C6D-C5D	-2.90	103.82	109.08
23	J	101	PL9	C22-C23-C24	-2.90	121.45	127.76
25	b	601	DGD	C1D-C2D-C3D	-2.90	104.26	109.97
24	b	621	BCR	C28-C27-C26	-2.90	109.27	113.87
22	c	507	CLA	O2D-CGD-O1D	-2.90	117.81	123.79
25	c	517	DGD	O5D-C6D-C5D	-2.89	103.83	109.08
22	b	612	CLA	CMB-C2B-C1B	-2.89	123.58	128.36
24	c	514	BCR	C33-C5-C6	-2.89	121.77	124.61
22	B	608	CLA	CMB-C2B-C1B	-2.89	123.58	128.36
30	B	624	LMT	C3'-C4'-C5'	-2.89	104.31	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	607	CLA	O2D-CGD-O1D	-2.88	117.83	123.79
23	d	407	PL9	C22-C23-C24	-2.88	121.49	127.76
22	C	505	CLA	O2D-CGD-O1D	-2.88	117.84	123.79
22	C	503	CLA	O2D-CGD-O1D	-2.87	117.85	123.79
25	c	517	DGD	CDB-CCB-CBB	-2.87	99.70	114.53
25	C	517	DGD	CDB-CCB-CBB	-2.87	99.70	114.53
22	c	504	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
22	B	608	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
22	b	610	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
22	C	502	CLA	O2D-CGD-O1D	-2.86	117.88	123.79
23	j	101	PL9	C22-C23-C24	-2.86	121.54	127.76
25	C	515	DGD	O6D-C1D-O3G	-2.86	103.16	110.05
24	B	617	BCR	C15-C16-C17	-2.86	117.07	123.39
25	B	625	DGD	C3G-C2G-C1G	-2.86	105.39	112.07
25	b	601	DGD	O3G-C3G-C2G	-2.85	104.20	110.99
22	B	606	CLA	O2D-CGD-O1D	-2.85	117.90	123.79
22	C	504	CLA	O2D-CGD-O1D	-2.85	117.91	123.79
22	b	605	CLA	O2D-CGD-O1D	-2.84	117.92	123.79
25	c	516	DGD	CDB-CCB-CBB	-2.82	99.97	114.53
24	c	514	BCR	C28-C27-C26	-2.81	109.41	113.87
22	b	611	CLA	O2D-CGD-O1D	-2.80	118.00	123.79
30	b	627	LMT	C3'-C4'-C5'	-2.80	104.50	110.84
24	b	621	BCR	C15-C16-C17	-2.79	117.21	123.39
27	D	408	LMG	O6-C1-O1	-2.79	103.33	110.05
25	C	516	DGD	CDB-CCB-CBB	-2.79	100.10	114.53
22	b	608	CLA	O2D-CGD-O1D	-2.79	118.02	123.79
25	B	625	DGD	O3G-C3G-C2G	-2.78	104.37	110.99
24	C	514	BCR	C28-C27-C26	-2.78	109.46	113.87
22	B	602	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
22	C	504	CLA	CMB-C2B-C1B	-2.77	123.78	128.36
22	B	604	CLA	O2D-CGD-O1D	-2.77	118.06	123.79
22	b	612	CLA	O2D-CGD-O1D	-2.77	118.08	123.79
22	c	504	CLA	CMB-C2B-C1B	-2.77	123.79	128.36
22	a	406	CLA	O2D-CGD-O1D	-2.77	118.08	123.79
22	c	505	CLA	O2D-CGD-O1D	-2.76	118.08	123.79
22	C	507	CLA	O2D-CGD-O1D	-2.76	118.08	123.79
22	C	506	CLA	O2D-CGD-O1D	-2.76	118.09	123.79
22	a	404	CLA	O2D-CGD-O1D	-2.75	118.10	123.79
25	D	410	DGD	CDB-CCB-CBB	-2.75	100.31	114.53
22	B	607	CLA	O2D-CGD-O1D	-2.74	118.13	123.79
22	c	520	CLA	O2D-CGD-O1D	-2.74	118.14	123.79
25	d	410	DGD	CDB-CCB-CBB	-2.74	100.39	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	501	CLA	O2D-CGD-O1D	-2.74	118.14	123.79
22	c	511	CLA	O2D-CGD-O1D	-2.74	118.14	123.79
25	A	408	DGD	O5D-C6D-C5D	-2.73	104.12	109.08
22	C	510	CLA	O2D-CGD-O1D	-2.73	118.15	123.79
22	c	501	CLA	O2D-CGD-O1D	-2.73	118.15	123.79
22	d	406	CLA	O2D-CGD-O1D	-2.73	118.15	123.79
24	J	102	BCR	C35-C13-C14	-2.73	118.87	122.90
22	b	616	CLA	O2D-CGD-O1D	-2.73	118.16	123.79
22	c	506	CLA	O2D-CGD-O1D	-2.73	118.16	123.79
22	A	402	CLA	O2D-CGD-O1D	-2.73	118.16	123.79
22	c	512	CLA	O2D-CGD-O1D	-2.72	118.16	123.79
22	A	403	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
22	c	510	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
22	b	613	CLA	O2D-CGD-O1D	-2.72	118.18	123.79
22	B	601	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
22	H	101	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
22	B	609	CLA	O2D-CGD-O1D	-2.69	118.23	123.79
27	M	101	LMG	C1-C2-C3	-2.69	104.67	109.97
22	B	612	CLA	O2D-CGD-O1D	-2.69	118.24	123.79
22	b	618	CLA	O2D-CGD-O1D	-2.68	118.25	123.79
22	c	502	CLA	O2D-CGD-O1D	-2.68	118.26	123.79
27	C	518	LMG	O6-C1-O1	-2.68	103.61	110.05
23	D	407	PL9	C27-C28-C29	-2.67	121.95	127.76
22	B	614	CLA	O2D-CGD-O1D	-2.67	118.27	123.79
24	B	618	BCR	C24-C23-C22	-2.67	122.14	126.22
22	C	520	CLA	O2D-CGD-O1D	-2.67	118.28	123.79
27	i	101	LMG	O6-C1-O1	-2.66	103.65	110.05
24	b	621	BCR	C15-C14-C13	-2.66	123.36	127.20
22	D	406	CLA	O2D-CGD-O1D	-2.66	118.30	123.79
30	M	102	LMT	C1'-O5'-C5'	-2.65	108.59	113.75
22	d	405	CLA	O2D-CGD-O1D	-2.65	118.32	123.79
25	C	517	DGD	C1D-O6D-C5D	-2.65	108.61	113.75
24	a	409	BCR	C33-C5-C6	-2.65	122.01	124.61
22	c	501	CLA	CMB-C2B-C1B	-2.65	123.99	128.36
24	y	101	BCR	C7-C8-C9	-2.64	122.19	126.22
25	c	517	DGD	C1D-O6D-C5D	-2.64	108.62	113.75
22	C	509	CLA	O2D-CGD-O1D	-2.64	118.34	123.79
22	A	404	CLA	O2D-CGD-O1D	-2.64	118.34	123.79
23	d	407	PL9	C7-C8-C9	-2.64	122.22	126.70
31	D	402	PHO	O2D-CGD-O1D	-2.64	118.34	123.79
27	I	101	LMG	O6-C1-O1	-2.64	103.71	110.05
24	j	102	BCR	C15-C14-C13	-2.63	123.40	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	408	PL9	C27-C28-C29	-2.63	122.05	127.76
24	j	102	BCR	C35-C13-C14	-2.63	119.02	122.90
27	B	621	LMG	C1-C2-C3	-2.63	104.79	109.97
23	J	101	PL9	C7-C8-C9	-2.63	122.25	126.70
30	B	623	LMT	C1'-O5'-C5'	-2.62	108.65	113.75
23	A	406	PL9	C27-C28-C29	-2.62	122.06	127.76
24	K	102	BCR	C33-C5-C6	-2.62	122.03	124.61
23	d	407	PL9	C27-C28-C29	-2.62	122.07	127.76
22	b	614	CLA	O2D-CGD-O1D	-2.61	118.39	123.79
22	h	101	CLA	O2D-CGD-O1D	-2.61	118.39	123.79
23	j	101	PL9	C7-C8-C9	-2.61	122.28	126.70
24	c	513	BCR	C11-C10-C9	-2.60	123.44	127.20
24	A	407	BCR	C33-C5-C6	-2.60	122.05	124.61
27	c	518	LMG	O6-C1-O1	-2.60	103.79	110.05
25	d	410	DGD	C3G-C2G-C1G	-2.60	105.99	112.07
22	C	512	CLA	O2D-CGD-O1D	-2.60	118.42	123.79
22	B	610	CLA	O2D-CGD-O1D	-2.59	118.45	123.79
22	C	511	CLA	O2D-CGD-O1D	-2.59	118.45	123.79
22	c	509	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
24	J	102	BCR	C15-C14-C13	-2.58	123.47	127.20
22	a	405	CLA	O2D-CGD-O1D	-2.58	118.47	123.79
24	g	101	BCR	C7-C8-C9	-2.57	122.29	126.22
23	D	407	PL9	C37-C38-C39	-2.57	122.17	127.76
23	D	407	PL9	C7-C8-C9	-2.57	122.34	126.70
25	a	410	DGD	O5D-C6D-C5D	-2.57	104.42	109.08
31	D	401	PHO	O2D-CGD-O1D	-2.57	118.49	123.79
27	a	402	LMG	O6-C1-O1	-2.56	103.88	110.05
22	C	501	CLA	CMB-C2B-C1B	-2.55	124.14	128.36
24	c	514	BCR	C11-C10-C9	-2.55	123.51	127.20
31	d	401	PHO	O2D-CGD-O1D	-2.55	118.53	123.79
24	K	102	BCR	C15-C16-C17	-2.55	117.75	123.39
23	d	407	PL9	C37-C38-C39	-2.55	122.22	127.76
24	c	521	BCR	C15-C16-C17	-2.55	117.76	123.39
24	C	513	BCR	C24-C23-C22	-2.54	122.34	126.22
24	c	521	BCR	C33-C5-C6	-2.54	122.11	124.61
30	b	626	LMT	C1'-O5'-C5'	-2.54	108.82	113.75
22	a	407	CLA	O2D-CGD-O1D	-2.54	118.55	123.79
24	b	623	BCR	C38-C26-C25	-2.54	122.11	124.61
24	C	514	BCR	C38-C26-C25	-2.54	122.11	124.61
23	d	407	PL9	C31-C32-C33	-2.53	105.05	111.69
30	M	103	LMT	C1'-O5'-C5'	-2.53	108.83	113.75
23	a	408	PL9	C7-C8-C9	-2.53	122.41	126.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	514	BCR	C15-C16-C17	-2.53	117.81	123.39
24	B	618	BCR	C11-C10-C9	-2.53	123.55	127.20
25	D	410	DGD	CFB-CEB-CDB	-2.52	101.50	114.53
24	B	619	BCR	C38-C26-C25	-2.52	122.13	124.61
31	D	402	PHO	CBD-CHA-C4D	-2.52	105.64	108.46
24	b	623	BCR	C33-C5-C6	-2.52	122.13	124.61
22	b	619	CLA	O2D-CGD-O1D	-2.52	118.59	123.79
31	D	401	PHO	CBD-CHA-C4D	-2.52	105.64	108.46
22	A	405	CLA	O2D-CGD-O1D	-2.51	118.60	123.79
23	D	407	PL9	C32-C33-C34	-2.51	122.30	127.76
27	E	101	LMG	C1-C2-C3	-2.51	105.02	109.97
31	d	401	PHO	CBD-CHA-C4D	-2.51	105.65	108.46
27	b	625	LMG	C1-C2-C3	-2.51	105.03	109.97
25	c	515	DGD	C3G-C2G-C1G	-2.50	106.22	112.07
25	c	516	DGD	C3G-C2G-C1G	-2.50	106.23	112.07
27	A	414	LMG	O6-C1-O1	-2.49	104.05	110.05
22	c	508	CLA	O2D-CGD-O1D	-2.49	118.65	123.79
31	d	402	PHO	CBD-CHA-C4D	-2.49	105.67	108.46
25	C	515	DGD	C3G-C2G-C1G	-2.49	106.25	112.07
24	B	619	BCR	C7-C8-C9	-2.49	122.42	126.22
30	D	411	LMT	C1'-O5'-C5'	-2.49	108.92	113.75
22	D	405	CLA	O2D-CGD-O1D	-2.49	118.66	123.79
25	d	410	DGD	CFB-CEB-CDB	-2.48	101.72	114.53
25	C	516	DGD	C3G-C2G-C1G	-2.48	106.27	112.07
24	B	618	BCR	C15-C14-C13	-2.48	123.62	127.20
24	b	622	BCR	C33-C5-C6	-2.47	122.17	124.61
31	d	402	PHO	O2D-CGD-O1D	-2.47	118.68	123.79
27	d	412	LMG	C38-C37-C36	-2.47	101.77	114.53
24	B	619	BCR	C33-C5-C6	-2.47	122.18	124.61
24	c	514	BCR	C38-C26-C25	-2.46	122.19	124.61
27	d	409	LMG	C38-C37-C36	-2.46	101.81	114.53
25	D	410	DGD	C3G-C2G-C1G	-2.46	106.31	112.07
27	D	412	LMG	C38-C37-C36	-2.46	101.83	114.53
25	a	410	DGD	CBB-CAB-C9B	-2.46	101.83	114.53
30	M	102	LMT	C3'-C4'-C5'	-2.46	105.28	110.84
24	C	513	BCR	C3-C4-C5	-2.45	109.97	113.87
24	b	623	BCR	C7-C8-C9	-2.45	122.47	126.22
27	A	410	LMG	C40-C39-C38	-2.45	101.86	114.53
24	C	514	BCR	C11-C10-C9	-2.45	123.66	127.20
25	A	408	DGD	CBB-CAB-C9B	-2.45	101.89	114.53
22	B	615	CLA	O2D-CGD-O1D	-2.44	118.74	123.79
24	A	407	BCR	C38-C26-C25	-2.43	122.22	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	519	LHG	C11-C10-C9	-2.43	101.99	114.53
27	e	101	LMG	C1-C2-C3	-2.43	105.19	109.97
27	m	101	LMG	O2-C2-C1	-2.43	104.70	110.02
23	d	407	PL9	C32-C33-C34	-2.43	122.48	127.76
24	c	521	BCR	C15-C14-C13	-2.43	123.69	127.20
30	b	603	LMT	C1'-O5'-C5'	-2.43	109.04	113.75
30	M	103	LMT	C3'-C4'-C5'	-2.43	105.35	110.84
23	A	406	PL9	C7-C8-C9	-2.42	122.59	126.70
24	B	617	BCR	C15-C14-C13	-2.42	123.70	127.20
24	C	514	BCR	C15-C14-C13	-2.42	123.70	127.20
24	K	102	BCR	C24-C23-C22	-2.42	122.52	126.22
24	b	622	BCR	C11-C10-C9	-2.42	123.70	127.20
23	D	407	PL9	C31-C32-C33	-2.42	105.35	111.69
24	C	513	BCR	C15-C14-C13	-2.41	123.71	127.20
24	a	409	BCR	C38-C26-C25	-2.41	122.24	124.61
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	A	410	LMG	O3-C3-C2	-2.41	104.91	110.34
27	D	409	LMG	C38-C37-C36	-2.41	102.10	114.53
27	d	408	LMG	C38-C37-C36	-2.41	102.10	114.53
25	B	620	DGD	CBB-CAB-C9B	-2.41	102.10	114.53
24	C	513	BCR	C15-C16-C17	-2.40	118.08	123.39
25	c	516	DGD	O6E-C1E-O5D	-2.40	104.27	110.05
25	b	624	DGD	CBB-CAB-C9B	-2.40	102.13	114.53
24	B	618	BCR	C33-C5-C6	-2.40	122.25	124.61
26	C	519	LHG	C11-C10-C9	-2.40	102.14	114.53
27	a	412	LMG	C40-C39-C38	-2.40	102.15	114.53
25	C	516	DGD	O6E-C1E-O5D	-2.39	104.29	110.05
30	B	627	LMT	C1'-O5'-C5'	-2.39	109.10	113.75
27	C	521	LMG	C40-C39-C38	-2.39	102.19	114.53
25	C	517	DGD	CFB-CEB-CDB	-2.39	102.19	114.53
25	c	517	DGD	CFB-CEB-CDB	-2.39	102.21	114.53
27	D	408	LMG	O2-C2-C1	-2.39	104.79	110.02
27	E	101	LMG	O6-C1-O1	-2.39	104.31	110.05
24	y	101	BCR	C1-C6-C5	-2.38	119.16	122.66
27	A	410	LMG	C1-C2-C3	-2.38	105.28	109.97
27	c	522	LMG	O6-C1-O1	-2.38	104.33	110.05
27	C	521	LMG	O2-C2-C1	-2.37	104.81	110.02
27	c	522	LMG	C40-C39-C38	-2.37	102.28	114.53
30	i	102	LMT	C1'-O5'-C5'	-2.37	109.14	113.75
25	B	620	DGD	C1D-C2D-C3D	-2.37	105.30	109.97
27	i	101	LMG	O2-C2-C1	-2.37	104.83	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	516	DGD	CFB-CEB-CDB	-2.37	102.32	114.53
27	D	408	LMG	C38-C37-C36	-2.36	102.34	114.53
27	B	621	LMG	O6-C1-O1	-2.36	104.37	110.05
24	c	514	BCR	C15-C16-C17	-2.36	118.17	123.39
25	A	408	DGD	C3G-C2G-C1G	-2.36	106.55	112.07
22	C	508	CLA	O2D-CGD-O1D	-2.36	118.92	123.79
24	B	618	BCR	C15-C16-C17	-2.36	118.17	123.39
24	c	513	BCR	C7-C8-C9	-2.36	122.62	126.22
27	m	101	LMG	C1-C2-C3	-2.35	105.33	109.97
27	I	101	LMG	O2-C2-C1	-2.35	104.87	110.02
27	a	412	LMG	O3-C3-C2	-2.35	105.05	110.34
25	d	410	DGD	C3D-C4D-C5D	-2.35	106.10	110.20
27	A	410	LMG	C38-C37-C36	-2.35	102.42	114.53
30	d	411	LMT	C3'-C4'-C5'	-2.34	105.54	110.84
27	D	412	LMG	C1-C2-C3	-2.34	105.36	109.97
25	a	410	DGD	C3G-C2G-C1G	-2.34	106.59	112.07
24	c	513	BCR	C15-C14-C13	-2.34	123.82	127.20
27	i	101	LMG	O1-C1-C2	-2.34	105.08	108.04
27	d	408	LMG	O2-C2-C1	-2.34	104.89	110.02
25	b	624	DGD	C1D-C2D-C3D	-2.34	105.36	109.97
22	B	611	CLA	O2D-CGD-O1D	-2.34	118.97	123.79
25	c	515	DGD	O5D-C6D-C5D	-2.33	104.85	109.08
24	J	102	BCR	C33-C5-C6	-2.33	122.31	124.61
24	j	102	BCR	C33-C5-C6	-2.33	122.31	124.61
30	d	411	LMT	C1'-O5'-C5'	-2.33	109.22	113.75
27	C	518	LMG	C38-C37-C36	-2.33	102.49	114.53
27	C	521	LMG	O6-C1-O1	-2.33	104.44	110.05
27	e	101	LMG	O6-C1-O1	-2.33	104.45	110.05
27	D	409	LMG	O6-C1-C2	-2.33	105.50	110.28
24	b	623	BCR	C11-C10-C9	-2.32	123.84	127.20
27	D	412	LMG	O3-C3-C2	-2.32	105.11	110.34
24	b	622	BCR	C15-C14-C13	-2.32	123.84	127.20
24	K	102	BCR	C15-C14-C13	-2.32	123.84	127.20
25	B	620	DGD	C3G-C2G-C1G	-2.32	106.64	112.07
27	B	621	LMG	C40-C39-C38	-2.32	102.58	114.53
24	K	102	BCR	C38-C26-C25	-2.31	122.33	124.61
27	c	518	LMG	C38-C37-C36	-2.31	102.58	114.53
25	C	516	DGD	CFB-CEB-CDB	-2.31	102.58	114.53
24	g	101	BCR	C1-C6-C5	-2.31	119.27	122.66
27	d	412	LMG	C1-C2-C3	-2.31	105.42	109.97
24	b	620	BCR	C11-C10-C9	-2.31	123.86	127.20
22	C	511	CLA	O2A-CGA-O1A	-2.30	117.55	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	622	BCR	C15-C16-C17	-2.30	118.31	123.39
27	c	522	LMG	O2-C2-C1	-2.30	104.98	110.02
27	a	412	LMG	C1-C2-C3	-2.30	105.44	109.97
24	j	102	BCR	C15-C16-C17	-2.30	118.31	123.39
27	a	412	LMG	C38-C37-C36	-2.30	102.68	114.53
25	a	410	DGD	C1D-C2D-C3D	-2.29	105.45	109.97
25	C	515	DGD	C1D-C2D-C3D	-2.29	105.45	109.97
27	b	625	LMG	C40-C39-C38	-2.29	102.70	114.53
23	d	407	PL9	C46-C47-C48	-2.29	105.69	111.69
27	d	412	LMG	O6-C1-O1	-2.29	104.55	110.05
27	i	101	LMG	O1-C7-C8	-2.29	105.55	110.99
24	B	616	BCR	C11-C10-C9	-2.29	123.90	127.20
24	c	513	BCR	C15-C16-C17	-2.29	118.34	123.39
25	b	624	DGD	C3G-C2G-C1G	-2.28	106.73	112.07
27	b	625	LMG	O6-C1-O1	-2.28	104.56	110.05
23	a	408	PL9	C31-C32-C33	-2.28	105.71	111.69
27	b	625	LMG	O2-C2-C1	-2.28	105.03	110.02
24	c	513	BCR	C24-C23-C22	-2.28	122.74	126.22
25	C	516	DGD	O3D-C3D-C4D	-2.28	105.21	110.34
23	D	407	PL9	C12-C13-C14	-2.28	122.81	127.76
30	D	411	LMT	C3'-C4'-C5'	-2.28	105.69	110.84
25	c	516	DGD	O3D-C3D-C4D	-2.28	105.21	110.34
25	b	601	DGD	O6D-C1D-O3G	-2.28	104.58	110.05
24	b	621	BCR	C35-C13-C14	-2.27	119.54	122.90
30	I	102	LMT	C1'-O5'-C5'	-2.27	109.33	113.75
27	C	521	LMG	C38-C37-C36	-2.27	102.82	114.53
24	c	514	BCR	C15-C14-C13	-2.27	123.92	127.20
27	M	101	LMG	O2-C2-C1	-2.27	105.05	110.02
27	d	408	LMG	O3-C3-C2	-2.26	105.25	110.34
24	b	621	BCR	C38-C26-C25	-2.26	122.39	124.61
23	D	407	PL9	C46-C47-C48	-2.25	105.79	111.69
27	b	625	LMG	C38-C37-C36	-2.25	102.91	114.53
24	B	616	BCR	C38-C26-C25	-2.24	122.40	124.61
24	C	513	BCR	C38-C26-C25	-2.24	122.41	124.61
27	D	412	LMG	O6-C1-O1	-2.24	104.66	110.05
34	F	101	HEM	C3B-C4B-NB	-2.24	107.35	111.63
24	c	521	BCR	C38-C26-C25	-2.23	122.41	124.61
27	D	408	LMG	O3-C3-C2	-2.23	105.31	110.34
25	c	515	DGD	C1D-C2D-C3D	-2.23	105.57	109.97
27	C	518	LMG	O2-C2-C1	-2.23	105.13	110.02
27	b	625	LMG	O3-C3-C2	-2.23	105.31	110.34
27	a	402	LMG	O3-C3-C2	-2.23	105.31	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	518	LMG	O2-C2-C1	-2.23	105.13	110.02
27	B	621	LMG	O3-C3-C2	-2.23	105.32	110.34
24	B	619	BCR	C11-C10-C9	-2.23	123.98	127.20
27	A	410	LMG	O1-C1-C2	-2.23	105.23	108.04
27	I	101	LMG	O3-C3-C2	-2.23	105.33	110.34
25	C	516	DGD	C3D-C4D-C5D	-2.23	106.32	110.20
23	d	407	PL9	O2-C1-C2	-2.23	116.88	121.89
27	a	402	LMG	O1-C7-C8	-2.23	105.69	110.99
27	c	522	LMG	C38-C37-C36	-2.23	103.04	114.53
24	F	102	BCR	C11-C10-C9	-2.22	123.99	127.20
23	j	101	PL9	O2-C1-C2	-2.22	116.89	121.89
24	B	617	BCR	C38-C26-C25	-2.22	122.42	124.61
34	f	101	HEM	C3B-C4B-NB	-2.22	107.38	111.63
27	d	412	LMG	O3-C3-C2	-2.22	105.34	110.34
27	m	101	LMG	C1-O6-C5	-2.22	109.44	113.75
30	B	624	LMT	C1'-O5'-C5'	-2.22	109.44	113.75
25	C	515	DGD	O5D-C6D-C5D	-2.22	105.06	109.08
34	f	101	HEM	CAA-CBA-CGA	-2.22	108.68	112.75
27	B	621	LMG	C38-C37-C36	-2.22	103.08	114.53
25	D	410	DGD	C3D-C4D-C5D	-2.22	106.33	110.20
22	c	511	CLA	O2A-CGA-O1A	-2.21	117.78	123.49
27	a	412	LMG	O2-C2-C1	-2.21	105.18	110.02
24	C	513	BCR	C11-C10-C9	-2.20	124.01	127.20
27	A	410	LMG	O2-C2-C1	-2.20	105.19	110.02
27	d	412	LMG	O2-C2-C1	-2.20	105.19	110.02
23	j	101	PL9	C12-C13-C14	-2.20	122.97	127.76
24	K	102	BCR	C11-C10-C9	-2.20	124.02	127.20
23	A	406	PL9	C11-C12-C13	-2.20	105.92	111.69
24	J	102	BCR	C20-C21-C22	-2.20	124.02	127.20
27	B	621	LMG	O2-C2-C1	-2.20	105.20	110.02
23	A	406	PL9	C31-C32-C33	-2.20	105.93	111.69
23	J	101	PL9	O2-C1-C2	-2.20	116.94	121.89
27	a	402	LMG	O2-C2-C1	-2.20	105.21	110.02
24	c	513	BCR	C33-C5-C6	-2.19	122.45	124.61
24	j	102	BCR	C20-C21-C22	-2.19	124.03	127.20
27	e	101	LMG	O1-C7-C8	-2.19	105.77	110.99
25	a	410	DGD	CAB-C9B-C8B	-2.19	103.22	114.53
23	J	101	PL9	C12-C13-C14	-2.19	123.01	127.76
27	c	522	LMG	O3-C3-C2	-2.19	105.42	110.34
25	A	408	DGD	C1D-C2D-C3D	-2.18	105.67	109.97
27	C	521	LMG	O3-C3-C2	-2.18	105.42	110.34
27	i	101	LMG	O3-C3-C2	-2.18	105.42	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	f	102	BCR	C11-C10-C9	-2.18	124.05	127.20
25	B	625	DGD	O6D-C1D-O3G	-2.18	104.81	110.05
25	c	516	DGD	CBB-CAB-C9B	-2.18	103.29	114.53
26	a	411	LHG	C27-C26-C25	-2.18	103.29	114.53
24	c	513	BCR	C38-C26-C25	-2.18	122.47	124.61
23	D	407	PL9	O2-C1-C2	-2.18	116.99	121.89
27	d	409	LMG	O6-C1-O1	-2.18	104.82	110.05
27	e	101	LMG	O3-C3-C2	-2.17	105.44	110.34
23	a	408	PL9	C11-C12-C13	-2.17	106.00	111.69
23	A	406	PL9	O2-C1-C2	-2.17	117.00	121.89
27	D	409	LMG	O6-C1-O1	-2.17	104.83	110.05
27	A	414	LMG	O3-C3-C2	-2.17	105.45	110.34
23	d	407	PL9	C36-C34-C33	-2.17	116.94	121.05
23	a	408	PL9	O2-C1-C2	-2.17	117.00	121.89
25	A	408	DGD	CAB-C9B-C8B	-2.17	103.33	114.53
25	C	516	DGD	CBB-CAB-C9B	-2.17	103.33	114.53
27	E	101	LMG	O1-C7-C8	-2.17	105.83	110.99
30	b	627	LMT	C1'-O5'-C5'	-2.17	109.54	113.75
24	B	616	BCR	C15-C14-C13	-2.17	124.07	127.20
27	c	518	LMG	O3-C3-C2	-2.17	105.46	110.34
25	C	517	DGD	CBB-CAB-C9B	-2.16	103.35	114.53
23	d	407	PL9	C12-C13-C14	-2.16	123.06	127.76
24	c	521	BCR	C11-C10-C9	-2.16	124.07	127.20
24	g	101	BCR	C3-C2-C1	-2.16	106.82	114.83
27	D	412	LMG	O2-C2-C1	-2.16	105.28	110.02
24	b	620	BCR	C15-C14-C13	-2.16	124.08	127.20
25	b	601	DGD	CBB-CAB-C9B	-2.16	103.38	114.53
24	f	102	BCR	C38-C26-C25	-2.16	122.49	124.61
27	A	414	LMG	O1-C7-C8	-2.16	105.86	110.99
24	c	521	BCR	C24-C23-C22	-2.15	122.94	126.22
24	b	622	BCR	C7-C8-C9	-2.15	122.94	126.22
25	C	516	DGD	CAB-C9B-C8B	-2.15	103.45	114.53
24	b	620	BCR	C38-C26-C25	-2.15	122.50	124.61
27	C	518	LMG	O3-C3-C2	-2.14	105.53	110.34
24	a	409	BCR	C15-C16-C17	-2.14	118.67	123.39
24	F	102	BCR	C38-C26-C25	-2.14	122.51	124.61
25	B	625	DGD	CBB-CAB-C9B	-2.13	103.51	114.53
24	B	617	BCR	C11-C10-C9	-2.13	124.12	127.20
25	c	517	DGD	CBB-CAB-C9B	-2.13	103.52	114.53
34	F	101	HEM	CAA-CBA-CGA	-2.13	108.84	112.75
23	A	406	PL9	C12-C13-C14	-2.13	123.13	127.76
26	A	409	LHG	C27-C26-C25	-2.13	103.54	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	BCR	C15-C14-C13	-2.13	124.12	127.20
24	B	617	BCR	C35-C13-C14	-2.13	119.76	122.90
27	a	412	LMG	O1-C1-C2	-2.13	105.36	108.04
24	b	621	BCR	C7-C8-C9	-2.13	122.97	126.22
27	E	101	LMG	O3-C3-C2	-2.12	105.56	110.34
24	b	623	BCR	C24-C23-C22	-2.12	122.98	126.22
25	b	601	DGD	CAB-C9B-C8B	-2.12	103.58	114.53
27	I	101	LMG	O1-C1-C2	-2.12	105.36	108.04
24	C	513	BCR	C7-C8-C9	-2.12	122.99	126.22
27	M	101	LMG	O3-C3-C2	-2.12	105.57	110.34
25	c	516	DGD	C3D-C4D-C5D	-2.12	106.51	110.20
24	a	409	BCR	C15-C14-C13	-2.12	124.14	127.20
27	d	409	LMG	O6-C1-C2	-2.11	105.94	110.28
23	a	408	PL9	C32-C33-C34	-2.11	123.17	127.76
24	y	101	BCR	C3-C2-C1	-2.11	107.01	114.83
24	F	102	BCR	C7-C8-C9	-2.11	123.00	126.22
25	d	410	DGD	C5B-C4B-C3B	-2.11	103.64	114.53
24	b	622	BCR	C38-C26-C25	-2.11	122.53	124.61
22	c	506	CLA	O2A-CGA-O1A	-2.11	118.06	123.49
25	c	517	DGD	CAB-C9B-C8B	-2.11	103.66	114.53
24	C	513	BCR	C33-C5-C6	-2.11	122.54	124.61
22	B	610	CLA	C4B-CHC-C1C	-2.10	124.75	129.26
24	J	102	BCR	C15-C16-C17	-2.10	118.74	123.39
25	B	625	DGD	CAB-C9B-C8B	-2.10	103.68	114.53
24	B	617	BCR	C7-C8-C9	-2.10	123.02	126.22
27	m	101	LMG	O3-C3-C2	-2.10	105.62	110.34
22	b	618	CLA	O2A-CGA-O1A	-2.09	118.09	123.49
24	B	618	BCR	C7-C8-C9	-2.09	123.02	126.22
27	A	414	LMG	O2-C2-C1	-2.09	105.43	110.02
26	C	519	LHG	C27-C26-C25	-2.09	103.73	114.53
25	c	516	DGD	O2D-C2D-C1D	-2.09	105.44	110.02
24	C	514	BCR	C24-C23-C22	-2.09	123.03	126.22
25	D	410	DGD	C5B-C4B-C3B	-2.09	103.75	114.53
27	M	101	LMG	C1-O6-C5	-2.09	109.70	113.75
23	a	408	PL9	C12-C13-C14	-2.08	123.23	127.76
22	b	614	CLA	C4B-CHC-C1C	-2.08	124.79	129.26
24	A	407	BCR	C15-C16-C17	-2.08	118.79	123.39
24	B	619	BCR	C24-C23-C22	-2.08	123.05	126.22
25	C	517	DGD	CAB-C9B-C8B	-2.08	103.79	114.53
24	B	616	BCR	C15-C16-C17	-2.08	118.80	123.39
25	c	516	DGD	CAB-C9B-C8B	-2.08	103.81	114.53
24	c	514	BCR	C24-C23-C22	-2.07	123.06	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	519	LHG	C27-C26-C25	-2.07	103.84	114.53
25	C	515	DGD	C5B-C4B-C3B	-2.07	103.85	114.53
25	C	516	DGD	O2D-C2D-C1D	-2.07	105.48	110.02
27	D	408	LMG	O1-C7-C8	-2.07	106.07	110.99
22	B	601	CLA	O2A-CGA-O1A	-2.07	118.16	123.49
24	B	618	BCR	C3-C4-C5	-2.07	110.59	113.87
25	c	515	DGD	C5B-C4B-C3B	-2.07	103.87	114.53
22	B	603	CLA	O2A-CGA-O1A	-2.06	118.17	123.49
24	b	621	BCR	C11-C10-C9	-2.06	124.22	127.20
27	e	101	LMG	O2-C2-C1	-2.06	105.50	110.02
27	E	101	LMG	O2-C2-C1	-2.06	105.51	110.02
24	F	102	BCR	C15-C16-C17	-2.06	118.85	123.39
34	f	101	HEM	CBD-CAD-C3D	-2.05	107.60	113.55
25	D	410	DGD	CAB-C9B-C8B	-2.05	103.96	114.53
23	D	407	PL9	C42-C43-C44	-2.05	123.31	127.76
25	c	515	DGD	O2D-C2D-C1D	-2.05	105.54	110.02
23	a	408	PL9	C3-C2-C1	-2.04	121.72	122.97
25	D	410	DGD	CBB-CAB-C9B	-2.04	103.98	114.53
23	A	406	PL9	C32-C33-C34	-2.04	123.32	127.76
25	C	517	DGD	O2D-C2D-C1D	-2.04	105.55	110.02
25	d	410	DGD	CAB-C9B-C8B	-2.04	104.00	114.53
23	D	407	PL9	C36-C34-C33	-2.04	117.19	121.05
24	a	409	BCR	C24-C23-C22	-2.04	123.11	126.22
25	b	624	DGD	CAB-C9B-C8B	-2.03	104.02	114.53
27	d	408	LMG	O1-C1-C2	-2.03	105.47	108.04
25	C	515	DGD	O3E-C3E-C2E	-2.03	105.76	110.34
22	c	509	CLA	O2A-CGA-O1A	-2.03	118.24	123.49
25	d	410	DGD	CBB-CAB-C9B	-2.03	104.03	114.53
22	B	602	CLA	O2A-CGA-O1A	-2.03	118.25	123.49
22	D	405	CLA	O2A-CGA-O1A	-2.03	118.25	123.49
22	b	607	CLA	O2A-CGA-O1A	-2.03	118.26	123.49
27	D	409	LMG	O3-C3-C2	-2.03	105.77	110.34
25	c	517	DGD	C5B-C4B-C3B	-2.02	104.08	114.53
25	C	517	DGD	C5B-C4B-C3B	-2.02	104.08	114.53
25	B	620	DGD	C5B-C4B-C3B	-2.02	104.09	114.53
23	a	408	PL9	C36-C37-C38	-2.02	106.39	111.69
24	x	101	BCR	C28-C27-C26	-2.02	110.66	113.87
25	C	516	DGD	C1D-C2D-C3D	-2.02	105.99	109.97
24	B	618	BCR	C38-C26-C25	-2.02	122.62	124.61
22	b	615	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
31	d	401	PHO	C2B-C1B-NB	-2.02	106.70	109.73
24	f	102	BCR	C15-C16-C17	-2.02	118.93	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	514	BCR	C7-C8-C9	-2.02	123.14	126.22
27	c	518	LMG	O1-C7-C8	-2.02	106.19	110.99
25	C	516	DGD	C5B-C4B-C3B	-2.02	104.12	114.53
22	C	506	CLA	O2A-CGA-O1A	-2.01	118.29	123.49
25	A	408	DGD	C5B-C4B-C3B	-2.01	104.14	114.53
24	K	102	BCR	C7-C8-C9	-2.01	123.15	126.22
27	a	412	LMG	C1-O6-C5	-2.01	109.84	113.75
25	a	410	DGD	C5B-C4B-C3B	-2.01	104.15	114.53
22	B	611	CLA	O2A-CGA-O1A	-2.01	118.30	123.49
23	d	407	PL9	C36-C37-C38	-2.01	106.42	111.69
27	I	101	LMG	O1-C7-C8	-2.01	106.21	110.99
25	B	620	DGD	CAB-C9B-C8B	-2.01	104.16	114.53
25	C	515	DGD	O2D-C2D-C1D	-2.01	105.62	110.02
22	B	612	CLA	O2A-CGA-O1A	-2.01	118.31	123.49
23	A	406	PL9	C36-C37-C38	-2.00	106.44	111.69
23	D	407	PL9	C3-C2-C1	-2.00	121.75	122.97
22	C	501	CLA	O2A-CGA-O1A	-2.00	118.33	123.49
22	c	520	CLA	CMD-C2D-C3D	2.00	129.00	125.09
31	D	401	PHO	CHB-C1B-NB	2.00	128.41	124.66
22	c	503	CLA	CMD-C2D-C3D	2.01	129.02	125.09
22	c	512	CLA	CMD-C2D-C3D	2.01	129.03	125.09
22	b	613	CLA	O2D-CGD-CBD	2.01	114.06	111.30
30	M	102	LMT	O1'-C1'-C2'	2.02	110.58	108.04
22	c	510	CLA	CMD-C2D-C3D	2.02	129.03	125.09
22	B	609	CLA	CMD-C2D-C3D	2.02	129.04	125.09
22	C	505	CLA	CMD-C2D-C3D	2.02	129.04	125.09
22	b	618	CLA	O2D-CGD-CBD	2.02	114.07	111.30
22	B	605	CLA	CMD-C2D-C3D	2.02	129.05	125.09
22	C	503	CLA	O1D-CGD-CBD	2.03	127.53	124.62
30	B	627	LMT	O1'-C1'-C2'	2.03	110.60	108.04
31	d	402	PHO	C1B-NB-C4B	2.03	110.53	106.51
22	c	504	CLA	CBA-CAA-C2A	2.03	119.47	113.73
22	b	616	CLA	CMD-C2D-C3D	2.03	129.06	125.09
29	d	403	SQD	C4-C3-C2	2.03	114.59	110.79
22	C	511	CLA	O1D-CGD-CBD	2.04	127.54	124.62
22	b	608	CLA	O1D-CGD-CBD	2.04	127.54	124.62
22	c	520	CLA	O1D-CGD-CBD	2.04	127.55	124.62
22	b	610	CLA	O1D-CGD-CBD	2.04	127.55	124.62
22	B	601	CLA	O1D-CGD-CBD	2.05	127.56	124.62
29	A	413	SQD	C1-O5-C5	2.05	117.72	113.75
22	C	520	CLA	O1D-CGD-CBD	2.05	127.56	124.62
31	D	401	PHO	C1B-NB-C4B	2.05	110.57	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	512	CLA	CMD-C2D-C3D	2.05	129.10	125.09
22	B	614	CLA	O2D-CGD-CBD	2.05	114.11	111.30
29	B	622	SQD	C4-C3-C2	2.05	114.62	110.79
22	B	614	CLA	CMD-C2D-C3D	2.06	129.11	125.09
22	C	520	CLA	CMD-C2D-C3D	2.06	129.11	125.09
31	d	401	PHO	C1B-NB-C4B	2.06	110.58	106.51
22	B	604	CLA	O1D-CGD-CBD	2.06	127.57	124.62
22	a	406	CLA	O1D-CGD-CBD	2.07	127.59	124.62
22	H	101	CLA	CMD-C2D-C3D	2.07	129.15	125.09
22	C	505	CLA	O1D-CGD-CBD	2.07	127.59	124.62
22	C	501	CLA	CMB-C2B-C3B	2.08	129.16	125.09
22	C	506	CLA	O2D-CGD-CBD	2.08	114.15	111.30
22	C	520	CLA	O2D-CGD-CBD	2.09	114.16	111.30
22	C	510	CLA	CMD-C2D-C3D	2.09	129.17	125.09
22	b	618	CLA	CMD-C2D-C3D	2.09	129.17	125.09
22	c	505	CLA	CMD-C2D-C3D	2.09	129.18	125.09
22	B	614	CLA	O1D-CGD-CBD	2.09	127.62	124.62
22	C	503	CLA	CMD-C2D-C3D	2.09	129.18	125.09
22	C	507	CLA	CMD-C2D-C3D	2.09	129.18	125.09
22	b	607	CLA	CMD-C2D-C3D	2.09	129.18	125.09
30	b	626	LMT	O1'-C1'-C2'	2.10	110.69	108.04
22	c	511	CLA	O1D-CGD-CBD	2.10	127.63	124.62
22	D	405	CLA	CHB-C4A-NA	2.10	127.41	124.51
22	B	615	CLA	O2D-CGD-CBD	2.10	114.18	111.30
31	D	402	PHO	C1B-NB-C4B	2.10	110.67	106.51
22	B	608	CLA	O1D-CGD-CBD	2.11	127.64	124.62
22	B	612	CLA	CMD-C2D-C3D	2.11	129.22	125.09
22	a	405	CLA	O2D-CGD-CBD	2.11	114.19	111.30
22	c	501	CLA	CMD-C2D-C3D	2.11	129.22	125.09
22	A	404	CLA	O2D-CGD-CBD	2.11	114.20	111.30
24	H	102	BCR	C29-C30-C25	2.12	113.71	110.36
22	b	617	CLA	O1D-CGD-CBD	2.12	127.66	124.62
22	d	405	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	B	613	CLA	O1D-CGD-CBD	2.12	127.66	124.62
22	c	506	CLA	CMD-C2D-C3D	2.12	129.24	125.09
29	f	103	SQD	O48-C23-C24	2.12	118.37	111.90
22	b	619	CLA	O2D-CGD-CBD	2.12	114.21	111.30
24	x	101	BCR	C27-C26-C25	2.13	125.49	122.78
22	b	618	CLA	O1D-CGD-CBD	2.13	127.68	124.62
22	b	606	CLA	O1D-CGD-CBD	2.13	127.68	124.62
29	A	412	SQD	C4-C3-C2	2.14	114.78	110.79
22	C	502	CLA	O1D-CGD-CBD	2.14	127.69	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	613	CLA	CMD-C2D-C3D	2.14	129.27	125.09
22	c	511	CLA	O2D-CGD-CBD	2.14	114.23	111.30
25	D	410	DGD	O5D-C1E-C2E	2.14	110.75	108.04
22	B	602	CLA	O2D-CGD-CBD	2.14	114.24	111.30
22	b	605	CLA	O1D-CGD-CBD	2.14	127.70	124.62
22	b	606	CLA	CMD-C2D-C3D	2.14	129.28	125.09
22	A	405	CLA	CMD-C2D-C3D	2.15	129.29	125.09
22	C	501	CLA	CMD-C2D-C3D	2.15	129.29	125.09
22	B	601	CLA	O2D-CGD-CBD	2.15	114.25	111.30
22	d	406	CLA	CMD-C2D-C3D	2.15	129.30	125.09
22	B	602	CLA	O1D-CGD-CBD	2.15	127.71	124.62
22	B	610	CLA	C4A-NA-C1A	2.16	109.14	106.36
22	B	613	CLA	CMD-C2D-C3D	2.16	129.31	125.09
22	b	605	CLA	CMD-C2D-C3D	2.18	129.34	125.09
22	c	501	CLA	CMB-C2B-C3B	2.18	129.35	125.09
30	M	103	LMT	O1'-C1'-C2'	2.18	110.79	108.04
22	D	406	CLA	CMD-C2D-C3D	2.18	129.35	125.09
30	b	627	LMT	O1'-C1'-C2'	2.18	110.80	108.04
22	B	603	CLA	CMD-C2D-C3D	2.19	129.36	125.09
22	C	506	CLA	O1D-CGD-CBD	2.19	127.76	124.62
24	x	101	BCR	C29-C30-C25	2.19	113.83	110.36
22	b	613	CLA	O1D-CGD-CBD	2.19	127.76	124.62
22	b	614	CLA	C4A-NA-C1A	2.19	109.19	106.36
22	B	602	CLA	CMD-C2D-C3D	2.19	129.37	125.09
22	B	601	CLA	CMD-C2D-C3D	2.19	129.37	125.09
24	H	102	BCR	C27-C26-C25	2.19	125.58	122.78
22	h	101	CLA	CMD-C2D-C3D	2.19	129.38	125.09
34	V	201	HEM	C2D-C3D-C4D	2.20	105.22	101.50
22	C	506	CLA	CMD-C2D-C3D	2.20	129.39	125.09
22	c	520	CLA	O2D-CGD-CBD	2.20	114.32	111.30
22	B	607	CLA	CMD-C2D-C3D	2.21	129.40	125.09
22	b	611	CLA	CMD-C2D-C3D	2.21	129.41	125.09
22	a	406	CLA	O2D-CGD-CBD	2.21	114.33	111.30
24	B	618	BCR	C27-C26-C25	2.21	125.60	122.78
22	C	509	CLA	O1D-CGD-CBD	2.22	127.81	124.62
22	c	502	CLA	O1D-CGD-CBD	2.22	127.81	124.62
22	C	508	CLA	O1D-CGD-CBD	2.23	127.82	124.62
30	B	623	LMT	O1'-C1'-C2'	2.23	110.86	108.04
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
29	F	103	SQD	O48-C23-C24	2.24	118.71	111.90
22	B	604	CLA	O2D-CGD-CBD	2.24	114.36	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	502	CLA	CMD-C2D-C3D	2.24	129.46	125.09
23	A	406	PL9	C41-C39-C40	2.24	120.14	114.64
29	a	415	SQD	C4-C3-C2	2.24	114.97	110.79
22	A	405	CLA	O1D-CGD-CBD	2.24	127.83	124.62
22	b	617	CLA	CMD-C2D-C3D	2.25	129.49	125.09
22	b	605	CLA	O2D-CGD-CBD	2.25	114.39	111.30
22	c	506	CLA	O1D-CGD-CBD	2.26	127.86	124.62
22	B	608	CLA	CMD-C2D-C3D	2.26	129.51	125.09
29	b	602	SQD	O48-C23-C24	2.27	118.80	111.90
29	f	103	SQD	C3-C4-C5	2.27	114.15	110.20
22	D	405	CLA	CMD-C2D-C3D	2.27	129.52	125.09
29	F	103	SQD	C3-C4-C5	2.27	114.15	110.20
22	c	507	CLA	CMD-C2D-C3D	2.27	129.54	125.09
24	J	102	BCR	C29-C30-C25	2.28	113.97	110.36
34	v	201	HEM	C2D-C3D-C4D	2.28	105.36	101.50
22	c	504	CLA	CMD-C2D-C3D	2.28	129.55	125.09
22	h	101	CLA	O1D-CGD-CBD	2.28	127.89	124.62
25	d	410	DGD	O5D-C1E-C2E	2.28	110.92	108.04
22	a	407	CLA	CMD-C2D-C3D	2.28	129.55	125.09
22	B	601	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	b	608	CLA	O2D-CGD-CBD	2.29	114.44	111.30
22	C	502	CLA	O2D-CGD-CBD	2.29	114.44	111.30
22	c	508	CLA	O1D-CGD-CBD	2.29	127.90	124.62
22	c	504	CLA	CMB-C2B-C3B	2.29	129.57	125.09
22	b	612	CLA	O2D-CGD-CBD	2.29	114.44	111.30
22	d	405	CLA	CMD-C2D-C3D	2.29	129.57	125.09
29	F	103	SQD	C44-O6-C1	2.29	118.64	113.82
34	F	101	HEM	C2D-C3D-C4D	2.30	105.39	101.50
22	b	605	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	B	612	CLA	O1D-CGD-CBD	2.30	127.92	124.62
22	c	505	CLA	O2D-CGD-CBD	2.31	114.46	111.30
22	A	403	CLA	O2D-CGD-CBD	2.31	114.47	111.30
23	a	408	PL9	C41-C39-C40	2.31	120.33	114.64
24	j	102	BCR	C29-C30-C25	2.32	114.03	110.36
22	b	616	CLA	O1D-CGD-CBD	2.32	127.94	124.62
22	B	609	CLA	O1D-CGD-CBD	2.32	127.94	124.62
22	b	619	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	A	413	SQD	O48-C23-C24	2.32	118.96	111.90
29	a	401	SQD	C1-O5-C5	2.32	118.25	113.75
22	B	608	CLA	O2D-CGD-CBD	2.32	114.48	111.30
24	b	622	BCR	C27-C26-C25	2.33	125.75	122.78
22	b	615	CLA	O1D-CGD-CBD	2.33	127.96	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	502	CLA	CMD-C2D-C3D	2.33	129.64	125.09
29	B	626	SQD	O48-C23-C24	2.33	119.00	111.90
24	B	616	BCR	C2-C1-C6	2.33	114.05	110.36
22	B	610	CLA	CMD-C2D-C3D	2.33	129.65	125.09
22	B	611	CLA	O1D-CGD-CBD	2.33	127.96	124.62
34	f	101	HEM	C2D-C3D-C4D	2.33	105.46	101.50
22	a	407	CLA	O1D-CGD-CBD	2.34	127.97	124.62
22	b	615	CLA	CMD-C2D-C3D	2.34	129.67	125.09
29	d	403	SQD	O48-C23-C24	2.35	119.05	111.90
22	B	611	CLA	CMD-C2D-C3D	2.35	129.68	125.09
22	C	504	CLA	CMB-C2B-C3B	2.35	129.69	125.09
22	b	619	CLA	CMB-C2B-C3B	2.36	129.70	125.09
22	B	615	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	B	615	CLA	CMB-C2B-C3B	2.36	129.71	125.09
30	B	624	LMT	O1'-C1'-C2'	2.36	111.02	108.04
22	d	406	CLA	O1D-CGD-CBD	2.36	128.01	124.62
22	D	406	CLA	O1D-CGD-CBD	2.37	128.01	124.62
29	A	413	SQD	O6-C1-C2	2.37	111.03	108.04
22	b	606	CLA	C4A-NA-C1A	2.37	109.42	106.36
22	a	404	CLA	C4A-NA-C1A	2.37	109.42	106.36
22	c	508	CLA	CMB-C2B-C3B	2.38	129.73	125.09
22	C	505	CLA	O2D-CGD-CBD	2.38	114.56	111.30
22	b	613	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	C	507	CLA	CHB-C4A-NA	2.38	127.81	124.51
29	a	415	SQD	O48-C23-C24	2.38	119.16	111.90
22	C	509	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	A	406	PL9	C20-C19-C21	2.39	119.05	115.41
22	b	606	CLA	O2D-CGD-CBD	2.39	114.57	111.30
22	b	612	CLA	C4A-NA-C1A	2.39	109.45	106.36
22	A	402	CLA	CMB-C2B-C3B	2.39	129.76	125.09
22	b	606	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	b	610	CLA	O2D-CGD-CBD	2.39	114.58	111.30
24	B	617	BCR	C29-C30-C25	2.39	114.15	110.36
24	b	621	BCR	C29-C30-C25	2.39	114.16	110.36
22	c	509	CLA	CHB-C4A-NA	2.40	127.82	124.51
22	C	508	CLA	CMB-C2B-C3B	2.40	129.78	125.09
22	B	606	CLA	CMB-C2B-C3B	2.40	129.78	125.09
22	b	605	CLA	C4A-NA-C1A	2.40	109.46	106.36
22	a	406	CLA	CMB-C2B-C3B	2.40	129.78	125.09
22	B	601	CLA	CMB-C2B-C3B	2.40	129.78	125.09
22	C	502	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	b	612	CLA	CHB-C4A-NA	2.40	127.83	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	H	101	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	d	405	CLA	C4A-NA-C1A	2.41	109.47	106.36
22	b	617	CLA	O2D-CGD-CBD	2.41	114.60	111.30
22	B	601	CLA	C4A-NA-C1A	2.41	109.47	106.36
22	C	507	CLA	O2D-CGD-CBD	2.41	114.61	111.30
22	C	504	CLA	CMD-C2D-C3D	2.41	129.81	125.09
22	C	511	CLA	CMD-C2D-C3D	2.41	129.81	125.09
22	B	608	CLA	CMB-C2B-C3B	2.41	129.81	125.09
22	b	613	CLA	C4A-NA-C1A	2.41	109.48	106.36
29	B	626	SQD	C4-C3-C2	2.41	115.30	110.79
22	D	406	CLA	C4A-NA-C1A	2.41	109.48	106.36
24	b	620	BCR	C2-C1-C6	2.42	114.19	110.36
22	c	507	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	B	606	CLA	O2D-CGD-CBD	2.42	114.62	111.30
22	C	503	CLA	O2D-CGD-CBD	2.42	114.62	111.30
22	c	509	CLA	C4A-NA-C1A	2.42	109.49	106.36
22	a	404	CLA	CMB-C2B-C3B	2.42	129.83	125.09
22	b	614	CLA	CMD-C2D-C3D	2.42	129.83	125.09
22	C	509	CLA	C4A-NA-C1A	2.42	109.49	106.36
22	B	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	b	612	CLA	CMB-C2B-C3B	2.43	129.83	125.09
22	b	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	a	401	SQD	O48-C23-C24	2.43	119.30	111.90
22	A	402	CLA	C4A-NA-C1A	2.43	109.50	106.36
22	c	511	CLA	CMD-C2D-C3D	2.43	129.84	125.09
24	F	102	BCR	C27-C26-C25	2.43	125.88	122.78
22	h	101	CLA	CHB-C4A-NA	2.43	127.88	124.51
29	B	622	SQD	O48-C23-C24	2.44	119.33	111.90
22	C	502	CLA	C4A-NA-C1A	2.44	109.51	106.36
22	c	510	CLA	O1D-CGD-CBD	2.44	128.12	124.62
22	A	405	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	b	605	CLA	CMB-C2B-C3B	2.44	129.87	125.09
24	f	102	BCR	C27-C26-C25	2.45	125.90	122.78
22	c	502	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	C	503	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	C	508	CLA	C4A-NA-C1A	2.45	109.52	106.36
22	B	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	b	617	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	D	406	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	A	402	CLA	CHB-C4A-NA	2.45	127.90	124.51
29	B	622	SQD	C44-O6-C1	2.45	118.97	113.82
22	b	611	CLA	C4A-NA-C1A	2.45	109.53	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	CMB-C2B-C3B	2.46	129.89	125.09
22	H	101	CLA	O1D-CGD-CBD	2.46	128.15	124.62
22	b	611	CLA	O1D-CGD-CBD	2.46	128.15	124.62
23	j	101	PL9	C20-C19-C21	2.46	119.17	115.41
22	A	404	CLA	CMB-C2B-C3B	2.46	129.91	125.09
22	D	405	CLA	O1D-CGD-CBD	2.46	128.15	124.62
22	C	501	CLA	O1D-CGD-CBD	2.47	128.16	124.62
22	c	509	CLA	CMB-C2B-C3B	2.47	129.92	125.09
22	a	404	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	c	520	CLA	CMB-C2B-C3B	2.47	129.92	125.09
22	b	609	CLA	CMB-C2B-C3B	2.47	129.93	125.09
22	d	406	CLA	C4A-NA-C1A	2.48	109.56	106.36
22	d	406	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	a	405	CLA	CMB-C2B-C3B	2.48	129.93	125.09
29	A	412	SQD	O48-C23-C24	2.48	119.44	111.90
22	B	613	CLA	O2D-CGD-CBD	2.48	114.70	111.30
22	A	403	CLA	CMB-C2B-C3B	2.48	129.94	125.09
22	D	405	CLA	C4A-NA-C1A	2.48	109.56	106.36
22	B	607	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	B	602	CLA	C4A-NA-C1A	2.48	109.57	106.36
24	C	513	BCR	C27-C26-C25	2.48	125.94	122.78
22	b	616	CLA	CHB-C4A-NA	2.48	127.95	124.51
24	c	513	BCR	C27-C26-C25	2.49	125.95	122.78
22	b	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	c	514	BCR	C29-C30-C25	2.49	114.30	110.36
22	C	508	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	509	CLA	CMB-C2B-C3B	2.49	129.96	125.09
22	h	101	CLA	CMB-C2B-C3B	2.49	129.96	125.09
22	B	606	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	c	512	CLA	C4A-NA-C1A	2.49	109.58	106.36
22	c	502	CLA	C4A-NA-C1A	2.49	109.58	106.36
22	c	508	CLA	C4A-NA-C1A	2.50	109.58	106.36
22	b	610	CLA	CMB-C2B-C3B	2.50	129.97	125.09
22	c	507	CLA	C4A-NA-C1A	2.50	109.59	106.36
22	c	503	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	b	620	BCR	C27-C26-C25	2.50	125.96	122.78
22	B	609	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	512	CLA	CHB-C4A-NA	2.50	127.97	124.51
29	f	103	SQD	C44-O6-C1	2.50	119.07	113.82
22	A	404	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	404	CLA	C4A-NA-C1A	2.50	109.59	106.36
22	H	101	CLA	CMB-C2B-C3B	2.51	129.99	125.09
22	c	512	CLA	O1D-CGD-CBD	2.51	128.21	124.62
22	C	520	CLA	CMB-C2B-C3B	2.51	129.99	125.09
22	c	501	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	b	602	SQD	C4-C3-C2	2.51	115.47	110.79
22	b	610	CLA	C4A-NA-C1A	2.51	109.60	106.36
24	C	514	BCR	C29-C30-C25	2.51	114.34	110.36
22	B	609	CLA	C4A-NA-C1A	2.51	109.60	106.36
22	B	610	CLA	O1D-CGD-CBD	2.51	128.22	124.62
22	c	510	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	b	607	CLA	CMB-C2B-C3B	2.52	130.01	125.09
22	B	608	CLA	C4A-NA-C1A	2.52	109.61	106.36
22	B	604	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	H	101	CLA	C4A-NA-C1A	2.52	109.61	106.36
24	B	616	BCR	C27-C26-C25	2.52	125.99	122.78
22	B	607	CLA	C4A-NA-C1A	2.52	109.62	106.36
22	b	618	CLA	CMB-C2B-C3B	2.52	130.02	125.09
22	B	613	CLA	C4A-NA-C1A	2.52	109.62	106.36
22	c	501	CLA	O1D-CGD-CBD	2.52	128.24	124.62
22	h	101	CLA	C4A-NA-C1A	2.52	109.62	106.36
22	a	407	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	c	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	b	619	CLA	C4A-NA-C1A	2.53	109.63	106.36
22	b	618	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	b	615	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	B	611	CLA	CHB-C4A-NA	2.54	128.02	124.51
29	d	403	SQD	C44-O6-C1	2.54	119.15	113.82
22	B	614	CLA	CMB-C2B-C3B	2.54	130.05	125.09
22	c	505	CLA	C4A-NA-C1A	2.54	109.65	106.36
22	a	407	CLA	C4A-NA-C1A	2.54	109.65	106.36
22	C	503	CLA	C4A-NA-C1A	2.54	109.65	106.36
22	C	511	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	C	510	CLA	O1D-CGD-CBD	2.55	128.27	124.62
22	B	608	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	C	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	C	507	CLA	C4A-NA-C1A	2.55	109.65	106.36
22	c	505	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	c	508	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	604	CLA	C4A-NA-C1A	2.55	109.65	106.36
22	c	510	CLA	C4A-NA-C1A	2.55	109.66	106.36
22	C	512	CLA	CHB-C4A-NA	2.55	128.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	C4A-NA-C1A	2.56	109.67	106.36
22	a	406	CLA	C4A-NA-C1A	2.56	109.67	106.36
22	b	617	CLA	C4A-NA-C1A	2.56	109.67	106.36
23	d	407	PL9	C20-C19-C21	2.56	119.32	115.41
22	b	608	CLA	CMB-C2B-C3B	2.56	130.10	125.09
22	B	605	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	c	506	CLA	C4A-NA-C1A	2.57	109.67	106.36
22	B	605	CLA	CMB-C2B-C3B	2.57	130.11	125.09
22	c	520	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	a	406	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	C	506	CLA	C4A-NA-C1A	2.57	109.69	106.36
22	d	406	CLA	CMB-C2B-C3B	2.57	130.12	125.09
22	c	511	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	B	612	CLA	C4A-NA-C1A	2.58	109.69	106.36
23	J	101	PL9	C20-C19-C21	2.58	119.34	115.41
23	D	407	PL9	C20-C19-C21	2.58	119.35	115.41
22	B	614	CLA	C4A-NA-C1A	2.58	109.70	106.36
22	B	615	CLA	C4A-NA-C1A	2.58	109.70	106.36
22	d	405	CLA	CMB-C2B-C3B	2.59	130.15	125.09
22	C	512	CLA	C4A-NA-C1A	2.59	109.70	106.36
22	B	604	CLA	CMB-C2B-C3B	2.59	130.15	125.09
22	A	405	CLA	C4A-NA-C1A	2.60	109.72	106.36
22	c	511	CLA	C4A-NA-C1A	2.60	109.72	106.36
22	c	520	CLA	C4A-NA-C1A	2.60	109.72	106.36
22	B	607	CLA	O1D-CGD-CBD	2.60	128.35	124.62
22	C	504	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	b	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	B	606	CLA	C4A-NA-C1A	2.61	109.73	106.36
22	b	608	CLA	C4A-NA-C1A	2.61	109.73	106.36
24	b	622	BCR	C29-C30-C25	2.61	114.49	110.36
22	c	506	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	C	520	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	C	505	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	C	510	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	C	511	CLA	CMB-C2B-C3B	2.62	130.21	125.09
22	C	511	CLA	C4A-NA-C1A	2.62	109.75	106.36
22	C	506	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	C	512	CLA	O1D-CGD-CBD	2.62	128.38	124.62
22	b	618	CLA	C4A-NA-C1A	2.62	109.75	106.36
22	C	502	CLA	CMB-C2B-C3B	2.63	130.23	125.09
22	c	502	CLA	CMB-C2B-C3B	2.63	130.23	125.09
23	a	408	PL9	C20-C19-C21	2.63	119.42	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	608	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	D	406	CLA	CMB-C2B-C3B	2.64	130.24	125.09
22	B	605	CLA	C4A-NA-C1A	2.64	109.77	106.36
22	c	501	CLA	C4A-NA-C1A	2.64	109.77	106.36
22	C	520	CLA	C4A-NA-C1A	2.64	109.77	106.36
22	b	616	CLA	C4A-NA-C1A	2.64	109.78	106.36
22	a	405	CLA	C4A-NA-C1A	2.65	109.78	106.36
22	D	405	CLA	CMB-C2B-C3B	2.65	130.26	125.09
22	B	609	CLA	CMB-C2B-C3B	2.65	130.27	125.09
22	c	503	CLA	O2D-CGD-CBD	2.65	114.93	111.30
22	c	503	CLA	CMB-C2B-C3B	2.65	130.27	125.09
22	c	511	CLA	CMB-C2B-C3B	2.65	130.27	125.09
22	b	607	CLA	CHB-C4A-NA	2.66	128.18	124.51
22	A	402	CLA	O1D-CGD-CBD	2.66	128.43	124.62
24	B	619	BCR	C27-C26-C25	2.66	126.17	122.78
22	c	503	CLA	C4A-NA-C1A	2.66	109.80	106.36
22	a	405	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	a	409	BCR	C27-C26-C25	2.67	126.18	122.78
22	A	403	CLA	C4A-NA-C1A	2.67	109.80	106.36
22	C	512	CLA	CMB-C2B-C3B	2.67	130.30	125.09
24	b	623	BCR	C27-C26-C25	2.67	126.18	122.78
26	c	519	LHG	O8-C23-C24	2.67	120.03	111.90
22	b	614	CLA	O1D-CGD-CBD	2.67	128.45	124.62
26	C	519	LHG	O8-C23-C24	2.67	120.04	111.90
22	B	611	CLA	CMB-C2B-C3B	2.68	130.34	125.09
22	C	501	CLA	C4A-NA-C1A	2.68	109.83	106.36
22	C	503	CLA	CMB-C2B-C3B	2.68	130.34	125.09
22	A	405	CLA	CMB-C2B-C3B	2.69	130.34	125.09
22	B	603	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	A	407	BCR	C27-C26-C25	2.69	126.21	122.78
22	a	404	CLA	O1D-CGD-CBD	2.70	128.49	124.62
22	A	403	CLA	CHB-C4A-NA	2.70	128.24	124.51
24	F	102	BCR	C29-C30-C25	2.70	114.64	110.36
22	b	607	CLA	C4A-NA-C1A	2.70	109.85	106.36
24	B	618	BCR	C29-C30-C25	2.70	114.64	110.36
22	C	510	CLA	C4A-NA-C1A	2.71	109.86	106.36
22	c	505	CLA	CMB-C2B-C3B	2.71	130.38	125.09
22	C	510	CLA	CMB-C2B-C3B	2.71	130.39	125.09
22	b	613	CLA	CMB-C2B-C3B	2.71	130.39	125.09
22	b	609	CLA	C4A-NA-C1A	2.71	109.87	106.36
22	c	512	CLA	CMB-C2B-C3B	2.72	130.41	125.09
22	b	615	CLA	C4A-NA-C1A	2.72	109.88	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	615	CLA	CMB-C2B-C3B	2.73	130.43	125.09
22	c	507	CLA	O2D-CGD-CBD	2.73	115.05	111.30
22	b	614	CLA	CMB-C2B-C3B	2.73	130.44	125.09
22	a	407	CLA	CMB-C2B-C3B	2.73	130.44	125.09
24	K	102	BCR	C27-C26-C25	2.74	126.28	122.78
22	b	617	CLA	CMB-C2B-C3B	2.75	130.46	125.09
22	C	505	CLA	CMB-C2B-C3B	2.75	130.47	125.09
24	c	521	BCR	C27-C26-C25	2.76	126.30	122.78
24	K	102	BCR	C2-C1-C6	2.76	114.74	110.36
22	B	603	CLA	C4A-NA-C1A	2.77	109.94	106.36
22	c	510	CLA	CMB-C2B-C3B	2.77	130.50	125.09
22	c	504	CLA	C4A-NA-C1A	2.78	109.95	106.36
22	B	613	CLA	CMB-C2B-C3B	2.79	130.55	125.09
22	C	504	CLA	O1D-CGD-CBD	2.80	128.63	124.62
22	c	506	CLA	CMB-C2B-C3B	2.80	130.56	125.09
22	C	506	CLA	CMB-C2B-C3B	2.80	130.57	125.09
24	f	102	BCR	C29-C30-C25	2.80	114.80	110.36
22	B	611	CLA	C4A-NA-C1A	2.81	109.99	106.36
26	a	411	LHG	O8-C23-C24	2.81	120.46	111.90
22	B	607	CLA	CMB-C2B-C3B	2.81	130.59	125.09
22	C	504	CLA	C4A-NA-C1A	2.81	110.00	106.36
22	b	606	CLA	CMB-C2B-C3B	2.83	130.63	125.09
24	b	623	BCR	C2-C1-C6	2.84	114.86	110.36
22	b	609	CLA	O1D-CGD-CBD	2.84	128.69	124.62
24	B	619	BCR	C2-C1-C6	2.84	114.86	110.36
22	B	602	CLA	CMB-C2B-C3B	2.84	130.65	125.09
22	B	610	CLA	CMB-C2B-C3B	2.84	130.65	125.09
26	A	409	LHG	O8-C23-C24	2.85	120.58	111.90
22	C	507	CLA	CMB-C2B-C3B	2.87	130.70	125.09
22	c	504	CLA	O1D-CGD-CBD	2.88	128.75	124.62
22	b	611	CLA	CMB-C2B-C3B	2.89	130.73	125.09
34	f	101	HEM	CMD-C2D-C3D	2.91	127.21	114.35
29	A	413	SQD	C44-O6-C1	2.91	119.94	113.82
29	B	622	SQD	C3-C4-C5	2.92	115.29	110.20
24	c	521	BCR	C2-C1-C6	2.92	114.99	110.36
29	a	415	SQD	C3-C4-C5	2.92	115.30	110.20
34	F	101	HEM	CMD-C2D-C3D	2.93	127.31	114.35
22	d	405	CLA	O1D-CGD-CBD	2.94	128.84	124.62
22	B	605	CLA	O1D-CGD-CBD	2.96	128.86	124.62
29	A	412	SQD	C3-C4-C5	2.97	115.38	110.20
23	D	407	PL9	C40-C39-C41	2.99	119.97	115.41
22	c	507	CLA	CMB-C2B-C3B	3.02	130.99	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	403	SQD	C3-C4-C5	3.05	115.51	110.20
24	b	622	BCR	C2-C1-C6	3.05	115.20	110.36
22	b	616	CLA	CMB-C2B-C3B	3.06	131.07	125.09
23	d	407	PL9	C40-C39-C41	3.06	120.08	115.41
24	g	101	BCR	C27-C26-C25	3.07	126.69	122.78
22	B	612	CLA	CMB-C2B-C3B	3.07	131.09	125.09
22	b	607	CLA	O1D-CGD-CBD	3.10	129.06	124.62
24	B	618	BCR	C2-C1-C6	3.11	115.28	110.36
24	y	101	BCR	C27-C26-C25	3.12	126.75	122.78
24	a	409	BCR	C2-C1-C6	3.15	115.34	110.36
34	v	201	HEM	CMD-C2D-C3D	3.15	128.29	114.35
29	a	401	SQD	O47-C7-C8	3.17	118.42	111.53
29	b	602	SQD	C3-C4-C5	3.20	115.78	110.20
29	a	401	SQD	C44-O6-C1	3.21	120.57	113.82
24	j	102	BCR	C27-C26-C25	3.22	126.88	122.78
34	V	201	HEM	CMD-C2D-C3D	3.23	128.66	114.35
29	B	626	SQD	C3-C4-C5	3.24	115.85	110.20
22	B	603	CLA	O1D-CGD-CBD	3.25	129.28	124.62
34	F	101	HEM	C3B-C4B-CHC	3.25	127.74	123.16
24	A	407	BCR	C2-C1-C6	3.26	115.53	110.36
24	J	102	BCR	C27-C26-C25	3.30	126.98	122.78
31	D	401	PHO	O1D-CGD-CBD	3.30	129.35	124.62
29	A	413	SQD	O47-C7-C8	3.30	118.70	111.53
29	f	103	SQD	O47-C7-C8	3.30	118.71	111.53
31	d	401	PHO	O1D-CGD-CBD	3.34	129.41	124.62
34	f	101	HEM	C3B-C4B-CHC	3.34	127.86	123.16
29	F	103	SQD	O47-C7-C8	3.38	118.88	111.53
31	D	402	PHO	O1D-CGD-CBD	3.40	129.49	124.62
31	d	402	PHO	O1D-CGD-CBD	3.40	129.50	124.62
29	B	622	SQD	O47-C7-C8	3.42	118.96	111.53
29	d	403	SQD	O47-C7-C8	3.42	118.96	111.53
29	A	412	SQD	O5-C5-C4	3.49	116.23	109.68
29	F	103	SQD	O5-C5-C4	3.51	116.27	109.68
29	f	103	SQD	O5-C5-C4	3.54	116.33	109.68
29	B	626	SQD	O47-C7-C8	3.55	119.24	111.53
29	b	602	SQD	O47-C7-C8	3.55	119.24	111.53
29	a	415	SQD	O5-C5-C4	3.58	116.41	109.68
29	A	412	SQD	O47-C7-C8	3.59	119.33	111.53
34	v	201	HEM	CMC-C2C-C3C	3.60	125.51	116.53
34	f	101	HEM	CMB-C2B-C3B	3.60	125.51	116.53
34	F	101	HEM	CMB-C2B-C3B	3.62	125.56	116.53
24	j	102	BCR	C2-C1-C6	3.64	116.12	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	102	BCR	C2-C1-C6	3.64	116.13	110.36
25	b	601	DGD	O5D-C1E-C2E	3.67	112.67	108.04
30	i	102	LMT	O1'-C1'-C2'	3.68	112.68	108.04
29	a	415	SQD	O47-C7-C8	3.68	119.53	111.53
29	b	602	SQD	O5-C5-C4	3.69	116.61	109.68
24	c	513	BCR	C2-C1-C6	3.72	116.25	110.36
30	I	102	LMT	O1'-C1'-C2'	3.74	112.76	108.04
29	a	401	SQD	O5-C5-C4	3.74	116.70	109.68
34	V	201	HEM	CMC-C2C-C3C	3.74	125.88	116.53
24	C	513	BCR	C2-C1-C6	3.75	116.29	110.36
29	B	626	SQD	O5-C5-C4	3.75	116.72	109.68
26	A	409	LHG	O4-P-O5	3.76	132.89	112.53
34	V	201	HEM	CAD-C3D-C4D	3.77	125.77	112.47
26	a	411	LHG	O4-P-O5	3.78	133.03	112.53
26	C	519	LHG	O4-P-O5	3.78	133.04	112.53
26	c	519	LHG	O4-P-O5	3.79	133.05	112.53
29	A	413	SQD	O5-C5-C4	3.80	116.81	109.68
25	B	625	DGD	O5D-C1E-C2E	3.85	112.90	108.04
34	v	201	HEM	CAD-C3D-C4D	3.86	126.07	112.47
34	F	101	HEM	CAD-C3D-C4D	3.99	126.53	112.47
34	f	101	HEM	CAD-C3D-C4D	4.03	126.68	112.47
29	f	103	SQD	O6-C1-C2	4.07	113.17	108.04
29	F	103	SQD	O6-C1-C2	4.31	113.48	108.04
29	B	622	SQD	O5-C5-C4	4.32	117.79	109.68
29	d	403	SQD	O5-C5-C4	4.40	117.94	109.68
29	F	103	SQD	O9-S-C6	4.68	110.89	106.94
34	f	101	HEM	CMC-C2C-C3C	4.73	128.34	116.53
29	A	413	SQD	O9-S-C6	4.77	110.96	106.94
34	F	101	HEM	CMC-C2C-C3C	4.78	128.46	116.53
29	a	401	SQD	O9-S-C6	4.79	110.98	106.94
29	f	103	SQD	O9-S-C6	4.84	111.02	106.94
34	V	201	HEM	CMB-C2B-C3B	4.90	128.77	116.53
34	v	201	HEM	CMB-C2B-C3B	4.92	128.81	116.53
29	d	403	SQD	O7-S-C6	5.02	111.17	106.94
29	B	622	SQD	O9-S-C6	5.04	111.19	106.94
34	f	101	HEM	CAD-C3D-C2D	5.09	127.86	113.22
34	F	101	HEM	CAD-C3D-C2D	5.17	128.08	113.22
29	a	415	SQD	O7-S-C6	5.23	111.35	106.94
29	d	403	SQD	O9-S-C6	5.24	111.36	106.94
29	B	626	SQD	O7-S-C6	5.28	111.39	106.94
29	B	622	SQD	O7-S-C6	5.32	111.42	106.94
29	A	412	SQD	O7-S-C6	5.33	111.44	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	v	201	HEM	CAD-C3D-C2D	5.34	128.57	113.22
29	B	622	SQD	O6-C1-C2	5.35	114.79	108.04
29	d	403	SQD	O6-C1-C2	5.36	114.81	108.04
29	b	602	SQD	O7-S-C6	5.48	111.56	106.94
34	V	201	HEM	CAD-C3D-C2D	5.49	129.01	113.22
29	B	626	SQD	O9-S-C6	5.71	111.75	106.94
29	b	602	SQD	O9-S-C6	5.71	111.76	106.94
29	A	413	SQD	O7-S-C6	5.74	111.78	106.94
29	a	401	SQD	O7-S-C6	5.77	111.81	106.94
29	F	103	SQD	O7-S-C6	5.95	111.95	106.94
29	f	103	SQD	O7-S-C6	5.99	111.99	106.94
29	B	626	SQD	O6-C1-C2	6.72	116.53	108.04
29	b	602	SQD	O6-C1-C2	6.89	116.74	108.04
29	a	415	SQD	O9-S-C6	6.96	112.81	106.94
29	A	412	SQD	O6-C1-C2	7.02	116.91	108.04
29	A	412	SQD	O9-S-C6	7.10	112.92	106.94
29	a	415	SQD	O6-C1-C2	7.20	117.13	108.04

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	c	520	CLA	NC
22	c	520	CLA	ND
22	c	520	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA

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Mol	Chain	Res	Type	Atom
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	ND
22	d	405	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	D	406	CLA	NC
22	D	406	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	c	508	CLA	NC

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Mol	Chain	Res	Type	Atom
22	c	508	CLA	ND
22	c	508	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	d	406	CLA	NC
22	d	406	CLA	ND
22	d	406	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	b	613	CLA	NC

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Mol	Chain	Res	Type	Atom
22	b	613	CLA	ND
22	b	613	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	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	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	D	405	CLA	NC

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Mol	Chain	Res	Type	Atom
22	D	405	CLA	ND
22	D	405	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND
22	b	619	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	C	520	CLA	NC
22	C	520	CLA	ND
22	C	520	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND
22	a	404	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	h	101	CLA	NC
22	h	101	CLA	ND
22	h	101	CLA	NA
22	C	512	CLA	NC

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Mol	Chain	Res	Type	Atom
22	C	512	CLA	ND
22	C	512	CLA	NA
22	a	407	CLA	NC
22	a	407	CLA	ND
22	a	407	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	c	516	DGD	C2G-O2G-C1B-C2B
25	C	516	DGD	C2G-O2G-C1B-C2B
29	d	403	SQD	C45-O47-C7-C8
29	B	622	SQD	C45-O47-C7-C8

There are no ring outliers.

79 monomers are involved in 296 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	10	0
22	A	403	CLA	13	0
22	A	404	CLA	15	0
22	A	405	CLA	9	0
23	A	406	PL9	4	0
24	A	407	BCR	3	0
25	A	408	DGD	1	0
26	A	409	LHG	3	0
27	A	410	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	412	SQD	3	0
29	A	413	SQD	3	0
27	A	414	LMG	1	0
22	B	601	CLA	1	0
22	B	602	CLA	11	0
22	B	603	CLA	3	0
22	B	604	CLA	7	0
22	B	605	CLA	7	0
22	B	606	CLA	16	0
22	B	607	CLA	9	0
22	B	608	CLA	13	0
22	B	609	CLA	3	0
22	B	610	CLA	6	0
22	B	611	CLA	11	0
22	B	612	CLA	10	0
22	B	613	CLA	4	0
22	B	614	CLA	2	0
22	B	615	CLA	6	0
24	B	616	BCR	4	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
29	B	622	SQD	3	0
30	B	623	LMT	2	0
25	B	625	DGD	2	0
29	B	626	SQD	1	0
30	B	627	LMT	2	0
30	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	2	0
22	C	506	CLA	6	0
22	C	507	CLA	4	0
22	C	508	CLA	2	0
22	C	509	CLA	6	0
22	C	510	CLA	10	0
22	C	511	CLA	2	0
22	C	512	CLA	3	0
24	C	513	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	514	BCR	7	0
25	C	515	DGD	3	0
25	C	516	DGD	3	0
25	C	517	DGD	5	0
27	C	518	LMG	4	0
26	C	519	LHG	2	0
22	C	520	CLA	4	0
31	D	401	PHO	10	0
31	D	402	PHO	5	0
22	D	405	CLA	8	0
22	D	406	CLA	3	0
23	D	407	PL9	12	0
27	D	408	LMG	4	0
27	D	409	LMG	6	0
25	D	410	DGD	2	0
27	D	412	LMG	1	0
27	E	101	LMG	1	0
34	F	101	HEM	4	0
24	F	102	BCR	4	0
29	F	103	SQD	3	0
22	H	101	CLA	9	0
24	H	102	BCR	2	0
27	I	101	LMG	1	0
30	I	102	LMT	1	0
24	J	102	BCR	1	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%)	0.50	31 (9%) 11 9	178, 179, 180, 181	0
1	a	335/344 (97%)	0.45	33 (9%) 9 8	178, 179, 180, 181	0
2	B	490/510 (96%)	0.25	27 (5%) 29 23	178, 179, 180, 181	0
2	b	490/510 (96%)	0.38	34 (6%) 20 15	178, 179, 180, 181	0
3	C	447/461 (96%)	0.32	30 (6%) 21 16	178, 179, 180, 181	0
3	c	447/461 (96%)	0.15	19 (4%) 39 31	178, 180, 180, 181	0
4	D	340/352 (96%)	0.24	15 (4%) 38 30	177, 179, 180, 181	0
4	d	340/352 (96%)	0.21	9 (2%) 59 49	177, 179, 180, 181	0
5	E	82/84 (97%)	0.12	2 (2%) 62 53	178, 180, 180, 181	0
5	e	82/84 (97%)	0.02	4 (4%) 33 26	178, 180, 181, 181	0
6	F	35/45 (77%)	-0.15	1 (2%) 55 45	179, 179, 180, 180	0
6	f	35/45 (77%)	-0.44	0 100 100	179, 180, 181, 181	0
7	H	65/66 (98%)	0.45	12 (18%) 2 3	179, 180, 180, 181	0
7	h	65/66 (98%)	0.57	10 (15%) 3 4	179, 180, 181, 181	0
8	I	35/38 (92%)	0.51	2 (5%) 27 21	178, 179, 180, 181	0
8	i	35/38 (92%)	-0.02	0 100 100	179, 179, 181, 181	0
9	J	34/40 (85%)	0.03	2 (5%) 26 19	178, 179, 180, 180	0
9	j	34/40 (85%)	-0.39	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	-0.02	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.52	5 (13%) 4 5	179, 180, 181, 181	0
11	L	37/37 (100%)	0.56	1 (2%) 58 48	178, 179, 180, 181	0
11	l	37/37 (100%)	0.17	0 100 100	178, 179, 180, 181	0
12	M	34/36 (94%)	0.34	2 (5%) 26 19	178, 179, 180, 181	0
12	m	34/36 (94%)	0.11	1 (2%) 55 45	178, 179, 180, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.62	25 (10%) 9 8	177, 179, 180, 181	0
13	o	243/272 (89%)	0.64	21 (8%) 13 11	177, 179, 181, 181	0
14	T	32/32 (100%)	0.23	2 (6%) 23 17	178, 179, 181, 181	0
14	t	32/32 (100%)	0.38	4 (12%) 5 6	178, 179, 180, 181	0
15	U	97/134 (72%)	0.59	7 (7%) 18 14	178, 179, 180, 181	0
15	u	97/134 (72%)	0.82	13 (13%) 4 6	178, 179, 180, 181	0
16	V	137/163 (84%)	0.17	3 (2%) 65 56	178, 179, 180, 181	0
16	v	137/163 (84%)	0.52	9 (6%) 22 16	178, 180, 181, 181	0
17	g	28/46 (60%)	0.46	2 (7%) 19 14	179, 180, 181, 182	0
17	y	28/46 (60%)	0.21	0 100 100	178, 180, 181, 181	0
18	X	37/41 (90%)	0.52	4 (10%) 8 7	179, 179, 181, 181	0
18	x	37/41 (90%)	0.84	6 (16%) 3 4	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.35	2 (3%) 51 41	179, 180, 181, 181	0
20	z	62/62 (100%)	0.95	4 (6%) 22 16	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.35	342 (6%) 22 16	177, 179, 180, 182	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	84	LYS	7.2
15	U	38	GLU	6.7
13	o	169	LYS	6.4
7	H	66	GLY	5.8
1	A	10	SER	5.7
3	C	148	GLY	5.5
3	C	149	TYR	5.3
5	e	82	GLN	5.0
1	A	299	GLY	4.8
3	c	201	ASN	4.4
2	b	490	GLN	4.4
18	x	11	THR	4.4
2	B	69	LEU	4.3
5	E	84	LYS	4.3
16	v	132	ASN	4.2
1	A	179	THR	4.2

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Mol	Chain	Res	Type	RSRZ
4	D	24	ARG	4.2
1	A	11	ALA	4.2
4	d	295	SER	4.1
13	o	168	PHE	4.1
13	O	84	ASN	4.0
3	c	202	PRO	4.0
13	O	90	GLU	4.0
4	d	13	GLY	3.9
15	U	39	LEU	3.9
1	a	175	GLY	3.9
13	o	31	LEU	3.9
3	c	372	PRO	3.9
1	a	137	LEU	3.9
17	g	27	MET	3.8
3	C	140	LEU	3.8
3	C	147	PHE	3.7
3	C	184	GLY	3.7
15	u	53	GLU	3.7
3	c	200	THR	3.7
3	C	141	GLU	3.7
13	o	124	GLU	3.7
2	B	411	PHE	3.6
1	A	175	GLY	3.6
1	a	224	ILE	3.6
2	B	295	GLY	3.6
2	b	218	LEU	3.5
1	a	190	HIS	3.5
4	D	190	ASN	3.5
3	C	266	TRP	3.5
3	c	260	ALA	3.5
1	a	19	ASN	3.5
1	A	195	HIS	3.5
3	C	143	TYR	3.4
1	A	294	ALA	3.4
2	B	83	GLU	3.4
13	O	91	PHE	3.3
4	D	174	GLY	3.3
1	a	239	PHE	3.3
13	o	154	SER	3.3
3	C	183	GLY	3.3
1	a	179	THR	3.3
2	b	302	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	139	THR	3.3
9	J	7	ARG	3.3
2	b	229	LEU	3.2
14	t	30	THR	3.2
4	d	191	TRP	3.2
1	A	198	HIS	3.2
13	O	170	GLY	3.2
1	a	165	GLN	3.2
7	H	6	TRP	3.2
1	A	12	ASN	3.2
14	t	31	LYS	3.2
2	b	338	GLN	3.2
1	A	177	SER	3.2
1	a	178	GLY	3.1
15	u	52	GLY	3.1
13	O	223	ILE	3.1
2	b	301	ALA	3.1
13	O	50	ASP	3.1
1	a	187	GLN	3.1
20	z	4	LEU	3.1
2	b	339	ALA	3.1
13	o	153	ALA	3.1
14	T	28	ARG	3.0
15	U	40	VAL	3.0
1	a	282	GLY	3.0
3	c	203	THR	3.0
14	t	32	LYS	3.0
10	k	14	ALA	3.0
15	u	58	ASN	3.0
1	a	299	GLY	3.0
15	u	72	TYR	3.0
2	B	84	THR	3.0
13	O	243	SER	2.9
3	C	142	GLU	2.9
3	C	473	ASP	2.9
1	a	183	MET	2.9
1	A	138	GLY	2.9
20	z	1	MET	2.9
18	x	12	ILE	2.9
2	B	161	LEU	2.9
2	b	303	SER	2.9
1	A	137	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	c	403	SER	2.9
13	o	32	THR	2.9
2	b	402	TYR	2.8
2	B	185	TRP	2.8
2	b	340	TRP	2.8
2	B	294	SER	2.8
7	h	2	ALA	2.8
2	B	183	PRO	2.8
3	C	212	TYR	2.8
2	B	378	LYS	2.8
1	A	293	MET	2.8
1	A	80	GLY	2.8
3	C	332	GLN	2.8
2	b	119	ASP	2.8
14	t	29	ILE	2.8
1	a	138	GLY	2.8
1	A	178	GLY	2.8
1	A	196	PRO	2.8
1	A	298	ASN	2.8
18	x	16	LEU	2.7
3	c	402	GLY	2.7
15	U	121	LEU	2.7
2	b	485	GLU	2.7
7	h	66	GLY	2.7
4	d	197	HIS	2.7
1	a	325	ASN	2.7
2	B	293	ALA	2.7
1	a	298	ASN	2.7
3	C	144	SER	2.7
3	C	137	PRO	2.7
16	v	133	LEU	2.7
4	D	197	HIS	2.7
1	A	165	GLN	2.7
7	h	14	LEU	2.7
18	x	47	GLN	2.6
7	H	5	THR	2.6
3	C	145	SER	2.6
13	o	35	ASP	2.6
16	v	47	LEU	2.6
3	C	464	GLU	2.6
1	A	191	ASN	2.6
2	b	133	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	b	298	LEU	2.6
15	u	51	TYR	2.6
4	d	194	ASN	2.6
2	b	482	ILE	2.6
6	F	11	VAL	2.6
7	H	56	ASP	2.6
15	U	42	VAL	2.6
13	O	58	ILE	2.6
10	k	17	ILE	2.6
15	u	47	LEU	2.6
7	H	63	LYS	2.6
1	a	177	SER	2.6
13	o	215	ARG	2.6
2	B	410	THR	2.6
2	b	487	SER	2.6
13	O	195	ASP	2.5
3	C	136	GLY	2.5
1	A	15	GLU	2.5
2	b	412	THR	2.5
13	O	169	LYS	2.5
2	B	165	GLY	2.5
1	a	198	HIS	2.5
3	C	27	ASP	2.5
13	O	46	PRO	2.5
3	c	209	ILE	2.5
13	o	213	VAL	2.5
8	I	30	ARG	2.5
13	O	268	SER	2.5
13	O	225	LEU	2.5
2	B	164	PRO	2.5
3	c	411	ALA	2.5
15	u	131	GLY	2.5
12	m	1	MET	2.5
1	a	286	THR	2.5
7	h	3	ARG	2.5
17	g	30	ILE	2.5
8	I	34	ARG	2.5
18	X	42	GLN	2.5
15	u	57	LEU	2.5
3	C	261	ARG	2.5
16	V	47	LEU	2.5
16	v	138	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
13	O	269	ILE	2.5
2	b	379	ALA	2.5
1	A	262	TYR	2.5
3	C	135	ARG	2.5
3	C	258	GLY	2.5
7	h	56	ASP	2.5
15	u	107	GLU	2.5
16	v	131	ARG	2.5
13	o	229	LYS	2.5
1	a	199	GLN	2.5
1	A	183	MET	2.4
7	h	26	GLY	2.4
2	B	474	LEU	2.4
15	u	65	PHE	2.4
4	D	176	ALA	2.4
4	D	170	ALA	2.4
2	b	120	LEU	2.4
10	k	43	VAL	2.4
16	v	142	ALA	2.4
2	B	326	ARG	2.4
2	b	393	GLU	2.4
7	H	62	TRP	2.4
4	D	194	ASN	2.4
4	D	199	MET	2.4
13	o	63	THR	2.4
1	a	201	GLY	2.4
13	o	224	SER	2.4
2	B	379	ALA	2.4
5	E	17	VAL	2.4
2	b	398	THR	2.4
2	b	219	VAL	2.4
2	b	397	VAL	2.4
2	B	412	THR	2.4
13	o	62	GLN	2.4
1	A	19	ASN	2.4
2	b	122	LEU	2.3
13	o	269	ILE	2.3
2	b	420	TYR	2.3
12	M	5	GLN	2.3
15	u	54	LYS	2.3
16	V	94	ASN	2.3
13	o	123	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	c	371	GLY	2.3
4	d	241	GLU	2.3
7	H	9	ASP	2.3
20	z	17	PHE	2.3
2	b	228	ALA	2.3
4	D	171	PRO	2.3
1	A	169	SER	2.3
18	x	42	GLN	2.3
3	C	44	ASN	2.3
13	O	68	ARG	2.3
13	O	262	GLN	2.3
3	C	151	TRP	2.3
11	L	33	SER	2.3
13	O	222	GLN	2.3
2	B	127	ARG	2.3
1	a	301	ASN	2.3
16	v	51	GLN	2.3
7	h	4	ARG	2.3
7	H	8	GLY	2.3
1	a	240	GLY	2.3
3	C	201	ASN	2.2
7	h	54	ILE	2.2
3	c	180	MET	2.2
2	B	129	GLY	2.2
1	a	172	MET	2.2
1	A	192	ILE	2.2
13	o	237	ILE	2.2
15	U	65	PHE	2.2
13	o	64	TYR	2.2
13	O	224	SER	2.2
18	X	45	LYS	2.2
2	b	337	ALA	2.2
5	e	83	LEU	2.2
3	c	211	GLY	2.2
2	b	217	ILE	2.2
2	B	8	VAL	2.2
2	b	431	GLU	2.2
1	a	225	ARG	2.2
4	D	295	SER	2.2
13	O	126	GLY	2.2
1	A	342	ASP	2.2
13	o	167	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	300	PHE	2.2
4	d	14	TRP	2.2
7	h	18	TYR	2.2
2	b	488	PRO	2.2
13	O	113	VAL	2.2
3	C	402	GLY	2.2
13	o	120	THR	2.2
4	d	200	GLY	2.2
1	A	13	LEU	2.2
15	U	69	ARG	2.2
2	B	353	GLU	2.2
1	A	181	ASN	2.2
1	a	191	ASN	2.2
7	H	64	ALA	2.2
18	X	11	THR	2.2
10	k	10	LYS	2.2
18	x	15	SER	2.1
20	Z	1	MET	2.1
3	c	259	TRP	2.1
2	B	120	LEU	2.1
4	D	177	ALA	2.1
7	H	27	THR	2.1
1	a	181	ASN	2.1
1	a	26	ASN	2.1
2	b	411	PHE	2.1
3	C	262	ARG	2.1
3	c	207	ARG	2.1
2	B	354	LEU	2.1
1	A	14	TRP	2.1
16	v	145	ILE	2.1
13	O	244	GLU	2.1
13	o	125	ASP	2.1
3	c	373	ASN	2.1
4	D	297	ASP	2.1
16	V	95	ILE	2.1
12	M	2	GLU	2.1
20	z	9	LEU	2.1
1	a	303	ASN	2.1
16	v	141	ILE	2.1
5	e	57	ALA	2.1
4	D	191	TRP	2.1
1	a	176	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
14	T	27	PRO	2.1
2	B	70	GLY	2.1
1	a	192	ILE	2.1
13	O	49	ASP	2.1
18	X	13	THR	2.1
9	J	8	ILE	2.1
3	C	146	PHE	2.1
1	a	322	ASN	2.1
13	O	51	THR	2.1
3	c	210	PHE	2.1
1	A	190	HIS	2.0
2	B	128	THR	2.0
3	c	405	ASN	2.0
20	Z	34	ASP	2.0
4	D	282	SER	2.0
7	h	23	PRO	2.0
13	O	234	THR	2.0
2	b	214	LEU	2.0
3	c	389	GLU	2.0
7	H	65	LEU	2.0
13	O	111	LEU	2.0
2	b	70	GLY	2.0
3	C	154	LYS	2.0
15	u	74	THR	2.0
4	D	172	SER	2.0
1	a	139	MET	2.0
2	B	162	PHE	2.0
4	d	201	VAL	2.0
15	u	76	ALA	2.0
7	H	10	ILE	2.0
2	b	409	GLN	2.0
10	k	13	GLU	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
30	LMT	i	102	35/35	0.51	1.11	7.54	178,181,183,183	0
30	LMT	I	102	35/35	0.48	1.09	7.13	178,180,182,183	0
27	LMG	C	518	45/55	0.65	1.11	5.83	178,179,180,181	0
24	BCR	c	521	40/40	0.85	1.25	5.60	178,179,181,181	0
27	LMG	c	518	45/55	0.74	1.01	5.58	178,180,181,181	0
24	BCR	y	101	40/40	0.76	1.00	5.52	177,179,180,180	0
25	DGD	D	410	63/66	0.74	0.87	5.39	178,181,182,183	0
24	BCR	B	619	40/40	0.73	0.82	5.25	178,179,180,180	0
25	DGD	d	410	63/66	0.64	0.84	5.06	178,180,183,183	0
24	BCR	b	623	40/40	0.73	0.73	4.61	177,178,180,180	0
22	CLA	A	405	65/65	0.80	0.70	4.44	177,179,180,181	0
30	LMT	b	627	35/35	0.67	1.10	4.35	178,180,182,182	0
24	BCR	C	513	40/40	0.88	0.74	4.14	177,179,180,180	0
23	PL9	J	101	35/55	0.25	0.59	4.10	177,180,181,181	0
22	CLA	b	605	65/65	0.59	1.12	3.73	179,180,182,183	0
30	LMT	D	411	31/35	0.66	0.87	3.33	179,180,182,182	0
22	CLA	c	512	65/65	0.76	0.80	3.26	178,180,181,182	0
22	CLA	B	603	65/65	0.78	0.53	3.16	176,179,180,180	0
24	BCR	H	102	40/40	0.67	1.01	3.15	178,180,181,182	0
22	CLA	D	406	65/65	0.89	0.67	2.96	177,179,180,181	0
23	PL9	j	101	35/55	0.52	0.35	2.92	179,180,181,181	0
24	BCR	a	409	40/40	0.69	0.69	2.84	177,178,180,180	0
22	CLA	a	407	65/65	0.77	0.71	2.71	178,179,180,181	0
24	BCR	c	513	40/40	0.76	0.89	2.71	178,179,180,180	0
22	CLA	B	601	65/65	0.61	0.95	2.70	177,180,181,182	0
24	BCR	g	101	40/40	0.57	0.89	2.67	178,179,180,180	0
25	DGD	b	601	52/66	0.71	0.55	2.57	178,180,181,182	0
22	CLA	c	511	65/65	0.87	0.68	2.52	178,180,181,182	0
30	LMT	d	411	31/35	0.49	0.79	2.46	178,181,182,183	0
25	DGD	B	625	52/66	0.76	0.59	2.43	177,180,182,182	0
27	LMG	M	101	42/55	0.69	0.55	2.36	178,180,181,182	0
30	LMT	B	624	35/35	0.80	0.50	2.32	178,180,182,183	0
24	BCR	B	617	40/40	0.67	0.50	2.31	177,179,180,180	0
24	BCR	K	102	40/40	0.71	0.89	2.27	178,180,181,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	BCR	J	102	40/40	0.53	0.37	2.26	178,180,181,181	0
30	LMT	B	627	35/35	0.64	0.64	2.25	178,180,182,182	0
29	SQD	f	103	45/54	0.86	0.57	2.12	177,179,181,182	0
24	BCR	C	514	40/40	0.81	0.77	2.10	178,179,180,181	0
24	BCR	F	102	40/40	0.61	0.53	2.09	177,179,180,180	0
22	CLA	b	606	65/65	0.88	0.59	2.07	177,179,180,181	0
22	CLA	c	503	65/65	0.82	0.56	2.04	177,179,180,181	0
30	LMT	b	604	35/35	0.71	0.57	2.04	177,179,181,182	0
24	BCR	f	102	40/40	0.78	0.33	2.02	177,179,181,181	0
27	LMG	e	101	44/55	0.77	0.37	1.97	177,179,181,181	0
22	CLA	B	611	65/65	0.92	0.41	1.95	177,179,180,180	0
29	SQD	B	626	47/54	0.74	0.56	1.95	175,179,181,183	0
22	CLA	b	613	65/65	0.86	0.76	1.94	178,179,180,181	0
24	BCR	A	407	40/40	0.76	0.53	1.92	177,179,180,180	0
27	LMG	a	402	42/55	0.64	0.49	1.82	177,180,181,182	0
22	CLA	c	508	65/65	0.86	0.46	1.80	177,179,180,181	0
22	CLA	c	501	65/65	0.86	0.49	1.79	177,179,180,181	0
22	CLA	C	506	65/65	0.81	0.75	1.75	177,179,180,180	0
22	CLA	C	502	65/65	0.68	0.54	1.70	178,179,180,180	0
22	CLA	B	604	65/65	0.89	0.72	1.70	177,179,180,180	0
22	CLA	d	406	65/65	0.83	0.56	1.68	177,179,180,181	0
24	BCR	c	514	40/40	0.73	0.78	1.65	177,179,180,180	0
22	CLA	b	609	65/65	0.85	0.64	1.65	178,179,180,181	0
29	SQD	a	401	54/54	0.84	0.65	1.64	178,180,181,183	0
29	SQD	d	403	43/54	0.67	0.86	1.59	178,180,182,186	0
22	CLA	c	502	65/65	0.55	0.64	1.59	178,179,180,181	0
22	CLA	C	508	65/65	0.83	0.85	1.58	177,179,180,180	0
22	CLA	c	506	65/65	0.88	0.58	1.58	178,179,180,181	0
22	CLA	b	607	65/65	0.82	0.43	1.48	177,179,180,181	0
30	LMT	b	603	35/35	0.68	0.50	1.47	178,179,181,182	0
25	DGD	b	624	58/66	0.72	0.43	1.47	177,178,180,180	0
22	CLA	B	608	65/65	0.86	0.58	1.44	177,179,180,180	0
22	CLA	b	608	65/65	0.88	0.52	1.41	178,179,180,181	0
24	BCR	B	618	40/40	0.87	0.32	1.41	177,178,179,179	0
27	LMG	A	414	42/55	0.62	0.52	1.39	177,179,182,182	0
22	CLA	c	510	65/65	0.80	0.56	1.38	178,179,181,181	0
24	BCR	B	616	40/40	0.68	0.47	1.36	176,178,180,180	0
22	CLA	B	614	65/65	0.85	0.67	1.32	177,179,180,181	0
22	CLA	B	609	65/65	0.90	0.51	1.29	178,179,180,181	0
27	LMG	E	101	44/55	0.63	0.61	1.24	176,179,181,182	0
22	CLA	C	501	65/65	0.86	0.47	1.22	178,179,180,180	0
22	CLA	h	101	65/65	0.84	0.46	1.19	176,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	BCR	x	101	40/40	0.74	0.86	1.16	178,179,180,181	0
22	CLA	b	619	65/65	0.67	0.76	1.16	177,179,180,181	0
22	CLA	C	512	65/65	0.81	0.91	1.12	177,180,181,182	0
22	CLA	b	615	65/65	0.88	0.40	1.12	177,179,180,180	0
29	SQD	b	602	47/54	0.80	0.42	1.08	176,179,182,185	0
22	CLA	C	511	65/65	0.90	0.88	1.05	178,179,180,181	0
24	BCR	b	622	40/40	0.75	0.37	1.03	176,178,179,179	0
25	DGD	a	410	56/66	0.71	0.41	0.97	178,180,181,182	0
22	CLA	B	605	65/65	0.87	0.69	0.93	178,179,180,180	0
22	CLA	B	615	65/65	0.83	0.73	0.93	176,179,180,181	0
29	SQD	A	413	54/54	0.87	0.38	0.91	178,180,182,184	0
29	SQD	F	103	45/54	0.82	0.64	0.90	178,180,182,182	0
22	CLA	C	510	65/65	0.77	0.54	0.88	177,179,180,181	0
25	DGD	A	408	56/66	0.73	0.42	0.88	178,179,181,182	0
22	CLA	b	612	65/65	0.84	0.63	0.85	176,179,181,181	0
27	LMG	m	101	42/55	0.79	0.42	0.83	175,179,181,181	0
27	LMG	a	412	51/55	0.78	0.36	0.81	177,179,180,180	0
34	HEM	f	101	43/43	0.89	0.35	0.80	178,180,180,181	0
24	BCR	b	621	40/40	0.79	0.38	0.79	178,178,179,179	0
22	CLA	C	505	65/65	0.81	0.47	0.74	177,179,180,181	0
30	LMT	B	628	35/35	0.57	0.49	0.74	177,180,182,183	0
22	CLA	b	618	65/65	0.81	0.68	0.72	177,179,180,180	0
34	HEM	F	101	43/43	0.94	0.42	0.70	178,180,181,182	0
22	CLA	C	503	65/65	0.86	0.40	0.69	177,179,180,180	0
23	PL9	a	408	45/55	0.81	0.30	0.67	176,179,180,180	0
34	HEM	V	201	43/43	0.91	0.39	0.61	176,178,180,180	0
23	PL9	A	406	45/55	0.72	0.41	0.59	177,179,180,180	0
22	CLA	B	602	65/65	0.92	0.50	0.59	176,178,180,180	0
22	CLA	c	505	65/65	0.81	0.51	0.59	177,179,180,181	0
25	DGD	c	515	53/66	0.83	0.40	0.56	176,179,181,182	0
22	CLA	C	504	65/65	0.87	0.39	0.46	177,179,180,180	0
34	HEM	v	201	43/43	0.91	0.53	0.45	177,179,180,180	0
24	BCR	b	620	40/40	0.85	0.37	0.44	177,179,179,180	0
22	CLA	c	504	65/65	0.89	0.31	0.42	177,179,180,180	0
22	CLA	b	616	65/65	0.94	0.30	0.41	177,179,180,180	0
22	CLA	a	404	65/65	0.76	0.61	0.41	177,178,180,180	0
22	CLA	b	617	65/65	0.83	0.42	0.41	178,179,180,182	0
27	LMG	C	521	48/55	0.77	0.31	0.33	177,179,180,181	0
29	SQD	B	622	43/54	0.85	0.43	0.31	177,180,182,185	0
22	CLA	a	405	65/65	0.80	0.58	0.29	174,178,179,180	0
22	CLA	B	607	65/65	0.89	0.38	0.27	178,179,180,181	0
22	CLA	C	509	65/65	0.85	0.36	0.27	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	B	613	65/65	0.74	0.44	0.24	177,179,180,180	0
27	LMG	d	412	46/55	0.92	0.24	0.24	177,178,180,180	0
27	LMG	D	412	46/55	0.80	0.32	0.19	178,179,180,181	0
22	CLA	b	611	65/65	0.86	0.35	0.18	177,179,180,180	0
22	CLA	C	507	65/65	0.84	0.36	0.14	178,179,180,181	0
23	PL9	d	407	55/55	0.60	0.41	0.11	177,179,180,181	0
31	PHO	d	401	64/64	0.73	0.42	0.08	178,179,180,180	0
23	PL9	D	407	55/55	0.71	0.40	0.08	177,178,179,180	0
31	PHO	D	402	64/64	0.79	0.36	0.06	177,179,180,181	0
29	SQD	a	415	51/54	0.79	0.31	0.04	178,179,181,182	0
27	LMG	A	410	51/55	0.81	0.32	0.03	177,178,180,181	0
22	CLA	H	101	65/65	0.87	0.32	0.02	177,179,180,181	0
25	DGD	B	620	58/66	0.83	0.33	0.02	176,179,181,182	0
24	BCR	j	102	40/40	0.69	0.30	0.00	179,180,182,183	0
27	LMG	D	409	48/55	0.88	0.28	-0.03	175,178,180,181	0
26	LHG	A	409	39/49	0.86	0.30	-0.04	178,179,181,181	0
22	CLA	b	614	65/65	0.91	0.28	-0.08	178,179,180,180	0
32	CL	a	413	1/1	0.94	0.54	-0.09	177,177,177,177	0
22	CLA	A	403	65/65	0.92	0.50	-0.09	177,179,179,180	0
25	DGD	C	517	66/66	0.74	0.41	-0.13	177,179,180,181	0
22	CLA	C	520	65/65	0.85	0.33	-0.16	178,179,180,181	0
27	LMG	d	409	48/55	0.84	0.30	-0.17	177,179,180,180	0
29	SQD	A	412	51/54	0.80	0.31	-0.18	178,179,180,181	0
31	PHO	D	401	64/64	0.87	0.35	-0.20	177,179,180,180	0
26	LHG	c	519	37/49	0.73	0.31	-0.21	178,180,183,187	0
22	CLA	B	610	65/65	0.87	0.36	-0.22	177,179,180,180	0
27	LMG	c	522	48/55	0.85	0.28	-0.25	178,180,180,181	0
22	CLA	A	402	65/65	0.92	0.41	-0.26	178,179,180,181	0
22	CLA	d	405	65/65	0.88	0.44	-0.30	177,178,179,180	0
25	DGD	C	515	53/66	0.87	0.31	-0.31	177,178,179,180	0
22	CLA	D	405	65/65	0.91	0.39	-0.32	177,179,180,180	0
22	CLA	c	509	65/65	0.86	0.32	-0.38	177,179,180,180	0
22	CLA	c	507	65/65	0.90	0.27	-0.44	177,179,180,181	0
27	LMG	D	408	49/55	0.78	0.32	-0.44	177,178,180,180	0
30	LMT	M	103	35/35	0.80	0.46	-0.44	177,179,180,180	0
22	CLA	B	606	65/65	0.86	0.34	-0.45	177,179,180,180	0
22	CLA	A	404	65/65	0.81	0.36	-0.52	176,178,180,181	0
26	LHG	C	519	37/49	0.77	0.34	-0.55	176,180,184,188	0
25	DGD	c	517	66/66	0.78	0.32	-0.58	177,179,181,181	0
22	CLA	c	520	65/65	0.90	0.30	-0.60	177,179,180,181	0
28	OEX	A	411	10/10	0.92	0.42	-0.60	172,175,178,178	0
26	LHG	a	411	39/49	0.85	0.26	-0.62	177,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	BCT	D	404	4/4	0.90	0.26	-0.64	178,179,179,179	0
22	CLA	b	610	65/65	0.89	0.28	-0.67	177,179,180,180	0
22	CLA	B	612	65/65	0.92	0.26	-0.76	176,178,180,181	0
27	LMG	b	625	49/55	0.86	0.29	-0.80	178,179,180,180	0
22	CLA	a	406	65/65	0.84	0.30	-0.88	177,179,180,181	0
31	PHO	d	402	64/64	0.86	0.24	-0.94	178,179,180,181	0
25	DGD	C	516	62/66	0.86	0.25	-1.02	177,179,180,181	0
27	LMG	d	408	49/55	0.94	0.20	-1.16	178,179,180,180	0
27	LMG	B	621	49/55	0.91	0.26	-1.22	177,179,180,180	0
30	LMT	M	102	35/35	0.73	0.36	-1.27	178,179,181,182	0
28	OEX	a	414	10/10	0.94	0.41	-1.36	174,177,179,182	0
32	CL	D	403	1/1	0.79	0.28	-1.56	180,180,180,180	0
25	DGD	c	516	62/66	0.88	0.27	-1.57	178,179,180,181	0
33	BCT	d	404	4/4	0.95	0.18	-1.88	178,180,180,180	0
21	FE2	A	401	1/1	0.92	0.20	-2.13	176,176,176,176	0
21	FE2	a	403	1/1	0.88	0.07	-3.50	182,182,182,182	0
30	LMT	b	626	35/35	0.65	0.67	-	178,180,182,183	0
30	LMT	B	623	35/35	0.69	0.86	-	177,181,182,183	0
27	LMG	I	101	43/55	0.59	1.02	-	178,180,181,182	0
35	CA	O	301	1/1	0.62	0.42	-	182,182,182,182	0
35	CA	k	101	1/1	0.87	0.27	-	180,180,180,180	0
35	CA	K	101	1/1	0.67	0.52	-	184,184,184,184	0
35	CA	o	301	1/1	0.77	0.56	-	184,184,184,184	0
27	LMG	i	101	43/55	0.77	0.79	-	177,180,182,184	0

6.5 Other polymers (i)

There are no such residues in this entry.