Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:45 PM GMT

PDB ID	:	4IXQ
Title	:	RT fs X-ray diffraction of Photosystem II, dark state
Authors	:	Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on	:	2013-01-27
Resolution	:	5.70 Å(reported)

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

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

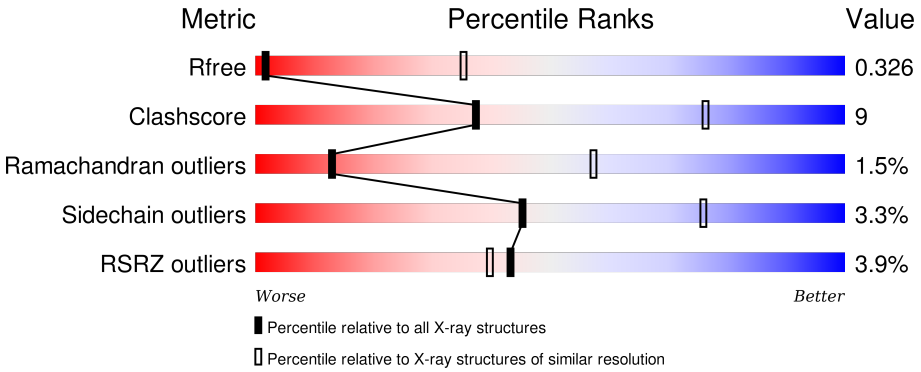
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.70 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	1006 (7.66-3.64)
Clashscore	102246	1037 (7.66-3.70)
Ramachandran outliers	100387	1011 (7.60-3.66)
Sidechain outliers	100360	1001 (7.60-3.64)
RSRZ outliers	91569	1005 (7.66-3.64)

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	360	2% 64% 28% 7%
1	a	360	% 91% 7%
2	B	510	5% 68% 27%
2	b	510	4% 93%

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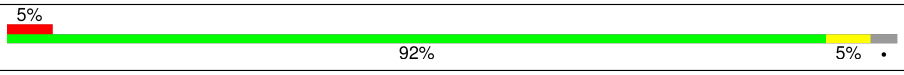
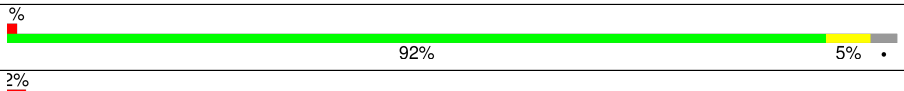
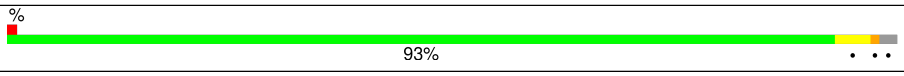
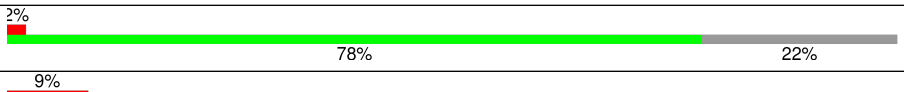
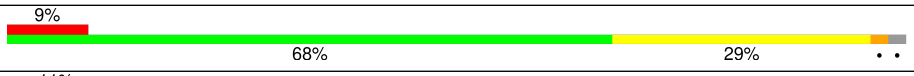
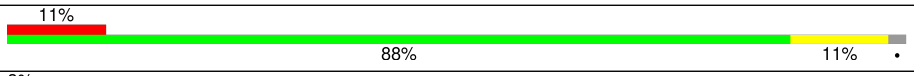
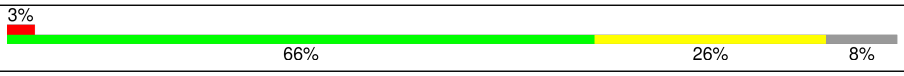
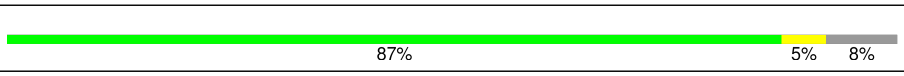
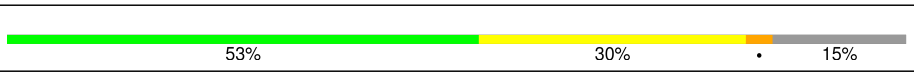
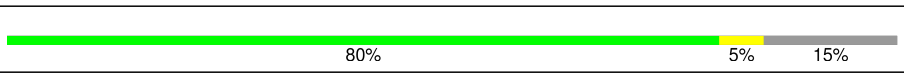
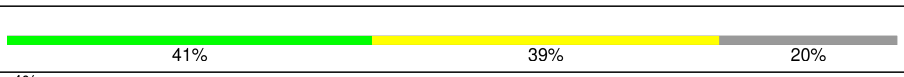
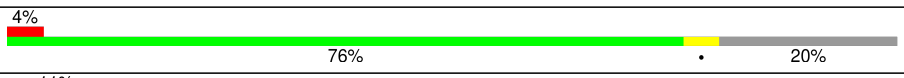
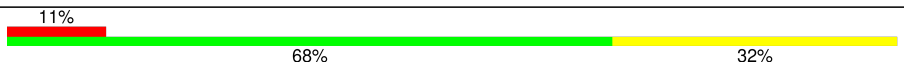
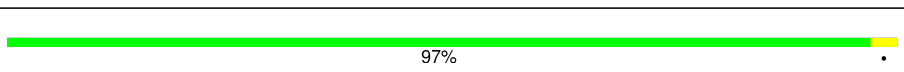
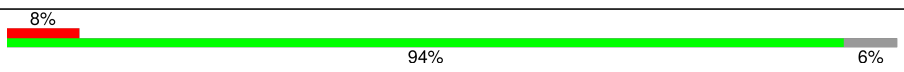
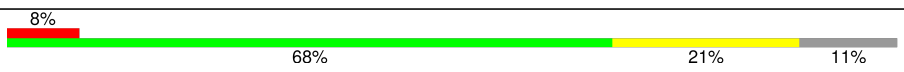
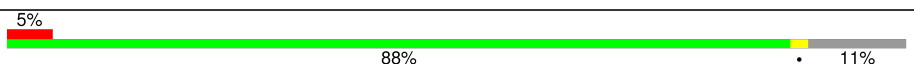
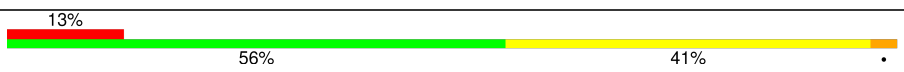
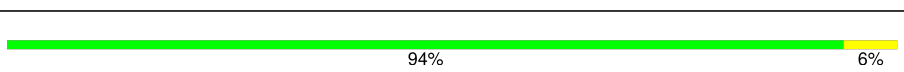
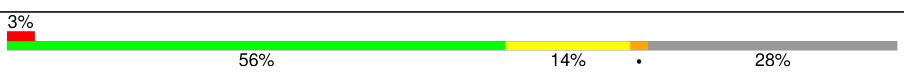
Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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Mol	Chain	Length	Quality of chain
15	u	134	69% 28%
16	V	163	4% 70% 13% 16%
16	v	163	2% 82% 16%
17	g	46	9% 54% 7% 39%
17	y	46	2% 54% 7% 39%
18	X	41	17% 61% 24% 10%
18	x	41	12% 83% 5% 10%
19	Z	62	10% 77% 18% 5%
19	z	62	2% 95% 5%
20	G	28	93% 7%
20	Y	28	100%

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	BCT	A	402	-	-	-	X
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	X	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	X
23	CLA	B	601	X	-	-	X
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	X
23	CLA	B	604	X	-	-	X
23	CLA	B	605	X	-	-	X
23	CLA	B	606	X	-	-	X
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	X
23	CLA	B	609	X	-	-	X
23	CLA	B	610	X	-	-	X
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	X
23	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	X
23	CLA	B	616	X	-	-	X
23	CLA	C	501	X	-	-	X
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	X
23	CLA	C	504	X	-	-	X
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	X
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	X
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	X
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	X
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	X
23	CLA	b	606	X	-	-	X
23	CLA	b	607	X	-	-	X
23	CLA	b	608	X	-	-	X
23	CLA	b	609	X	-	-	X
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	X
23	CLA	b	612	X	-	-	X
23	CLA	b	613	X	-	-	X
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	X
23	CLA	b	619	X	-	-	X
23	CLA	c	501	X	-	-	X
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	X
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	X
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	X
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	X
23	CLA	c	512	X	-	-	X
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	X
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	j	101	-	-	-	X
26	OEC	A	409	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	514	-	-	-	X
27	BCR	C	515	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	K	102	-	-	-	X
27	BCR	Z	101	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	621	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	c	516	-	-	-	X
27	BCR	f	102	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	x	101	-	-	-	X
28	DGD	B	621	-	-	-	X
28	DGD	B	626	-	-	-	X
28	DGD	D	410	-	-	-	X
28	DGD	b	602	-	-	-	X
28	DGD	d	408	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	417	-	-	-	X
30	SQD	D	409	-	-	-	X
30	SQD	F	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	a	401	-	-	-	X
30	SQD	d	407	-	-	-	X
30	SQD	f	103	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	520	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	M	102	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	520	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	k	103	-	-	-	X
33	LMT	B	624	-	-	-	X
33	LMT	B	627	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	D	411	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	T	101	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	626	-	-	-	X
33	LMT	i	102	-	-	-	X
33	LMT	m	101	-	-	-	X
33	LMT	x	102	-	-	-	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 50232 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
			2627	1720	432	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	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 Z.

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

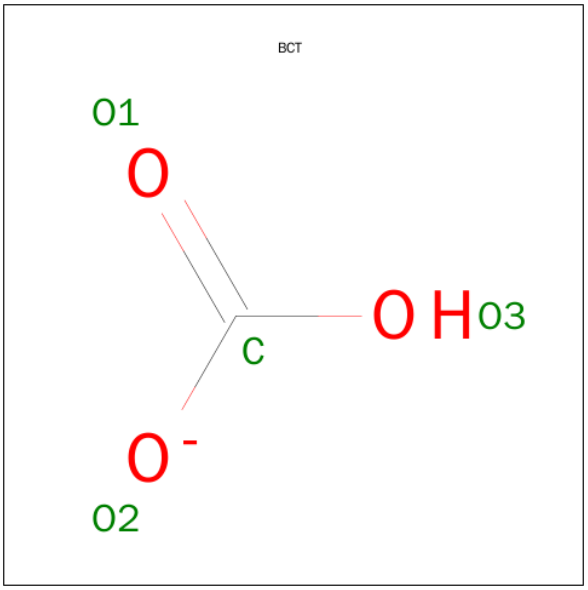
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

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

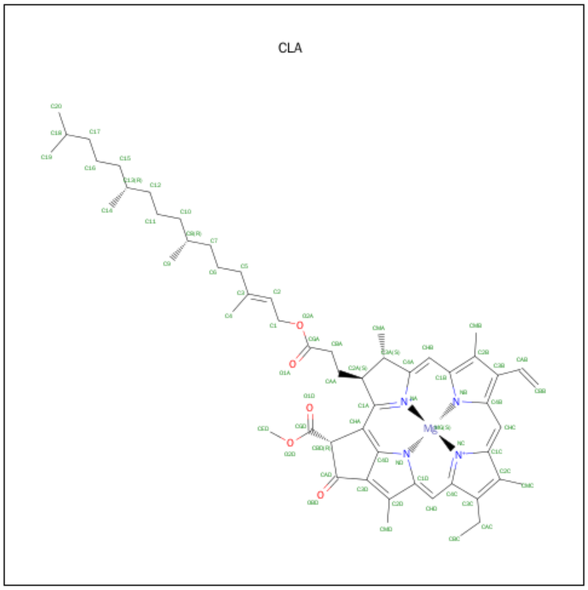
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe 1 1	0	0
21	a	1	Total Fe 1 1	0	0

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O 4 1 3	0	0
22	d	1	Total C O 4 1 3	0	0

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



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

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

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

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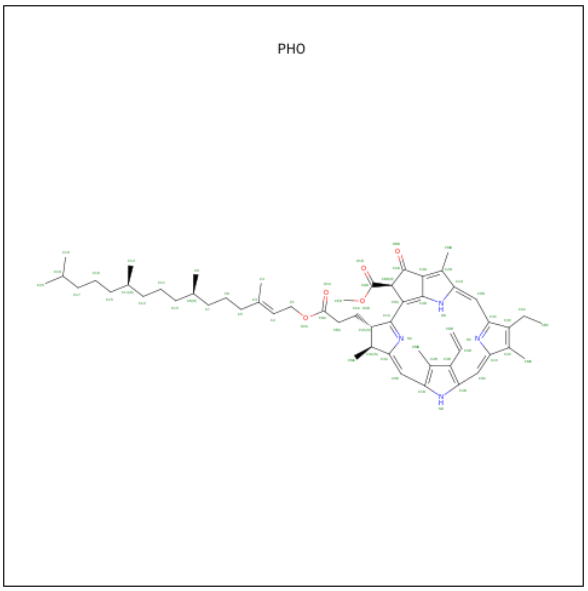
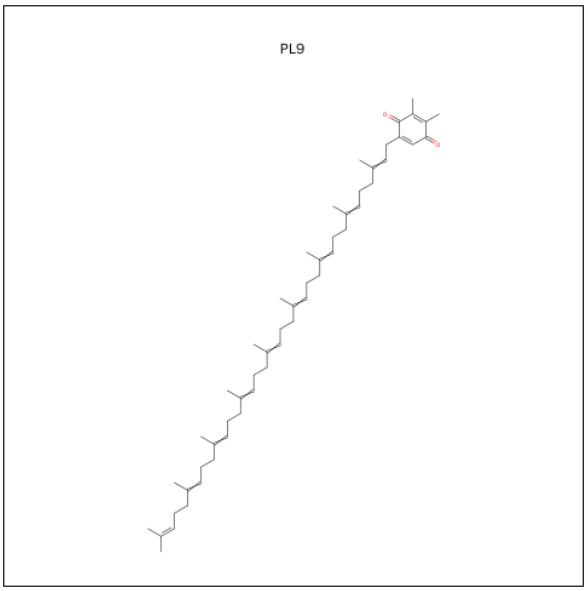
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4 5	0	0
23	c	1	Total C Mg N O 65 55 1 4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

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



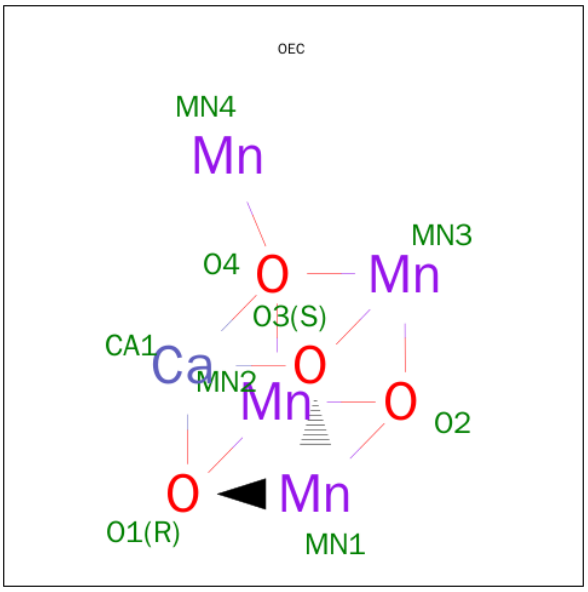
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 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: $C_{53}H_{80}O_2$).



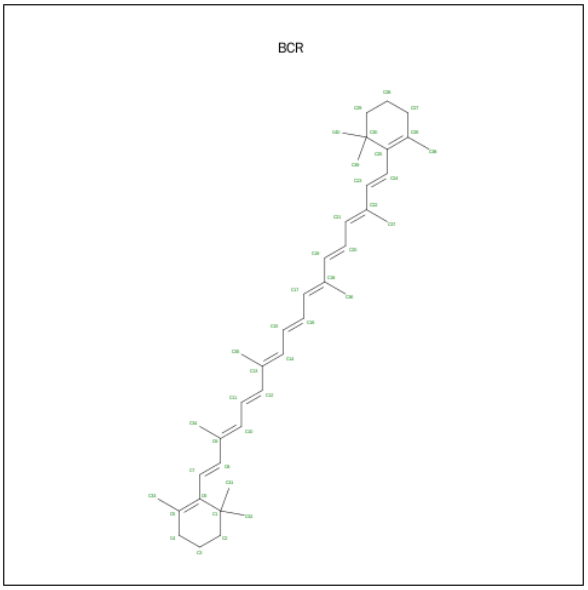
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 45 43 2	0	0
25	D	1	Total C O 55 53 2	0	0
25	J	1	Total C O 35 33 2	0	0
25	a	1	Total C O 45 43 2	0	0
25	d	1	Total C O 55 53 2	0	0
25	j	1	Total C O 35 33 2	0	0

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total Ca Mn 5 1 4	0	0
26	a	1	Total Ca Mn 5 1 4	0	0

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Z	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	f	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

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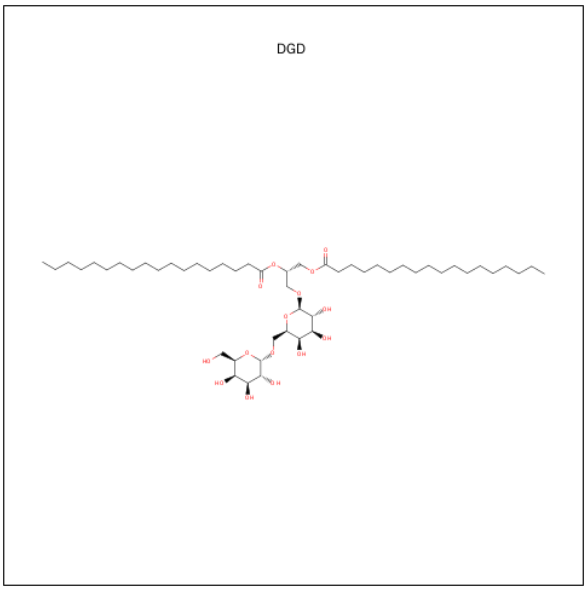
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	x	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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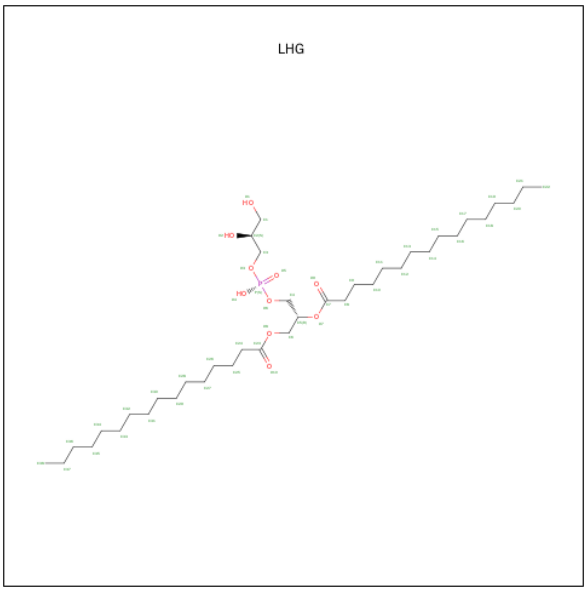
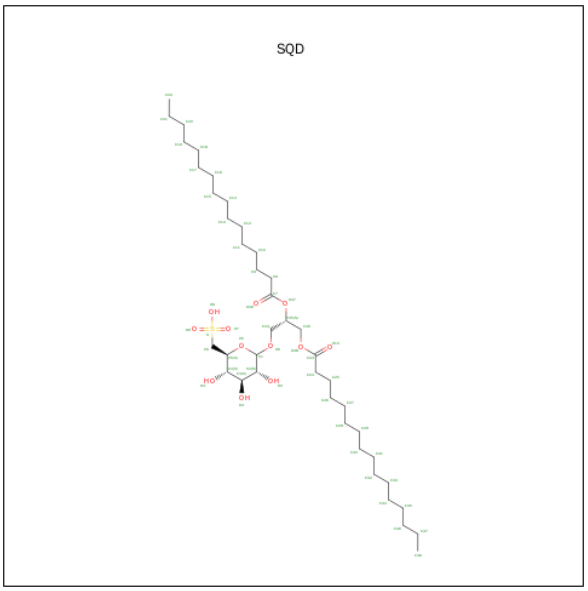
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C O 53 38 15	0	0
28	c	1	Total C O 62 47 15	0	0
28	c	1	Total C O 66 51 15	0	0
28	d	1	Total C O 63 48 15	0	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



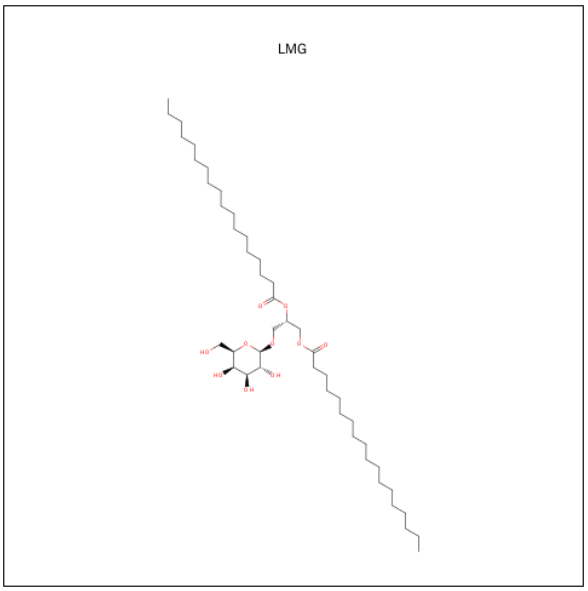
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O P 39 28 10 1	0	0
29	A	1	Total C O P 37 26 10 1	0	0
29	a	1	Total C O P 39 28 10 1	0	0
29	a	1	Total C O P 37 26 10 1	0	0

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



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

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 51 41 10	0	0
31	A	1	Total C O 42 32 10	0	0
31	B	1	Total C O 49 39 10	0	0
31	C	1	Total C O 48 38 10	0	0
31	C	1	Total C O 45 35 10	0	0
31	D	1	Total C O 46 36 10	0	0
31	D	1	Total C O 49 39 10	0	0
31	D	1	Total C O 48 38 10	0	0
31	E	1	Total C O 44 34 10	0	0
31	I	1	Total C O 43 33 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	a	1	Total C O 42 32 10	0	0
31	a	1	Total C O 51 41 10	0	0

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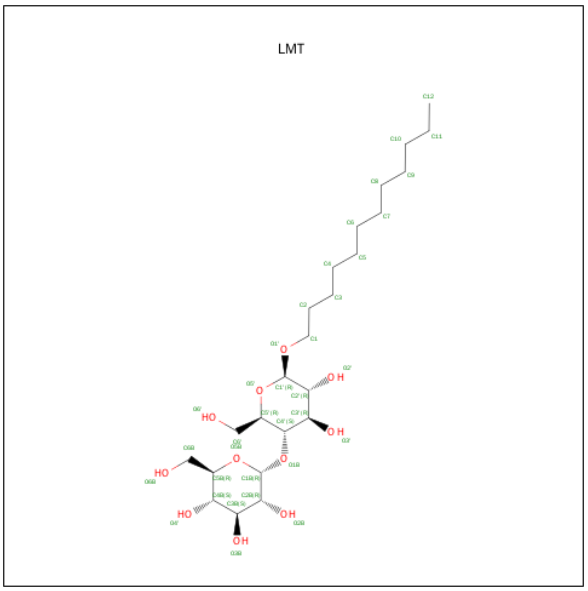
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C O 49 39 10	0	0
31	b	1	Total C O 49 39 10	0	0
31	c	1	Total C O 45 35 10	0	0
31	d	1	Total C O 46 36 10	0	0
31	d	1	Total C O 48 38 10	0	0
31	e	1	Total C O 44 34 10	0	0
31	i	1	Total C O 43 33 10	0	0
31	k	1	Total C O 48 38 10	0	0

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

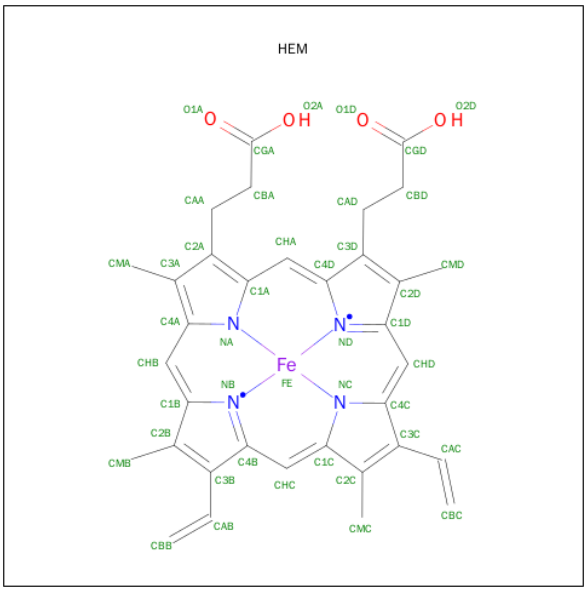
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Cl 1 1	0	0
32	d	1	Total Cl 1 1	0	0

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	B	1	Total C O 35 24 11	0	0
33	D	1	Total C O 31 20 11	0	0
33	I	1	Total C O 35 24 11	0	0
33	M	1	Total C O 35 24 11	0	0
33	T	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	b	1	Total C O 35 24 11	0	0
33	i	1	Total C O 35 24 11	0	0
33	m	1	Total C O 35 24 11	0	0
33	x	1	Total C O 31 20 11	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	0	0
			43	34	1	4	4		
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).

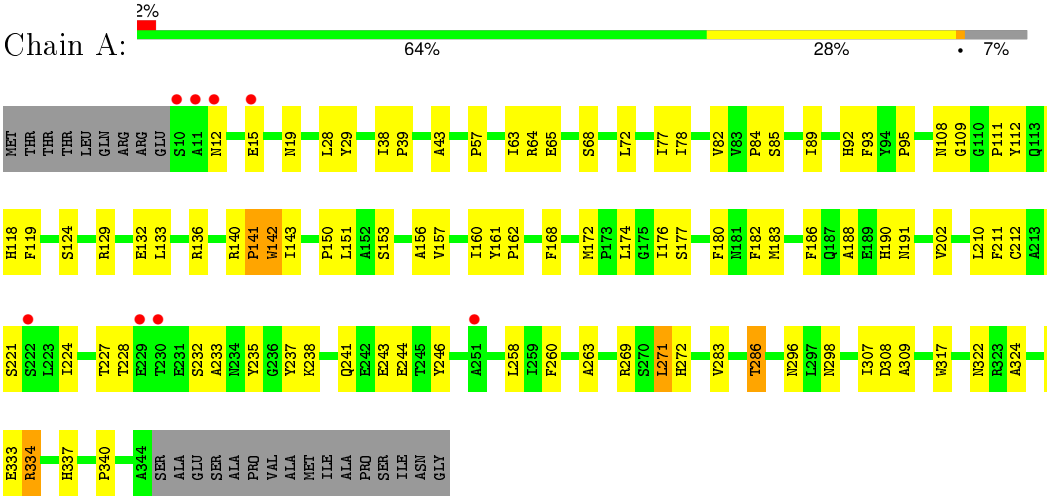
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	K	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		

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.

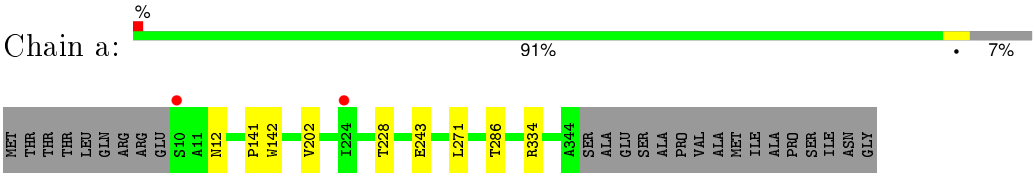
- Molecule 1: Photosystem Q(B) protein 1

Chain A:



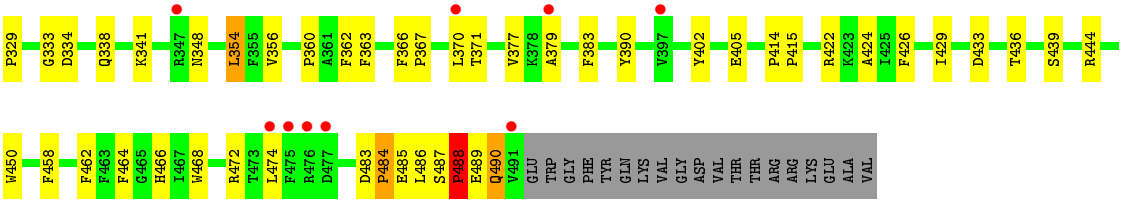
- Molecule 1: Photosystem Q(B) protein 1

Chain a:

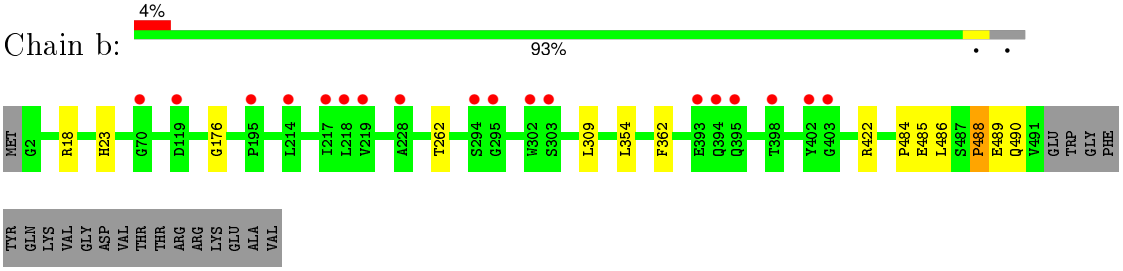


- Molecule 2: Photosystem II core light harvesting protein

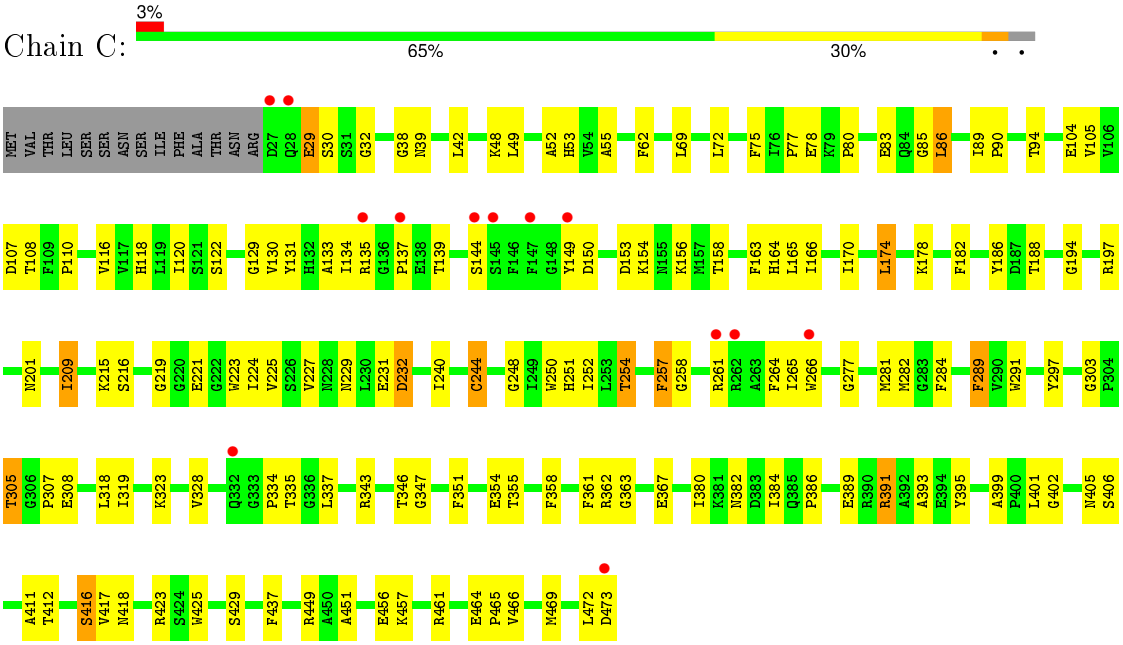
Chain B:



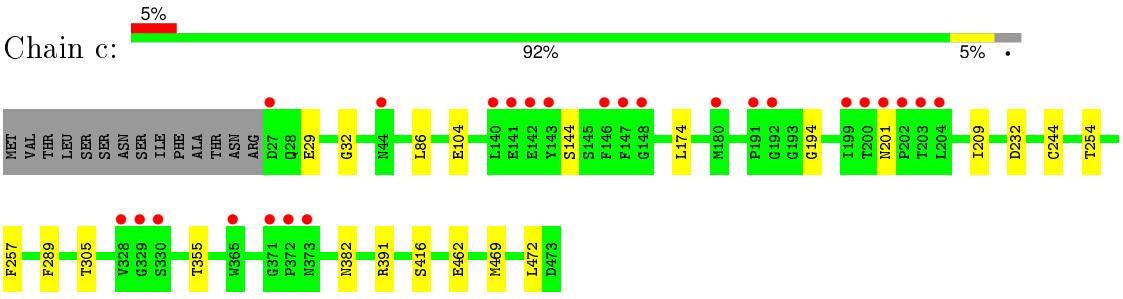
• Molecule 2: Photosystem II core light harvesting protein



• Molecule 3: Photosystem II CP43 protein

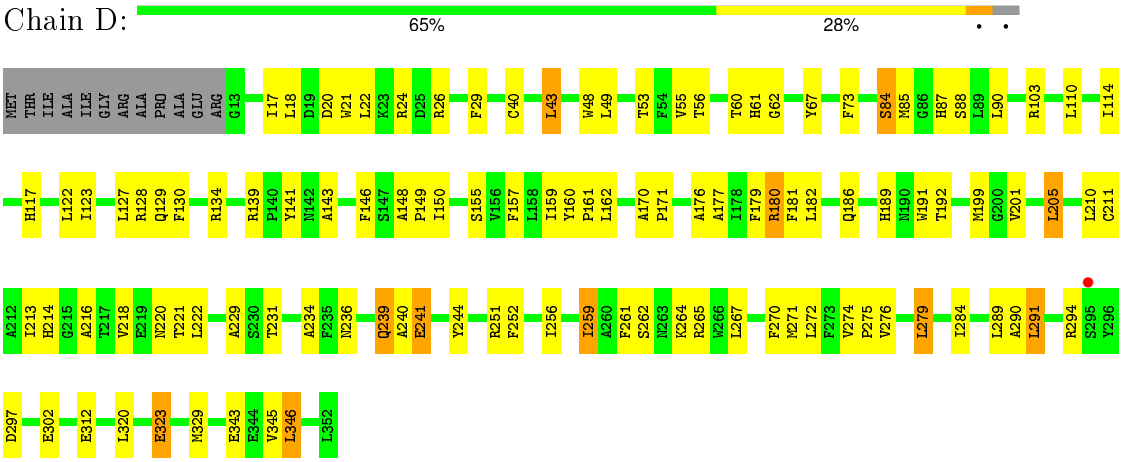


• Molecule 3: Photosystem II CP43 protein



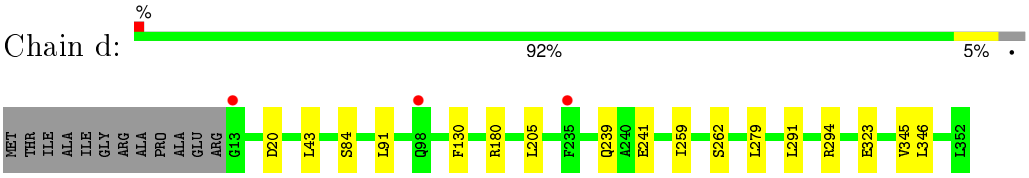
• Molecule 4: Photosystem II D2 protein

Chain D:



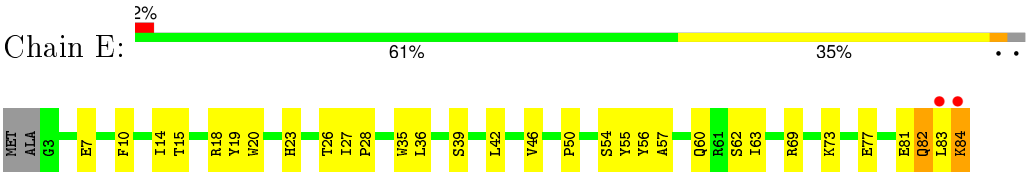
• Molecule 4: Photosystem II D2 protein

Chain d:



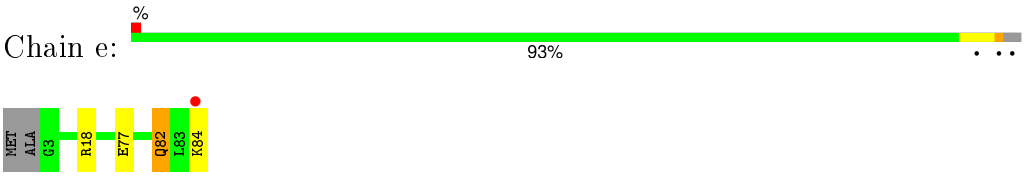
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



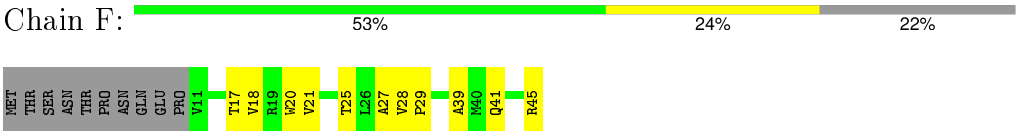
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



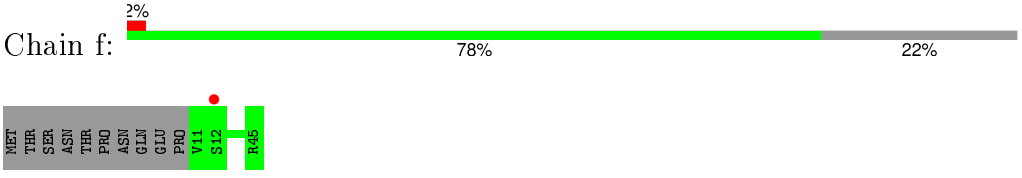
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



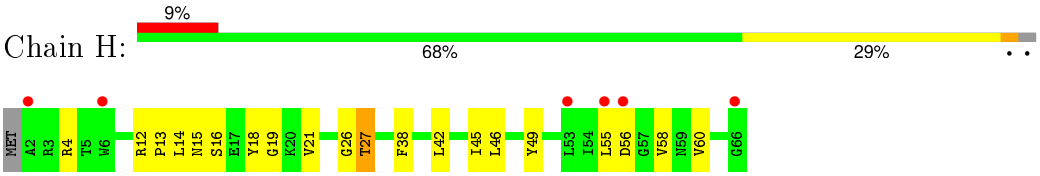
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



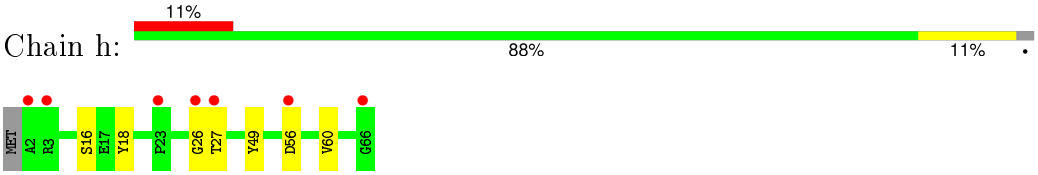
• Molecule 7: Photosystem II reaction center protein H

Chain H:



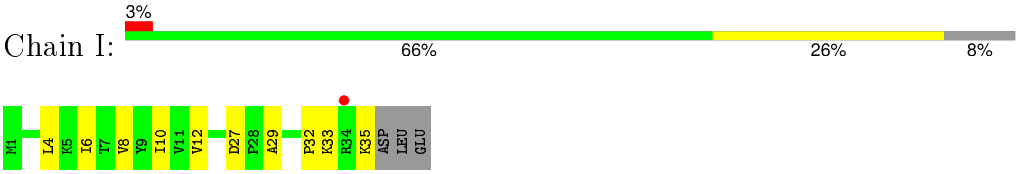
• Molecule 7: Photosystem II reaction center protein H

Chain h:



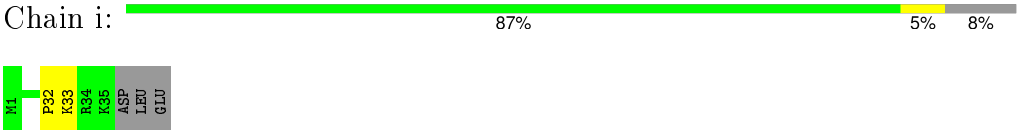
• Molecule 8: Photosystem II reaction center protein I

Chain I:



• Molecule 8: Photosystem II reaction center protein I

Chain i:

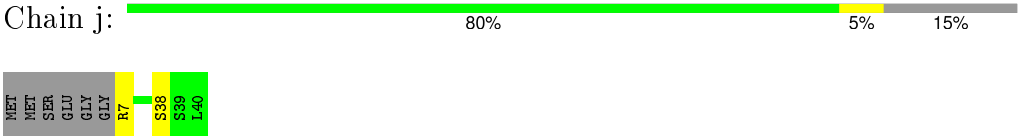


• Molecule 9: Photosystem II reaction center protein J

Chain J:

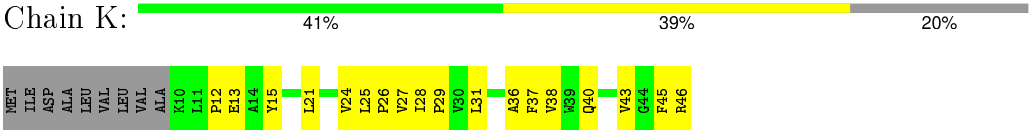
• Molecule 9: Photosystem II reaction center protein J

Chain j:



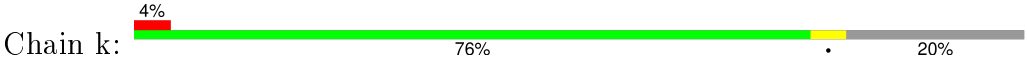
• Molecule 10: Photosystem II reaction center protein K

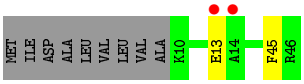
Chain K:



• Molecule 10: Photosystem II reaction center protein K

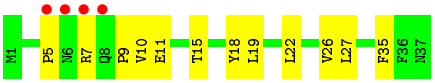
Chain k:





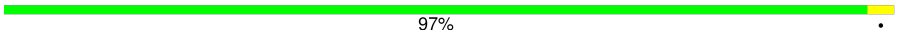
• Molecule 11: Photosystem II reaction center protein L

Chain L:



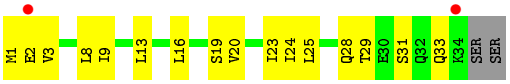
• Molecule 11: Photosystem II reaction center protein L

Chain l:



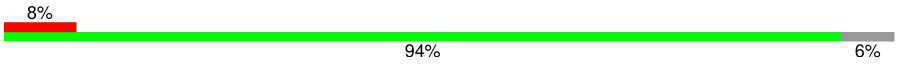
• Molecule 12: Photosystem II reaction center protein M

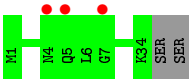
Chain M:



• Molecule 12: Photosystem II reaction center protein M

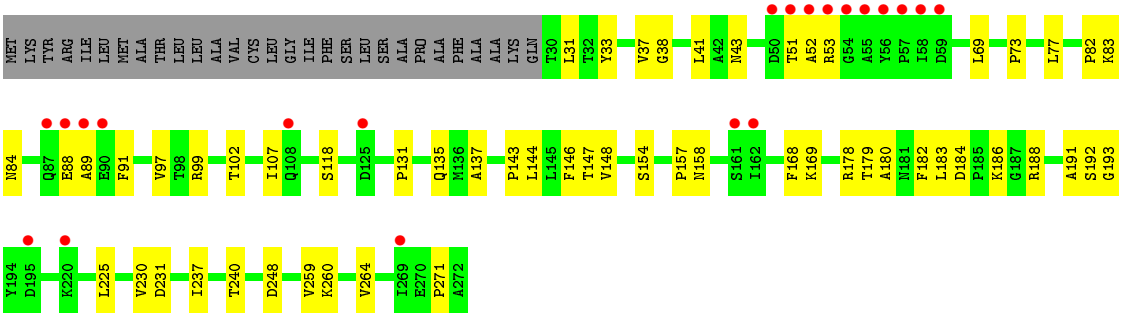
Chain m:





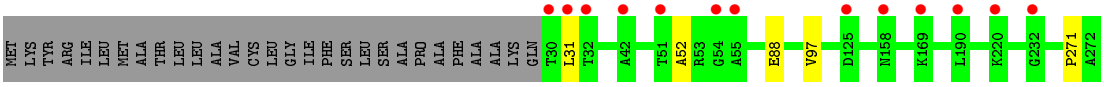
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



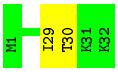
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

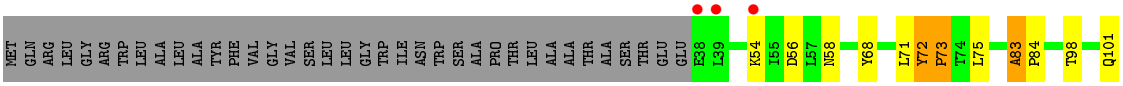


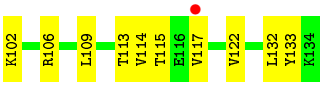
• Molecule 14: Photosystem II reaction center protein T

• Molecule 14: Photosystem II reaction center protein T

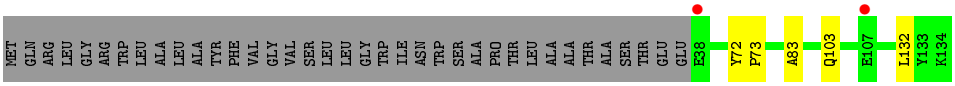


• Molecule 15: Photosystem II 12 kDa extrinsic protein

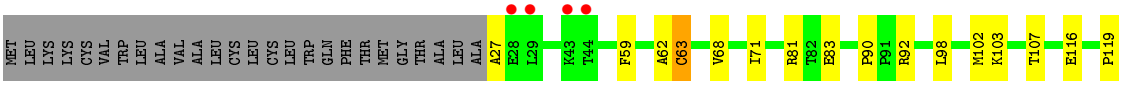


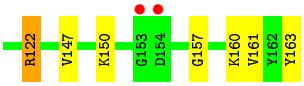


• Molecule 15: Photosystem II 12 kDa extrinsic protein

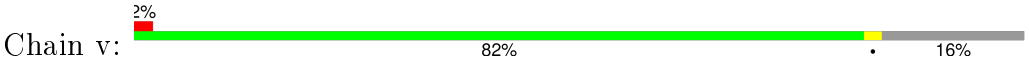


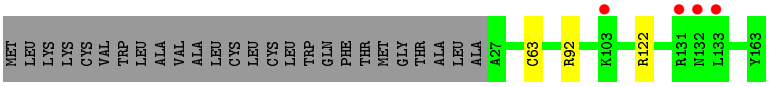
• Molecule 16: Cytochrome c-550





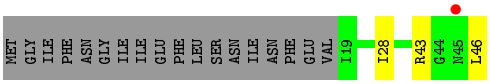
• Molecule 16: Cytochrome c-550





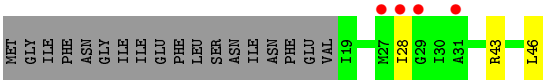
• Molecule 17: Photosystem II reaction center protein ycf12

Chain y:



• Molecule 17: Photosystem II reaction center protein ycf12

Chain g:

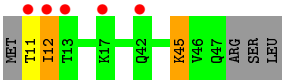


• Molecule 18: Photosystem II reaction center X protein

Chain X:

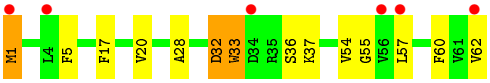
• Molecule 18: Photosystem II reaction center X protein

Chain x:



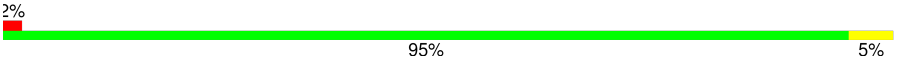
• Molecule 19: Photosystem II reaction center protein Z

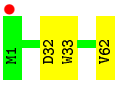
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

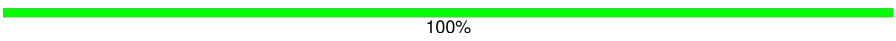
Chain z:





• Molecule 20: Photosystem II reaction center protein Y

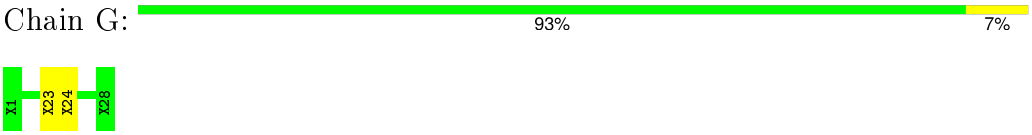
Chain Y:



There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Y

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.86Å 227.51Å 307.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.94 – 5.70 82.94 – 5.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.94-5.70) 98.3 (82.94-5.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.75 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.277 , 0.314 0.306 , 0.326	Depositor DCC
R_{free} test set	1325 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	7.8	Xtriage
Anisotropy	7.673	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.16$	Xtriage
Outliers	1 of 27220 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.29	0/3986	0.46	0/5433
3	C	0.29	0/3556	0.46	0/4842
3	c	0.28	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.28	0/685	0.48	0/933
5	e	0.27	0/685	0.46	0/933
6	F	0.26	0/291	0.44	0/397
6	f	0.26	0/291	0.42	0/397
7	H	0.27	0/520	0.50	0/709
7	h	0.28	0/520	0.51	0/709
8	I	0.28	0/293	0.47	0/395
8	i	0.31	0/293	0.49	0/395
9	J	0.25	0/255	0.44	0/346
9	j	0.27	0/255	0.45	0/346
10	K	0.28	0/303	0.53	0/416
10	k	0.29	0/303	0.53	0/416
11	L	0.27	0/311	0.47	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.66	0/367
12	m	0.41	0/270	0.66	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.35	0/284	0.47	0/381
14	t	0.36	0/284	0.48	0/381
15	U	0.28	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.31	0/1081	0.51	0/1468
16	v	0.26	0/1081	0.47	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	g	0.24	0/202	0.52	0/272
17	y	0.25	0/202	0.51	0/272
18	X	0.31	0/273	0.49	0/370
18	x	0.31	0/273	0.53	0/370
19	Z	0.29	0/490	0.50	0/669
19	z	0.27	0/490	0.47	0/669
All	All	0.29	0/41948	0.48	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

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	2627	0	2524	96	0
1	a	2627	0	2524	0	0
2	B	3850	0	3718	132	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	122	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	101	0
4	d	2706	0	2608	0	0
5	E	666	0	651	25	0
5	e	666	0	651	0	0
6	F	282	0	291	12	0
6	f	282	0	291	0	0
7	H	507	0	521	21	0
7	h	507	0	521	0	0
8	I	286	0	308	5	0
8	i	286	0	308	0	0
9	J	249	0	262	11	0
9	j	249	0	262	0	0
10	K	293	0	305	14	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	15	0
11	l	304	0	316	0	0
12	M	267	0	289	15	0
12	m	267	0	289	0	0
13	O	1845	0	1801	37	0
13	o	1845	0	1801	0	0
14	T	275	0	288	16	0
14	t	275	0	288	0	0
15	U	774	0	773	13	0
15	u	774	0	773	0	0
16	V	1060	0	1068	16	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	12	0
18	x	270	0	299	0	0
19	Z	479	0	516	13	0
19	z	479	0	516	0	0
20	G	140	0	32	1	0
20	Y	140	0	32	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	1	0	0
22	d	4	0	1	0	0
23	A	260	0	288	49	0
23	B	1040	0	1152	144	0
23	C	845	0	936	56	0
23	D	130	0	144	12	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	4	0
24	D	64	0	74	7	0
24	a	128	0	148	0	0
25	A	45	0	61	2	0
25	D	55	0	80	11	0
25	J	35	0	45	1	0
25	a	45	0	61	0	0
25	d	55	0	80	0	0
25	j	35	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	5	0	0	0	0
26	a	5	0	0	0	0
27	A	40	0	56	5	0
27	B	160	0	224	28	0
27	C	80	0	112	21	0
27	D	40	0	56	3	0
27	H	40	0	56	4	0
27	J	40	0	56	5	0
27	K	40	0	56	10	0
27	T	80	0	112	12	0
27	Z	40	0	56	5	0
27	a	40	0	56	0	0
27	b	80	0	112	0	0
27	c	120	0	168	0	0
27	f	40	0	56	0	0
27	j	40	0	56	0	0
27	k	40	0	56	0	0
27	x	40	0	56	0	0
28	A	56	0	70	1	0
28	B	110	0	136	5	0
28	C	181	0	245	21	0
28	D	63	0	87	3	0
28	a	56	0	70	0	0
28	b	110	0	136	0	0
28	c	181	0	245	0	0
28	d	63	0	87	0	0
29	A	76	0	95	6	0
29	a	76	0	95	0	0
30	A	105	0	147	10	0
30	B	47	0	61	1	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	A	93	0	124	5	0
31	B	49	0	67	4	0
31	C	93	0	124	4	0
31	D	143	0	194	17	0
31	E	44	0	57	1	0
31	I	43	0	55	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	M	84	0	107	6	0
31	a	93	0	124	0	0
31	b	98	0	134	0	0
31	c	45	0	59	0	0
31	d	94	0	126	0	0
31	e	44	0	58	0	0
31	i	43	0	55	0	0
31	k	48	0	66	0	0
32	A	1	0	0	0	0
32	d	1	0	0	0	0
33	B	140	0	184	4	0
33	D	31	0	35	2	0
33	I	35	0	46	2	0
33	M	35	0	46	0	0
33	T	35	0	46	2	0
33	b	105	0	138	0	0
33	i	35	0	46	0	0
33	m	35	0	46	0	0
33	x	31	0	35	0	0
34	F	43	0	30	4	0
34	V	43	0	30	4	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	50232	0	51358	824	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 9.

All (824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.91
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.51	0.89
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.57	0.89
3:C:362:ARG:H	28:C:516:DGD:HE4	1.40	0.86
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.84
3:C:362:ARG:H	28:C:517:DGD:HE4	24.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.62	0.82
4:D:199:MET:HG2	25:D:404:PL9:H322	1.79	0.79
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.65	0.78
23:B:606:CLA:H72	27:B:620:BCR:H311	1.68	0.75
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.75
14:T:18:PHE:HB2	27:T:103:BCR:H10C	1.67	0.75
1:A:63:ILE:HB	3:C:335:THR:HG21	1.67	0.75
2:B:103:LEU:HD21	23:B:608:CLA:HMC3	30.59	0.74
2:B:187:PRO:HB3	23:B:604:CLA:HMB2	35.98	0.74
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.69	0.74
3:C:297:TYR:O	3:C:423:ARG:NH2	2.48	0.73
3:C:449:ARG:HE	23:C:505:CLA:HED1	1.54	0.73
4:D:29:PHE:O	4:D:128:ARG:NH2	2.26	0.73
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.71	0.72
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.84	0.72
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.26	0.71
23:C:508:CLA:HBC3	23:C:510:CLA:H92	1.80	0.71
4:D:236:ASN:ND2	4:D:239:GLN:O	2.24	0.71
12:M:25:LEU:O	12:M:28:GLN:HG3	1.97	0.71
23:B:611:CLA:H42	4:D:127:LEU:HD11	30.60	0.70
2:B:187:PRO:HB3	23:B:601:CLA:HMB2	1.71	0.70
3:C:250:TRP:O	3:C:254:THR:OG1	2.08	0.70
24:A:406:PHO:HBC3	4:D:279:LEU:HG	1.73	0.70
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.57	0.69
23:B:602:CLA:H42	7:H:45:ILE:HD11	1.73	0.69
2:B:262:THR:HG22	2:B:263:THR:HG23	1.79	0.69
23:C:511:CLA:HMB2	27:C:514:BCR:H382	1.74	0.69
2:B:271:THR:HG22	2:B:273:TYR:H	1.56	0.69
23:A:405:CLA:HED1	25:D:404:PL9:H372	28.46	0.69
23:C:507:CLA:H112	27:C:515:BCR:H362	1.74	0.69
1:A:64:ARG:O	13:O:178:ARG:NH2	2.26	0.68
23:C:503:CLA:H172	23:C:510:CLA:HBB2	1.74	0.68
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.68
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.74	0.68
27:B:620:BCR:H363	27:T:103:BCR:H19C	52.07	0.68
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.68
27:B:618:BCR:H10C	14:T:18:PHE:HB2	43.74	0.67
1:A:29:TYR:O	1:A:129:ARG:NH1	2.34	0.67
23:D:403:CLA:H43	18:X:23:LEU:HA	1.77	0.67
23:A:403:CLA:H71	23:A:404:CLA:HAB	1.76	0.67
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.67
2:B:103:LEU:HD21	23:B:605:CLA:HMC3	1.77	0.66
3:C:303:GLY:O	3:C:423:ARG:NE	2.23	0.66
1:A:183:MET:HB3	23:A:403:CLA:HBC2	1.77	0.66
23:B:608:CLA:H42	4:D:127:LEU:HD11	1.76	0.66
27:B:617:BCR:H383	30:B:625:SQD:H92	1.77	0.65
6:F:17:THR:HG23	6:F:20:TRP:H	1.61	0.65
23:B:608:CLA:HBA2	30:D:409:SQD:H101	1.78	0.65
4:D:259:ILE:HG12	31:D:406:LMG:H292	45.27	0.65
23:A:404:CLA:HED1	25:D:404:PL9:H372	1.78	0.65
3:C:49:LEU:O	3:C:53:HIS:ND1	2.29	0.65
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.23	0.65
23:B:603:CLA:H193	7:H:42:LEU:HD12	1.78	0.65
1:A:329:GLU:O	1:A:332:HIS:ND1	2.32	0.65
23:B:607:CLA:HBD	23:B:608:CLA:H43	37.76	0.64
27:C:514:BCR:H391	10:K:36:ALA:HB2	2.02	0.64
29:A:415:LHG:H271	29:A:415:LHG:H101	1.78	0.64
11:L:9:PRO:HB3	31:M:102:LMG:HC61	1.80	0.64
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.91	0.64
23:B:608:CLA:HBB1	23:B:609:CLA:H51	11.75	0.64
23:C:513:CLA:HAB	27:C:515:BCR:H24C	27.52	0.64
14:T:21:ILE:HD12	27:T:103:BCR:H332	1.80	0.64
3:C:118:HIS:CE1	31:C:520:LMG:H192	2.33	0.63
4:D:186:GLN:HB2	23:D:401:CLA:HBC1	1.79	0.63
3:C:48:LYS:NZ	3:C:133:ALA:O	2.31	0.63
4:D:259:ILE:HG12	31:D:408:LMG:H292	1.79	0.63
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.80	0.63
2:B:149:LEU:HG	23:B:603:CLA:HBC1	1.79	0.63
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.79	0.63
23:B:606:CLA:H193	7:H:42:LEU:HD12	40.04	0.63
30:D:409:SQD:H301	30:D:409:SQD:H171	1.81	0.63
12:M:20:VAL:O	12:M:24:ILE:HG13	1.98	0.63
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.81	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.62
1:A:183:MET:HA	23:A:403:CLA:HMD2	1.81	0.62
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.24	0.62
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.80	0.62
23:A:404:CLA:H203	24:D:402:PHO:H71	1.81	0.62
31:A:418:LMG:H112	2:B:43:ALA:HA	42.25	0.62
3:C:165:LEU:HD21	23:C:506:CLA:HAB	1.86	0.62
23:B:608:CLA:H151	23:B:609:CLA:H203	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:618:BCR:H19C	27:B:619:BCR:H363	1.81	0.61
1:A:183:MET:HA	23:A:404:CLA:HMD2	8.53	0.61
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.83	0.61
23:A:403:CLA:H122	24:D:402:PHO:H3A	1.83	0.61
23:A:405:CLA:H42	25:D:404:PL9:H162	18.95	0.61
23:A:405:CLA:H142	23:D:401:CLA:H151	1.82	0.61
23:D:403:CLA:H42	18:X:26:GLY:HA3	1.82	0.61
1:A:217:SER:HA	4:D:272:LEU:HD12	1.91	0.61
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.91	0.61
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.35	0.60
1:A:140:ARG:HH22	29:A:412:LHG:P	2.23	0.60
7:H:38:PHE:HB2	27:H:101:BCR:H10C	1.82	0.60
11:L:10:VAL:O	12:M:28:GLN:NE2	2.29	0.60
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.84	0.60
31:A:414:LMG:H231	25:D:404:PL9:H352	1.82	0.60
23:B:606:CLA:C2D	23:B:608:CLA:H2	40.54	0.60
10:K:26:PRO:O	10:K:29:PRO:HD2	2.15	0.60
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.60
23:B:605:CLA:H42	7:H:45:ILE:HD11	17.52	0.60
1:A:183:MET:HB3	23:A:404:CLA:HBC2	6.06	0.59
4:D:24:ARG:NH2	18:X:44:ASP:O	2.35	0.59
3:C:284:PHE:HB3	28:C:517:DGD:HA51	19.73	0.59
1:A:132:GLU:O	1:A:136:ARG:HG2	2.02	0.59
30:A:413:SQD:H311	23:C:508:CLA:H71	1.84	0.59
2:B:222:PRO:HG3	7:H:27:THR:H	1.67	0.59
23:B:602:CLA:HBD	23:B:602:CLA:H2	1.82	0.59
23:A:403:CLA:H202	23:A:404:CLA:H93	1.83	0.59
23:C:513:CLA:HAB	27:Z:101:BCR:H24C	1.83	0.59
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.85	0.59
1:A:153:SER:HB3	23:A:404:CLA:HED1	17.27	0.59
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.90	0.59
23:C:509:CLA:HBD	23:C:509:CLA:H121	1.84	0.59
23:C:501:CLA:H193	23:C:507:CLA:H111	2.00	0.59
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.69	0.59
23:B:606:CLA:C3D	23:B:608:CLA:H2	40.76	0.59
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	1.85	0.58
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.85	0.58
16:V:62:ALA:O	34:V:201:HEM:HAB	2.03	0.58
2:B:271:THR:HB	2:B:274:GLN:HG3	1.87	0.58
3:C:361:PHE:HD1	28:C:516:DGD:HE61	1.68	0.58
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.37	0.58
23:B:608:CLA:H202	23:B:612:CLA:HBB2	38.91	0.58
12:M:31:SER:HA	31:M:101:LMG:HC1	1.86	0.58
30:A:413:SQD:H223	28:C:518:DGD:HAE1	1.85	0.58
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.90	0.58
3:C:405:ASN:HB2	28:C:518:DGD:HG31	1.86	0.57
1:A:227:THR:HG21	1:A:233:ALA:HA	1.85	0.57
23:B:605:CLA:H2	23:B:605:CLA:HBD	7.34	0.57
12:M:31:SER:HA	31:M:102:LMG:HC1	10.19	0.57
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.47	0.57
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.86	0.57
1:A:174:LEU:HD22	24:D:402:PHO:H151	1.85	0.57
13:O:73:PRO:HG2	13:O:102:THR:HB	1.85	0.57
23:B:615:CLA:H172	23:B:615:CLA:H111	1.85	0.57
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.94	0.57
2:B:212:ALA:HB2	23:B:612:CLA:HMC3	28.12	0.57
2:B:149:LEU:HG	23:B:606:CLA:HBC1	9.35	0.57
28:D:410:DGD:HO5E	28:D:410:DGD:HO4E	1.52	0.57
1:A:78:ILE:O	1:A:176:ILE:HB	2.05	0.57
23:C:501:CLA:C2D	23:C:503:CLA:H2	2.34	0.57
1:A:72:LEU:HD13	31:A:418:LMG:H111	1.87	0.57
1:A:176:ILE:HD12	23:A:404:CLA:HED3	1.86	0.57
23:A:404:CLA:HAA1	25:D:404:PL9:H362	1.86	0.56
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.79	0.56
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.93	0.56
18:X:12:ILE:HA	18:X:16:LEU:HD12	2.03	0.56
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.98	0.56
2:B:150:CYS:HB2	23:B:606:CLA:HMC3	8.11	0.56
23:A:404:CLA:HHC	23:A:404:CLA:HBB1	2.48	0.56
23:C:511:CLA:H171	19:Z:20:VAL:HA	1.88	0.56
3:C:361:PHE:HA	28:C:516:DGD:HE62	1.86	0.56
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.04	0.56
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.56
23:A:405:CLA:H93	23:D:401:CLA:H152	1.88	0.56
3:C:158:THR:O	3:C:251:HIS:HB3	2.10	0.56
1:A:244:GLU:HG3	1:A:246:TYR:H	1.69	0.56
2:B:458:PHE:HB3	23:B:607:CLA:HBC2	15.80	0.56
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.39	0.56
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.56
2:B:329:PRO:HB3	23:B:610:CLA:HED1	37.85	0.55
31:I:101:LMG:H181	33:I:102:LMT:H42	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:408:LMG:H111	11:L:19:LEU:HD21	1.88	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.88	0.55
4:D:261:PHE:HB2	25:D:404:PL9:H522	1.88	0.55
2:B:120:LEU:HD13	23:B:616:CLA:HMD2	1.88	0.55
2:B:212:ALA:HB2	23:B:609:CLA:HMC3	1.87	0.55
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.71	0.55
13:O:118:SER:HB3	13:O:157:PRO:HA	2.06	0.55
1:A:77:ILE:HD11	14:T:6:TYR:HB3	2.03	0.55
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.41	0.55
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.89	0.55
2:B:327:THR:HG21	31:B:622:LMG:H111	1.88	0.55
2:B:122:LEU:O	7:H:15:ASN:ND2	2.41	0.55
3:C:406:SER:O	3:C:418:ASN:ND2	2.43	0.55
30:A:413:SQD:H162	25:J:101:PL9:H533	1.89	0.55
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.87	0.54
2:B:329:PRO:HB3	23:B:607:CLA:HED1	1.89	0.54
2:B:462:PHE:CZ	23:B:613:CLA:HMB3	2.43	0.54
28:C:517:DGD:HA41	31:C:519:LMG:H391	1.89	0.54
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.23	0.54
30:A:413:SQD:H241	29:A:415:LHG:HC81	1.89	0.54
23:B:610:CLA:HBC3	27:B:620:BCR:HC8	30.45	0.54
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.89	0.54
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.97	0.54
23:B:608:CLA:H18	23:B:609:CLA:H192	1.89	0.54
23:B:607:CLA:H192	31:D:407:LMG:H342	1.89	0.54
4:D:274:VAL:HA	25:D:404:PL9:H253	2.12	0.54
1:A:141:PRO:O	1:A:143:ILE:N	2.40	0.54
23:B:605:CLA:HBB1	23:B:606:CLA:H51	1.89	0.54
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.43	0.54
14:T:7:VAL:HG12	33:T:101:LMT:H122	1.90	0.54
2:B:241:SER:HB3	23:B:615:CLA:HED3	13.93	0.54
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.88	0.54
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.97	0.54
23:B:603:CLA:C2D	23:B:605:CLA:H2	2.38	0.53
11:L:9:PRO:HB3	31:M:101:LMG:HC61	14.32	0.53
2:B:121:GLU:O	7:H:12:ARG:NH2	2.45	0.53
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.08	0.53
23:C:504:CLA:H121	28:C:517:DGD:HBE2	1.89	0.53
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.08	0.53
2:B:184:GLU:H	2:B:200:ALA:HB2	1.73	0.53
23:A:405:CLA:HBA1	23:A:405:CLA:CHA	3.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:604:CLA:HBB1	23:B:607:CLA:CBB	2.39	0.53
2:B:150:CYS:HA	23:B:606:CLA:HBC2	11.26	0.53
23:C:506:CLA:HMC2	23:C:507:CLA:H102	1.90	0.53
31:D:408:LMG:O6	11:L:15:THR:HG21	2.09	0.53
13:O:83:LYS:HG2	13:O:84:ASN:H	1.73	0.53
3:C:361:PHE:HD1	28:C:517:DGD:HE61	20.63	0.53
2:B:96:VAL:HG22	23:B:609:CLA:HBA1	35.34	0.53
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.97	0.53
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.43	0.53
23:B:608:CLA:H51	23:B:609:CLA:H101	1.91	0.53
23:C:501:CLA:HMB3	27:C:515:BCR:H403	1.90	0.53
31:D:406:LMG:H111	11:L:19:LEU:HD21	43.59	0.53
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.91	0.53
2:B:474:LEU:O	4:D:134:ARG:NH1	2.46	0.53
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.74	0.53
16:V:59:PHE:HA	16:V:63:CYS:SG	2.49	0.53
23:A:403:CLA:HBB1	23:A:403:CLA:HHC	1.90	0.53
31:D:406:LMG:O6	11:L:15:THR:HG21	54.24	0.53
9:J:9:PRO:HB2	9:J:12:ILE:HG13	1.91	0.53
23:B:601:CLA:HMB3	27:H:101:BCR:H281	1.90	0.52
9:J:14:ALA:O	9:J:18:GLY:N	2.51	0.52
1:A:298:ASN:ND2	3:C:402:GLY:O	2.42	0.52
13:O:230:VAL:HG12	13:O:231:ASP:H	1.75	0.52
1:A:190:HIS:O	1:A:298:ASN:HB3	2.18	0.52
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.45	0.52
23:B:611:CLA:HAB	4:D:123:ILE:HG23	20.54	0.52
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.92	0.52
3:C:337:LEU:HA	13:O:131:PRO:HG3	1.97	0.52
1:A:140:ARG:NH2	29:A:412:LHG:O5	2.40	0.52
2:B:239:SER:O	2:B:466:HIS:ND1	2.43	0.52
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.51	0.52
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	1.90	0.52
27:A:410:BCR:H311	30:A:417:SQD:H351	1.91	0.52
23:C:504:CLA:H202	28:C:518:DGD:HAF2	1.92	0.52
4:D:192:THR:HG23	23:D:401:CLA:HBC2	1.92	0.52
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.48	0.52
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.96	0.52
3:C:284:PHE:HB3	28:C:516:DGD:HA51	1.91	0.51
1:A:334:ARG:NH1	13:O:183:LEU:O	2.52	0.51
1:A:177:SER:HA	1:A:180:PHE:CD2	2.45	0.51
30:A:417:SQD:H332	23:B:609:CLA:H203	71.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:HIS:ND1	23:C:507:CLA:OBD	2.37	0.51
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.92	0.51
15:U:98:THR:O	15:U:102:LYS:HG3	2.94	0.51
23:B:607:CLA:H193	11:L:27:LEU:HD11	1.92	0.51
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	1.99	0.51
2:B:201:HIS:HD2	2:B:202:HIS:CE1	2.41	0.51
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.05	0.51
23:B:611:CLA:H151	23:B:612:CLA:H203	14.40	0.51
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.91	0.51
16:V:119:PRO:HG2	34:V:201:HEM:HMC2	2.08	0.51
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.56	0.51
16:V:98:LEU:O	16:V:102:MET:HG3	2.11	0.51
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.52	0.51
28:A:411:DGD:HAT2	3:C:281:MET:HG3	1.93	0.51
2:B:464:PHE:HD2	23:B:614:CLA:HAC2	17.84	0.51
1:A:85:SER:HA	1:A:109:GLY:HA3	2.02	0.51
2:B:135:LEU:HD23	2:B:138:MET:HE3	1.92	0.51
23:B:603:CLA:C3D	23:B:605:CLA:H2	2.41	0.51
2:B:68:ARG:HH22	23:B:604:CLA:HED1	1.75	0.51
3:C:282:MET:HG2	23:C:501:CLA:H61	2.06	0.51
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.93	0.51
2:B:18:ARG:NH1	2:B:115:TRP:O	2.47	0.50
27:B:618:BCR:H352	27:B:619:BCR:H382	1.92	0.50
1:A:211:PHE:HA	1:A:214:MET:HB2	1.93	0.50
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.95	0.50
3:C:380:ILE:HA	3:C:384:ILE:HD11	2.05	0.50
27:B:618:BCR:H381	14:T:4:ILE:HD13	25.32	0.50
30:F:102:SQD:H162	18:X:33:THR:HA	1.94	0.50
3:C:224:ILE:O	3:C:227:VAL:HG23	2.20	0.50
23:B:611:CLA:HBA1	23:B:611:CLA:CHA	4.24	0.50
13:O:240:THR:HG22	13:O:264:VAL:HG12	2.05	0.50
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.50
2:B:213:GLY:O	2:B:217:ILE:HG13	2.12	0.50
24:A:406:PHO:H151	23:D:401:CLA:H172	1.93	0.50
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	2.47	0.50
27:B:618:BCR:H332	14:T:21:ILE:HD12	49.26	0.50
10:K:21:LEU:HD21	27:K:102:BCR:HC31	1.92	0.50
1:A:153:SER:HB3	23:A:403:CLA:HED1	1.93	0.50
1:A:176:ILE:HD12	23:A:405:CLA:HED3	27.20	0.50
3:C:361:PHE:HA	28:C:517:DGD:HE62	22.85	0.50
23:A:404:CLA:H42	25:D:404:PL9:H162	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:LEU:HD13	27:D:405:BCR:C15	2.41	0.50
12:M:13:LEU:HD12	27:T:102:BCR:H333	12.25	0.50
2:B:12:LEU:HB2	23:B:615:CLA:HMC2	18.85	0.50
27:B:620:BCR:H382	27:T:103:BCR:H352	52.61	0.50
28:B:626:DGD:HB22	33:B:628:LMT:H72	1.93	0.50
3:C:130:VAL:O	3:C:134:ILE:HG12	2.26	0.50
23:B:610:CLA:H193	11:L:27:LEU:HD11	29.72	0.50
23:C:505:CLA:H11	27:C:515:BCR:H312	1.94	0.50
31:D:408:LMG:H392	27:T:103:BCR:HC32	1.94	0.50
23:B:616:CLA:H72	23:B:616:CLA:H12	1.92	0.49
28:D:410:DGD:O5E	28:D:410:DGD:O4E	2.29	0.49
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.77	0.49
23:B:611:CLA:H41	23:B:614:CLA:HBC3	1.92	0.49
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.95	0.49
19:Z:33:TRP:HA	19:Z:36:SER:HB3	1.94	0.49
2:B:137:LYS:HD2	7:H:14:LEU:O	2.12	0.49
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.98	0.49
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.94	0.49
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.61	0.49
23:C:505:CLA:HBA1	23:C:505:CLA:HBD	1.94	0.49
6:F:21:VAL:O	6:F:25:THR:HG23	2.12	0.49
27:K:102:BCR:H332	19:Z:17:PHE:CD1	2.48	0.49
16:V:90:PRO:O	16:V:92:ARG:HD3	2.13	0.49
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.03	0.49
2:B:78:TRP:HB3	13:O:137:ALA:HB1	59.84	0.49
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.95	0.49
2:B:5:TRP:HZ3	23:B:611:CLA:H51	1.77	0.49
4:D:49:LEU:O	4:D:53:THR:HG23	2.12	0.49
10:K:31:LEU:HB3	27:K:102:BCR:C15	2.43	0.49
23:B:606:CLA:C1D	23:B:608:CLA:H52	39.04	0.49
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.09	0.49
2:B:25:MET:HG2	27:T:102:BCR:C23	36.59	0.49
6:F:27:ALA:HB1	34:F:101:HEM:CAC	2.42	0.49
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.46	0.49
33:B:627:LMT:H122	14:T:7:VAL:HG12	34.54	0.49
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.02	0.49
2:B:150:CYS:HB2	23:B:603:CLA:HMC3	1.95	0.49
23:C:512:CLA:H143	23:C:513:CLA:H162	1.99	0.49
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.49
2:B:25:MET:HG2	27:B:617:BCR:C23	2.43	0.49
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:363:GLY:O	3:C:367:GLU:HG2	2.13	0.49
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.47	0.49
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.45	0.49
1:A:283:VAL:O	1:A:286:THR:HG22	2.13	0.48
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.48
2:B:241:SER:HB3	23:B:612:CLA:HED3	1.95	0.48
13:O:77:LEU:HB2	13:O:260:LYS:HB3	1.95	0.48
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.95	0.48
23:A:405:CLA:H11	23:A:405:CLA:H51	4.37	0.48
23:A:404:CLA:H71	23:A:405:CLA:HAB	27.68	0.48
3:C:425:TRP:CE2	23:C:504:CLA:HBA1	2.49	0.48
27:C:514:BCR:H343	27:C:514:BCR:H311	1.98	0.48
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.07	0.48
12:M:8:LEU:HG	12:M:9:ILE:HD12	7.07	0.48
23:A:404:CLA:CHA	23:A:404:CLA:HBA1	2.42	0.48
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.48
2:B:280:PHE:O	2:B:284:ILE:HG13	2.14	0.48
1:A:114:LEU:O	1:A:118:HIS:ND1	2.47	0.48
23:B:603:CLA:CBB	23:B:605:CLA:H152	2.42	0.48
23:A:405:CLA:HAB	23:D:401:CLA:H72	1.95	0.48
23:B:605:CLA:H122	23:B:605:CLA:H162	4.55	0.48
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.94	0.48
2:B:25:MET:HG2	27:B:617:BCR:H23C	1.95	0.48
23:B:606:CLA:H41	23:B:606:CLA:H61	2.96	0.48
23:B:609:CLA:HMD1	7:H:27:THR:HB	1.96	0.48
23:B:611:CLA:H51	23:B:612:CLA:H101	18.80	0.48
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.48
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.72	0.48
33:D:411:LMT:H72	18:X:26:GLY:HA2	1.96	0.48
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.95	0.48
7:H:19:GLY:O	7:H:21:VAL:HG13	2.15	0.48
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.79	0.48
23:A:404:CLA:H101	31:D:408:LMG:H221	1.96	0.48
19:Z:1:MET:HE3	19:Z:60:PHE:CD2	2.49	0.48
23:C:504:CLA:H151	28:C:517:DGD:HBW1	1.96	0.47
1:A:337:HIS:NE2	3:C:354:GLU:OE1	2.47	0.47
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.53	0.47
4:D:320:LEU:HD23	4:D:323:GLU:OE1	2.14	0.47
2:B:462:PHE:CZ	23:B:616:CLA:HMB3	23.45	0.47
2:B:464:PHE:HD2	23:B:611:CLA:HAC2	1.79	0.47
2:B:89:GLY:HA2	28:B:626:DGD:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:267:LEU:O	4:D:271:MET:HG3	2.14	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.47
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.01	0.47
1:A:116:ILE:HG13	1:A:117:PHE:N	2.29	0.47
2:B:91:TRP:CH2	23:B:606:CLA:H12	2.49	0.47
2:B:25:MET:HG2	27:T:102:BCR:H23C	37.34	0.47
33:T:101:LMT:H1B	33:T:101:LMT:H3'	1.56	0.47
30:A:417:SQD:H152	27:T:103:BCR:HC22	1.97	0.47
23:C:501:CLA:H171	23:C:507:CLA:HMB3	1.98	0.47
2:B:468:TRP:HH2	31:D:407:LMG:HO2	1.63	0.47
23:B:612:CLA:HMD1	7:H:27:THR:HB	21.28	0.47
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.49	0.47
23:A:405:CLA:HAA1	25:D:404:PL9:H362	24.29	0.47
23:B:604:CLA:HBB1	23:B:607:CLA:HBB2	1.95	0.47
27:B:620:BCR:H351	27:B:620:BCR:H15C	1.80	0.47
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.97	0.47
23:B:611:CLA:HBC2	31:D:407:LMG:H222	1.96	0.47
23:B:606:CLA:H18	23:B:616:CLA:H121	1.96	0.47
2:B:257:TRP:CD2	4:D:291:LEU:HD12	2.50	0.47
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.06	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.58	0.47
27:B:617:BCR:H341	27:B:618:BCR:H24C	1.96	0.47
3:C:240:ILE:HD11	27:C:515:BCR:H372	1.97	0.47
30:D:409:SQD:H241	30:D:409:SQD:H111	1.97	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	1.97	0.47
30:A:413:SQD:H112	29:A:415:LHG:H111	1.97	0.47
12:M:19:SER:O	12:M:23:ILE:HG13	2.15	0.47
2:B:450:TRP:NE1	23:B:607:CLA:HBA1	2.30	0.47
24:A:406:PHO:H161	4:D:48:TRP:CE2	2.50	0.47
27:J:102:BCR:H11C	27:J:102:BCR:H341	1.71	0.47
5:E:60:GLN:HG2	5:E:62:SER:H	1.83	0.47
23:B:603:CLA:HBB2	23:B:603:CLA:H92	1.97	0.46
3:C:209:ILE:HG23	27:C:515:BCR:H382	1.97	0.46
14:T:4:ILE:HD13	27:T:103:BCR:H381	1.96	0.46
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.61	0.46
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.85	0.46
23:A:405:CLA:H122	23:A:405:CLA:HMA1	8.80	0.46
24:D:402:PHO:H61	24:D:402:PHO:H92	1.75	0.46
4:D:252:PHE:O	4:D:256:ILE:HG22	2.15	0.46
3:C:229:ASN:ND2	3:C:231:GLU:HB2	2.41	0.46
6:F:45:ARG:NH2	9:J:40:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:147:VAL:O	16:V:150:LYS:HB2	2.23	0.46
23:B:614:CLA:H112	23:B:614:CLA:H91	1.73	0.46
4:D:214:HIS:ND1	25:D:404:PL9:O2	2.37	0.46
3:C:38:GLY:HA3	23:C:511:CLA:HMD3	1.97	0.46
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.46
4:D:84:SER:HB2	4:D:85:MET:HE2	1.97	0.46
1:A:111:PRO:O	1:A:115:ILE:HG13	2.15	0.46
23:B:603:CLA:H41	23:B:603:CLA:H61	1.67	0.46
23:B:611:CLA:HMA1	4:D:130:PHE:CE1	17.32	0.46
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.59	0.46
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.06	0.46
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.06	0.46
23:C:510:CLA:H61	23:C:510:CLA:H2	1.67	0.46
27:C:515:BCR:H341	27:C:515:BCR:H11C	1.82	0.46
2:B:333:GLY:O	2:B:439:SER:HB3	2.23	0.46
2:B:450:TRP:NE1	23:B:610:CLA:HBA1	27.99	0.46
28:C:518:DGD:HAW2	28:C:518:DGD:HA91	4.32	0.46
27:J:102:BCR:H351	27:J:102:BCR:H15C	1.63	0.46
9:J:33:TYR:HB3	27:J:102:BCR:H383	1.97	0.46
23:C:511:CLA:H141	19:Z:20:VAL:HG13	1.98	0.46
13:O:192:SER:OG	13:O:193:GLY:N	2.49	0.46
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.48	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.98	0.46
4:D:216:ALA:O	4:D:220:ASN:ND2	2.52	0.46
1:A:153:SER:HB2	23:A:404:CLA:H43	14.47	0.46
4:D:146:PHE:O	4:D:149:PRO:HD2	2.16	0.46
19:Z:32:ASP:CG	19:Z:33:TRP:H	2.22	0.46
13:O:51:THR:O	13:O:53:ARG:N	2.56	0.46
23:B:606:CLA:H92	23:B:606:CLA:HBB2	13.67	0.46
23:B:615:CLA:H162	23:B:615:CLA:H122	4.48	0.46
3:C:429:SER:HB3	28:C:517:DGD:HA81	1.97	0.46
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.32	0.46
27:C:514:BCR:H353	27:K:102:BCR:H321	2.00	0.46
31:C:520:LMG:H111	31:C:520:LMG:H292	1.98	0.46
2:B:135:LEU:HA	2:B:138:MET:HE3	2.04	0.46
23:B:608:CLA:HBA1	23:B:608:CLA:CHA	2.46	0.46
27:B:617:BCR:H371	27:B:617:BCR:H24C	1.74	0.46
33:B:628:LMT:H62	8:I:4:LEU:HD22	81.54	0.46
3:C:174:LEU:HD13	23:C:502:CLA:H111	2.01	0.46
3:C:451:ALA:HA	3:C:456:GLU:CD	2.36	0.46
23:C:501:CLA:C1D	23:C:503:CLA:H2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.44	0.46
3:C:257:PHE:HB3	3:C:258:GLY:H	1.59	0.46
27:A:410:BCR:H342	30:A:417:SQD:H311	1.98	0.45
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.51	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.45
23:A:403:CLA:H62	23:A:403:CLA:H102	1.79	0.45
2:B:208:VAL:HG21	23:B:605:CLA:HMC1	26.22	0.45
23:B:614:CLA:H72	31:M:102:LMG:H352	1.98	0.45
3:C:163:PHE:CG	23:C:512:CLA:HAB	2.52	0.45
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.78	0.45
23:D:403:CLA:H61	23:D:403:CLA:H41	1.88	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.45
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.62	0.45
2:B:198:VAL:O	2:B:202:HIS:ND1	2.42	0.45
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.81	0.45
23:A:403:CLA:H191	31:D:408:LMG:H352	1.98	0.45
2:B:247:PHE:HE1	23:B:605:CLA:H101	11.54	0.45
23:B:608:CLA:HMA1	23:B:609:CLA:HBA2	15.98	0.45
2:B:137:LYS:O	2:B:141:ILE:HG13	2.29	0.45
2:B:487:SER:N	2:B:488:PRO:HD2	2.32	0.45
14:T:1:MET:HB3	14:T:2:GLU:OE2	2.17	0.45
1:A:150:PRO:HB2	23:A:404:CLA:H61	9.28	0.45
4:D:148:ALA:HB1	4:D:279:LEU:HB2	1.99	0.45
27:C:514:BCR:HC7	27:C:514:BCR:H331	1.60	0.45
8:I:8:VAL:O	8:I:12:VAL:HG23	2.23	0.45
29:A:412:LHG:HC32	4:D:229:ALA:O	2.16	0.45
31:B:622:LMG:H421	4:D:284:ILE:HD13	1.99	0.45
23:A:404:CLA:H71	31:D:408:LMG:H202	1.98	0.45
3:C:120:ILE:HD11	27:C:514:BCR:HC8	2.01	0.45
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.62	0.45
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.45
23:A:403:CLA:HBA1	23:A:403:CLA:H3A	1.57	0.45
23:A:403:CLA:H51	24:D:402:PHO:C3B	2.47	0.45
27:D:405:BCR:H11C	27:D:405:BCR:H341	1.75	0.45
27:J:102:BCR:H20C	27:J:102:BCR:H361	1.85	0.45
27:T:102:BCR:H24C	27:T:102:BCR:H371	1.73	0.45
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.99	0.45
5:E:19:TYR:O	5:E:23:HIS:ND1	2.41	0.45
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.92	0.45
3:C:319:ILE:HG21	3:C:389:GLU:HG3	1.99	0.45
23:B:605:CLA:H202	23:B:609:CLA:HBB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:618:BCR:H341	27:B:618:BCR:H11C	1.70	0.45
3:C:240:ILE:O	3:C:244:CYS:HB2	2.18	0.45
3:C:405:ASN:CB	28:C:518:DGD:HG31	2.46	0.45
5:E:55:TYR:O	5:E:84:LYS:HE3	2.22	0.45
2:B:256:MET:HA	2:B:263:THR:HG21	1.99	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.19	0.45
2:B:125:ASP:HB2	2:B:132:ALA:HB3	1.99	0.45
27:B:618:BCR:HC32	31:D:406:LMG:H392	78.78	0.45
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.07	0.45
3:C:248:GLY:O	3:C:252:ILE:HG12	2.16	0.45
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.51	0.45
5:E:42:LEU:O	5:E:46:VAL:HG23	2.29	0.45
2:B:247:PHE:HB2	23:B:611:CLA:HBC1	15.95	0.44
2:B:354:LEU:HB3	2:B:370:LEU:HB3	1.98	0.44
2:B:155:ALA:O	2:B:159:THR:OG1	2.22	0.44
1:A:124:SER:HA	1:A:151:LEU:HD21	1.99	0.44
3:C:343:ARG:NH1	3:C:347:GLY:O	2.51	0.44
1:A:238:LYS:HD2	14:T:32:LYS:HB3	2.07	0.44
2:B:150:CYS:HA	23:B:603:CLA:HBC2	2.00	0.44
3:C:86:LEU:HB3	3:C:90:PRO:HD3	2.00	0.44
1:A:210:LEU:HG	24:A:406:PHO:NC	2.32	0.44
2:B:458:PHE:CG	23:B:604:CLA:HMC3	2.51	0.44
23:B:605:CLA:H41	23:B:605:CLA:H62	1.75	0.44
4:D:40:CYS:HB3	4:D:117:HIS:O	2.18	0.44
23:D:403:CLA:HMD2	33:D:411:LMT:H22	1.99	0.44
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.83	0.44
23:C:509:CLA:H11	23:C:509:CLA:H51	1.74	0.44
2:B:201:HIS:HD2	2:B:202:HIS:ND1	2.28	0.44
1:A:224:ILE:O	4:D:265:ARG:NH2	2.50	0.44
23:B:605:CLA:H72	7:H:46:LEU:HD13	19.03	0.44
23:B:607:CLA:HBB1	31:B:622:LMG:H341	2.00	0.44
2:B:89:GLY:HA2	28:B:626:DGD:HD61	1.98	0.44
6:F:17:THR:OG1	6:F:18:VAL:N	2.50	0.44
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.44
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.81	0.44
23:B:602:CLA:H62	23:B:602:CLA:H93	1.90	0.44
23:B:606:CLA:H2	23:B:608:CLA:H93	40.30	0.44
23:B:607:CLA:HBB1	23:B:610:CLA:CBB	28.21	0.44
23:B:615:CLA:H171	23:B:616:CLA:HBB2	5.25	0.44
4:D:146:PHE:C	4:D:149:PRO:HD2	2.38	0.44
3:C:52:ALA:HA	23:C:511:CLA:HMB3	2.03	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.00	0.44
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.71	0.44
23:B:616:CLA:H191	27:B:620:BCR:H333	4.68	0.44
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.04	0.44
4:D:275:PRO:O	4:D:279:LEU:HD23	2.23	0.44
4:D:180:ARG:HG3	4:D:181:PHE:N	2.33	0.44
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.60	0.44
2:B:488:PRO:O	2:B:490:GLN:N	2.43	0.44
1:A:28:LEU:HB2	30:A:417:SQD:H91	1.99	0.44
1:A:43:ALA:HB1	27:A:410:BCR:H362	2.00	0.44
7:H:12:ARG:HD3	7:H:12:ARG:O	2.19	0.44
2:B:338:GLN:HB3	13:O:84:ASN:HB3	38.65	0.44
2:B:462:PHE:CE1	23:B:616:CLA:HMB3	23.45	0.44
1:A:214:MET:HA	1:A:214:MET:CE	2.62	0.44
1:A:238:LYS:O	1:A:241:GLN:HG3	2.18	0.44
2:B:360:PRO:HB2	2:B:363:PHE:HD2	1.83	0.44
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.44
23:B:607:CLA:HBA2	23:B:607:CLA:C4A	2.44	0.44
24:D:402:PHO:H102	24:D:402:PHO:H13	1.77	0.44
27:C:514:BCR:H11C	27:K:102:BCR:H322	2.00	0.44
9:J:14:ALA:HB3	27:K:102:BCR:H393	2.00	0.44
5:E:23:HIS:HA	5:E:26:THR:OG1	2.23	0.44
4:D:110:LEU:O	4:D:114:ILE:HG13	2.18	0.44
12:M:1:MET:HG2	12:M:2:GLU:H	1.99	0.44
23:B:602:CLA:H162	23:B:602:CLA:H122	1.57	0.43
3:C:85:GLY:N	28:C:517:DGD:HE4	2.33	0.43
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.06	0.43
16:V:103:LYS:O	16:V:122:ARG:HG2	2.19	0.43
16:V:83:GLU:H	16:V:83:GLU:CD	2.21	0.43
23:B:604:CLA:HBD	23:B:605:CLA:H43	2.00	0.43
23:B:610:CLA:H12	23:B:610:CLA:H51	1.82	0.43
23:B:613:CLA:H191	27:B:619:BCR:H333	1.99	0.43
27:B:619:BCR:H351	27:B:619:BCR:H15C	1.78	0.43
1:A:141:PRO:HB2	1:A:142:TRP:H	1.60	0.43
3:C:72:LEU:HD11	3:C:108:THR:HB	2.11	0.43
27:A:410:BCR:H24C	27:A:410:BCR:H371	1.84	0.43
31:A:414:LMG:H172	4:D:270:PHE:HE1	1.83	0.43
23:B:603:CLA:H2	23:B:605:CLA:H93	2.01	0.43
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.76	0.43
27:D:405:BCR:H351	27:D:405:BCR:H15C	1.82	0.43
27:C:514:BCR:H371	27:C:514:BCR:H24C	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:K:102:BCR:H351	27:K:102:BCR:H15C	1.84	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43
1:A:340:PRO:HD3	15:U:133:TYR:CZ	2.54	0.43
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.16	0.43
1:A:191:ASN:HB2	3:C:411:ALA:HB1	1.99	0.43
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.68	0.43
4:D:90:LEU:HA	4:D:90:LEU:HD23	1.89	0.43
23:A:404:CLA:H202	23:A:404:CLA:H162	1.72	0.43
1:A:271:LEU:HD11	25:A:408:PL9:C4	2.48	0.43
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.48	0.43
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.58	0.43
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.56	0.43
2:B:30:VAL:HG12	23:B:608:CLA:HHD	23.76	0.43
3:C:80:PRO:HB2	3:C:83:GLU:HG3	1.99	0.43
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.83	0.43
23:B:603:CLA:HBB2	23:B:605:CLA:H152	2.01	0.43
28:B:626:DGD:O2D	28:B:626:DGD:O1B	2.37	0.43
23:C:504:CLA:H151	28:C:518:DGD:HBW1	9.30	0.43
23:C:507:CLA:H62	23:C:507:CLA:H92	1.76	0.43
3:C:163:PHE:CD2	23:C:512:CLA:HAB	2.53	0.43
31:A:414:LMG:H211	11:L:26:VAL:HG21	2.01	0.43
27:C:514:BCR:H353	27:K:102:BCR:C32	2.52	0.43
5:E:7:GLU:H	5:E:7:GLU:CD	2.22	0.43
23:B:606:CLA:H71	27:B:620:BCR:H342	2.00	0.43
1:A:221:SER:HB2	4:D:139:ARG:O	2.18	0.43
1:A:182:PHE:O	1:A:186:PHE:HB2	2.18	0.43
4:D:239:GLN:HB3	4:D:240:ALA:H	1.55	0.43
27:K:102:BCR:H11C	27:K:102:BCR:H341	1.90	0.43
23:B:607:CLA:H202	23:B:607:CLA:H161	4.72	0.43
2:B:247:PHE:HB2	23:B:608:CLA:HBC1	2.00	0.43
23:D:401:CLA:H61	23:D:401:CLA:H41	1.66	0.43
31:I:101:LMG:H221	33:I:102:LMT:H81	2.00	0.43
10:K:37:PHE:HB3	27:K:102:BCR:C40	2.48	0.43
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.53	0.43
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.73	0.43
8:I:6:ILE:O	8:I:10:ILE:HG12	2.23	0.43
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.34	0.43
18:X:34:PHE:O	18:X:38:ILE:HG12	2.18	0.43
23:A:404:CLA:H191	31:D:406:LMG:H352	46.05	0.43
23:B:611:CLA:H52	23:B:614:CLA:HBC3	2.01	0.43
23:C:513:CLA:HBA2	23:C:513:CLA:H3A	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:22:LEU:O	11:L:26:VAL:HG22	2.19	0.43
3:C:89:ILE:N	3:C:90:PRO:HD2	2.34	0.43
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.54	0.43
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.36	0.43
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.50	0.43
1:A:269:ARG:NH1	4:D:231:THR:HB	2.38	0.43
27:Z:101:BCR:H24C	27:Z:101:BCR:H371	1.77	0.42
4:D:85:MET:HA	5:E:69:ARG:HB3	2.17	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.56	0.42
13:O:41:LEU:HD12	13:O:41:LEU:HA	2.01	0.42
3:C:62:PHE:HZ	10:K:28:ILE:HD12	1.83	0.42
2:B:472:ARG:NE	23:B:611:CLA:HED3	2.34	0.42
3:C:265:ILE:HG12	23:C:505:CLA:HED1	2.00	0.42
27:C:515:BCR:H24C	27:C:515:BCR:H371	2.08	0.42
1:A:258:LEU:O	4:D:128:ARG:NH1	2.52	0.42
3:C:416:SER:OG	3:C:417:VAL:N	2.52	0.42
2:B:458:PHE:CD2	23:B:604:CLA:HMC3	2.54	0.42
23:B:602:CLA:H72	7:H:46:LEU:HD13	2.01	0.42
23:B:608:CLA:H143	23:B:608:CLA:H161	1.86	0.42
27:B:620:BCR:H20C	27:B:620:BCR:H361	1.94	0.42
23:C:511:CLA:H151	19:Z:20:VAL:O	2.20	0.42
5:E:50:PRO:HB3	5:E:54:SER:O	2.32	0.42
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.06	0.42
2:B:148:LEU:HA	2:B:210:ILE:HD11	2.04	0.42
11:L:11:GLU:HA	12:M:29:THR:OG1	2.18	0.42
5:E:10:PHE:N	31:E:101:LMG:O3	2.51	0.42
23:B:602:CLA:H61	7:H:46:LEU:HB2	2.01	0.42
23:B:616:CLA:HMB1	23:B:616:CLA:HBB1	3.73	0.42
23:C:506:CLA:H202	23:C:506:CLA:H161	1.80	0.42
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.54	0.42
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.00	0.42
2:B:334:ASP:N	2:B:334:ASP:OD1	2.53	0.42
1:A:119:PHE:HZ	23:A:403:CLA:H8	1.84	0.42
27:B:620:BCR:H331	33:B:623:LMT:H122	2.01	0.42
2:B:7:ARG:O	2:B:10:THR:OG1	2.31	0.42
27:C:514:BCR:H351	27:C:514:BCR:H15C	1.69	0.42
1:A:322:ASN:OD1	3:C:412:THR:HA	2.20	0.42
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.01	0.42
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.59	0.42
23:A:405:CLA:H143	23:A:405:CLA:H161	1.89	0.42
23:B:614:CLA:H43	31:M:102:LMG:H332	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.45	0.42
23:C:509:CLA:H92	23:C:509:CLA:H62	1.71	0.42
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.05	0.42
3:C:29:GLU:HB2	3:C:30:SER:H	1.65	0.42
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.59	0.42
2:B:170:ASP:OD1	2:B:175:THR:N	2.50	0.42
19:Z:5:PHE:CE1	19:Z:54:VAL:HG13	2.56	0.42
5:E:14:ILE:HG22	9:J:13:VAL:HG11	2.09	0.42
23:A:404:CLA:H92	23:A:404:CLA:H61	1.77	0.42
23:B:614:CLA:H162	23:B:614:CLA:H141	4.50	0.42
31:B:622:LMG:H142	11:L:35:PHE:CE1	2.54	0.42
5:E:26:THR:HB	34:F:101:HEM:CAB	2.50	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.10	0.42
13:O:33:TYR:O	13:O:37:VAL:HG23	2.26	0.42
23:B:609:CLA:HMC2	27:H:101:BCR:H343	2.01	0.42
27:B:619:BCR:H341	27:B:619:BCR:H11C	1.85	0.42
3:C:425:TRP:CZ2	23:C:504:CLA:HBA1	2.56	0.42
27:C:514:BCR:H11C	27:C:514:BCR:H341	1.79	0.42
3:C:261:ARG:HA	3:C:266:TRP:CZ2	2.61	0.42
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.55	0.42
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.01	0.42
3:C:334:PRO:HA	13:O:179:THR:OG1	2.31	0.42
1:A:324:ALA:HB2	4:D:329:MET:SD	2.60	0.42
2:B:462:PHE:CE1	23:B:613:CLA:HMB3	2.54	0.42
19:Z:55:GLY:HA2	27:Z:101:BCR:H312	2.01	0.42
14:T:3:THR:O	14:T:7:VAL:HG23	2.25	0.42
2:B:133:LEU:HB3	2:B:138:MET:CE	2.50	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.12	0.42
13:O:147:THR:OG1	13:O:148:VAL:N	2.53	0.42
2:B:41:GLU:HB3	2:B:60:MET:SD	2.62	0.42
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.01	0.42
15:U:83:ALA:HB1	15:U:84:PRO:HD2	2.00	0.42
23:B:615:CLA:H72	23:B:616:CLA:HBB1	2.02	0.42
3:C:277:GLY:C	23:C:505:CLA:HBC2	2.47	0.42
23:C:502:CLA:CGA	23:C:503:CLA:H42	2.55	0.42
27:Z:101:BCR:H351	27:Z:101:BCR:H15C	1.75	0.42
10:K:25:LEU:HB2	10:K:26:PRO:HD3	2.11	0.42
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.88	0.42
13:O:144:LEU:HD13	13:O:259:VAL:HG11	2.09	0.42
1:A:180:PHE:HA	1:A:183:MET:HE2	2.08	0.41
1:A:271:LEU:HD21	25:A:408:PL9:HC71	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:606:CLA:H192	23:B:606:CLA:H162	4.43	0.41
23:C:513:CLA:HMC2	27:Z:101:BCR:H372	2.02	0.41
23:C:511:CLA:H93	23:C:511:CLA:H61	1.78	0.41
15:U:73:PRO:HG2	16:V:107:THR:HB	2.01	0.41
2:B:45:PHE:HB2	2:B:60:MET:SD	2.59	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.02	0.41
3:C:69:LEU:HD21	3:C:116:VAL:HG13	2.02	0.41
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.61	0.41
23:A:404:CLA:HBD	23:A:405:CLA:HAC2	15.25	0.41
23:B:612:CLA:H162	23:B:612:CLA:H122	1.82	0.41
2:B:238:LEU:HB2	23:B:612:CLA:HMD3	2.02	0.41
27:B:620:BCR:H11C	27:B:620:BCR:H341	1.82	0.41
27:T:102:BCR:H15C	27:T:102:BCR:H351	1.75	0.41
13:O:73:PRO:HG3	13:O:146:PHE:CE2	2.59	0.41
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.08	0.41
2:B:238:LEU:HB2	23:B:615:CLA:HMD3	11.71	0.41
23:B:610:CLA:C4A	23:B:610:CLA:HBA2	4.47	0.41
3:C:457:LYS:HG2	4:D:229:ALA:HA	2.06	0.41
2:B:118:TRP:CH2	11:L:5:PRO:HD2	2.71	0.41
16:V:160:LYS:HA	16:V:163:TYR:CG	2.70	0.41
10:K:43:VAL:HG22	10:K:46:ARG:HE	1.88	0.41
5:E:81:GLU:C	5:E:83:LEU:H	2.24	0.41
23:A:405:CLA:H162	23:A:405:CLA:H202	4.13	0.41
23:A:405:CLA:HMD3	4:D:182:LEU:HD11	2.02	0.41
27:A:410:BCR:H15C	27:A:410:BCR:H351	1.78	0.41
23:B:605:CLA:H61	7:H:46:LEU:HB2	20.14	0.41
23:B:615:CLA:H12	23:B:615:CLA:H52	1.74	0.41
4:D:73:PHE:CZ	31:D:406:LMG:H172	2.56	0.41
3:C:107:ASP:O	3:C:110:PRO:HD2	2.20	0.41
23:A:405:CLA:H62	23:A:405:CLA:H41	3.11	0.41
2:B:247:PHE:HE1	23:B:602:CLA:H101	1.86	0.41
31:C:519:LMG:H112	27:J:102:BCR:H373	2.02	0.41
7:H:55:LEU:O	7:H:58:VAL:HG12	2.20	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.76	0.41
23:B:604:CLA:H41	23:B:604:CLA:H61	1.85	0.41
23:B:608:CLA:H41	23:B:608:CLA:H62	2.05	0.41
3:C:305:THR:HG22	3:C:308:GLU:CB	2.51	0.41
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.91	0.41
1:A:308:ASP:O	6:F:45:ARG:NE	2.70	0.41
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.56	0.41
27:B:617:BCR:H341	27:B:617:BCR:H11C	1.84	0.41
28:C:517:DGD:HAW2	28:C:517:DGD:HA91	1.78	0.41
27:H:101:BCR:H15C	27:H:101:BCR:H351	1.87	0.41
3:C:319:ILE:O	3:C:323:LYS:HG3	2.20	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.20	0.41
23:A:405:CLA:H92	23:A:405:CLA:H61	4.47	0.41
4:D:43:LEU:HD23	4:D:117:HIS:CE1	4.03	0.41
19:Z:33:TRP:O	19:Z:33:TRP:HD1	2.04	0.41
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.34	0.41
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.05	0.41
3:C:437:PHE:HZ	23:C:510:CLA:HMB3	1.85	0.41
3:C:53:HIS:HB3	23:C:512:CLA:OBD	2.29	0.41
24:D:402:PHO:H62	24:D:402:PHO:H41	1.32	0.41
23:B:606:CLA:H41	23:B:606:CLA:H62	1.79	0.41
23:C:504:CLA:H112	23:C:504:CLA:H142	1.78	0.41
4:D:43:LEU:HD21	23:D:403:CLA:C3C	2.51	0.41
4:D:294:ARG:HG2	4:D:294:ARG:H	1.75	0.41
12:M:16:LEU:O	12:M:20:VAL:HG23	2.20	0.41
1:A:235:TYR:C	1:A:237:TYR:H	2.25	0.41
14:T:29:ILE:O	14:T:31:LYS:N	2.53	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.91	0.41
4:D:155:SER:HA	4:D:159:ILE:HB	2.12	0.41
4:D:346:LEU:HD12	4:D:346:LEU:HA	1.90	0.41
2:B:12:LEU:HD13	2:B:19:LEU:HA	2.03	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.95	0.41
23:B:610:CLA:H62	23:B:610:CLA:H41	1.78	0.41
23:B:602:CLA:H152	28:B:621:DGD:HAW2	2.03	0.41
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.57	0.41
1:A:337:HIS:CD2	3:C:354:GLU:OE1	2.74	0.41
12:M:20:VAL:HG13	12:M:20:VAL:HG13	0.00	0.41
5:E:56:TYR:O	16:V:27:ALA:HB2	2.20	0.41
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.10	0.41
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.03	0.41
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.02	0.41
23:B:606:CLA:H3A	23:B:606:CLA:HBA2	1.30	0.40
23:C:501:CLA:H52	23:C:503:CLA:H92	2.10	0.40
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.59	0.40
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.08	0.40
2:B:33:TRP:CD1	27:B:618:BCR:H391	2.56	0.40
23:B:608:CLA:H161	23:B:608:CLA:H141	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:609:CLA:H3A	23:B:609:CLA:HBA2	3.15	0.40
23:B:613:CLA:HMB1	23:B:613:CLA:HBB1	2.03	0.40
23:C:501:CLA:H162	23:C:501:CLA:H141	1.83	0.40
3:C:122:SER:OG	27:C:514:BCR:H14C	2.22	0.40
18:X:12:ILE:O	18:X:12:ILE:HG23	2.21	0.40
4:D:218:VAL:HA	4:D:221:THR:HG22	2.23	0.40
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.12	0.40
2:B:41:GLU:O	2:B:45:PHE:N	2.59	0.40
2:B:153:PHE:O	2:B:157:HIS:HB3	2.28	0.40
2:B:86:ILE:H	2:B:86:ILE:HG13	1.78	0.40
3:C:77:PRO:HG2	3:C:78:GLU:OE2	2.21	0.40
23:A:403:CLA:H162	23:A:404:CLA:C9	2.51	0.40
23:A:404:CLA:H3A	23:A:404:CLA:HBA1	3.95	0.40
23:B:612:CLA:H8	23:B:612:CLA:H122	1.85	0.40
3:C:264:PHE:HE1	23:C:507:CLA:HAB	1.87	0.40
23:A:407:CLA:HBC1	31:I:101:LMG:H341	2.01	0.40
10:K:24:VAL:O	10:K:27:VAL:HG12	2.21	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.38	0.40
3:C:42:LEU:HD13	23:C:511:CLA:HMA3	2.04	0.40
4:D:18:LEU:O	4:D:22:LEU:HG	2.41	0.40
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.02	0.40
5:E:36:LEU:HA	5:E:39:SER:OG	2.37	0.40
23:B:603:CLA:H192	23:B:603:CLA:H162	1.77	0.40
23:B:609:CLA:H41	23:B:609:CLA:H62	4.42	0.40
23:B:610:CLA:H152	23:B:615:CLA:HBD	2.04	0.40
23:B:614:CLA:H152	23:B:614:CLA:H112	1.85	0.40
3:C:284:PHE:CZ	28:C:517:DGD:HA91	15.54	0.40
20:G:23:UNK:O	20:G:24:UNK:C	2.70	0.40
1:A:307:ILE:HD11	6:F:45:ARG:NH2	2.45	0.40
4:D:18:LEU:HD13	18:X:38:ILE:HD13	2.12	0.40
19:Z:5:PHE:HB2	19:Z:57:LEU:HG	2.16	0.40
2:B:356:VAL:HG21	2:B:424:ALA:HB3	2.05	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.03	0.40
31:D:406:LMG:O5	31:D:406:LMG:O4	2.74	0.40
3:C:75:PHE:CD1	3:C:86:LEU:HD21	2.55	0.40
28:D:410:DGD:HG32	28:D:410:DGD:O2D	2.21	0.40
2:B:134:ASP:OD2	2:B:137:LYS:HE3	2.21	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.91	0.40
3:C:399:ALA:O	3:C:401:LEU:N	2.51	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	333/360 (92%)	311 (93%)	18 (5%)	4 (1%)	16	61
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	16	61
2	B	488/510 (96%)	448 (92%)	35 (7%)	5 (1%)	19	65
2	b	488/510 (96%)	448 (92%)	36 (7%)	4 (1%)	24	70
3	C	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	15	60
3	c	445/461 (96%)	405 (91%)	33 (7%)	7 (2%)	12	56
4	D	338/352 (96%)	315 (93%)	20 (6%)	3 (1%)	21	67
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	30	74
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	15	60
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	60
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	31
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	31
8	I	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	5	42
8	i	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	5	42
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	41
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	41
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	27
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	27
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%)	207 (86%)	30 (12%)	4 (2%)	11	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	241/272 (89%)	209 (87%)	29 (12%)	3 (1%)	16	61
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	40
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	40
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	41
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	41
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4	37
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	37
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	27
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	27
19	Z	60/62 (97%)	54 (90%)	4 (7%)	2 (3%)	5	40
19	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	55
All	All	5138/5650 (91%)	4681 (91%)	382 (7%)	75 (2%)	13	57

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA
14	T	30	THR
18	X	45	LYS
1	a	12	ASN
1	a	142	TRP
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
14	t	30	THR
18	x	45	LYS
1	A	141	PRO
1	A	142	TRP
2	B	489	GLU
3	C	32	GLY

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Mol	Chain	Res	Type
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
7	H	26	GLY
17	y	43	ARG
19	Z	32	ASP
1	a	141	PRO
2	b	489	GLU
3	c	32	GLY
3	c	144	SER
3	c	257	PHE
3	c	416	SER
4	d	239	GLN
7	h	26	GLY
17	g	43	ARG
19	z	32	ASP
2	B	176	GLY
4	D	262	SER
5	E	82	GLN
9	J	38	SER
13	O	88	GLU
1	a	334	ARG
2	b	176	GLY
3	c	194	GLY
5	e	82	GLN
9	j	38	SER
13	o	88	GLU
3	C	194	GLY
13	O	271	PRO
15	U	72	TYR
15	U	83	ALA
4	d	262	SER
7	h	16	SER
13	o	271	PRO
15	u	72	TYR
15	u	83	ALA
1	A	334	ARG
2	B	230	ARG
7	H	16	SER
10	K	13	GLU
13	O	158	ASN

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Mol	Chain	Res	Type
18	X	12	ILE
10	k	13	GLU
10	k	45	PHE
18	x	12	ILE
4	D	234	ALA
10	K	45	PHE
19	Z	28	ALA
3	c	462	GLU
15	u	73	PRO
15	U	73	PRO
8	I	32	PRO
3	c	209	ILE
3	C	209	ILE
8	i	32	PRO

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	271/291 (93%)	266 (98%)	5 (2%)	66	87
1	a	271/291 (93%)	266 (98%)	5 (2%)	66	87
2	B	390/407 (96%)	379 (97%)	11 (3%)	51	78
2	b	390/407 (96%)	379 (97%)	11 (3%)	51	78
3	C	347/362 (96%)	332 (96%)	15 (4%)	35	70
3	c	347/362 (96%)	332 (96%)	15 (4%)	35	70
4	D	275/283 (97%)	262 (95%)	13 (5%)	32	68
4	d	275/283 (97%)	260 (94%)	15 (6%)	27	64
5	E	72/73 (99%)	68 (94%)	4 (6%)	26	62
5	e	72/73 (99%)	68 (94%)	4 (6%)	26	62
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	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	h	53/55 (96%)	49 (92%)	4 (8%)	17 54
8	I	32/35 (91%)	31 (97%)	1 (3%)	47 77
8	i	32/35 (91%)	31 (97%)	1 (3%)	47 77
9	J	24/28 (86%)	23 (96%)	1 (4%)	36 70
9	j	24/28 (86%)	23 (96%)	1 (4%)	36 70
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 78
11	l	35/35 (100%)	34 (97%)	1 (3%)	50 78
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 75
14	t	29/29 (100%)	28 (97%)	1 (3%)	44 75
15	U	84/112 (75%)	83 (99%)	1 (1%)	78 90
15	u	84/112 (75%)	82 (98%)	2 (2%)	57 82
16	V	116/138 (84%)	114 (98%)	2 (2%)	68 87
16	v	116/138 (84%)	113 (97%)	3 (3%)	54 80
17	g	20/37 (54%)	18 (90%)	2 (10%)	9 38
17	y	20/37 (54%)	18 (90%)	2 (10%)	9 38
18	X	30/34 (88%)	27 (90%)	3 (10%)	9 38
18	x	30/34 (88%)	27 (90%)	3 (10%)	9 38
19	Z	52/52 (100%)	49 (94%)	3 (6%)	25 61
19	z	52/52 (100%)	50 (96%)	2 (4%)	40 73
All	All	4244/4616 (92%)	4103 (97%)	141 (3%)	45 76

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	VAL
1	A	228	THR
1	A	243	GLU

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Mol	Chain	Res	Type
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	354	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	488	PRO
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	232	ASP
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	469	MET
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	84	SER
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	323	GLU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG

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Mol	Chain	Res	Type
5	E	77	GLU
5	E	82	GLN
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	63	CYS
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	45	LYS
19	Z	1	MET
19	Z	33	TRP
19	Z	62	VAL
1	a	202	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	354	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	488	PRO
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU

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Mol	Chain	Res	Type
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	232	ASP
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	305	THR
3	c	355	THR
3	c	382	ASN
3	c	391	ARG
3	c	469	MET
3	c	472	LEU
4	d	20	ASP
4	d	43	LEU
4	d	84	SER
4	d	91	LEU
4	d	130	PHE
4	d	180	ARG
4	d	205	LEU
4	d	241	GLU
4	d	259	ILE
4	d	279	LEU
4	d	291	LEU
4	d	294	ARG
4	d	323	GLU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	77	GLU
5	e	82	GLN
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

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Mol	Chain	Res	Type
15	u	103	GLN
15	u	132	LEU
16	v	63	CYS
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	11	THR
18	x	12	ILE
18	x	45	LYS
19	z	33	TRP
19	z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	261	GLN
2	B	201	HIS
2	B	409	GLN
4	D	117	HIS
4	D	332	GLN
1	a	241	GLN
2	b	201	HIS
4	d	142	ASN

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 (i)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	BCT	A	402	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	403	-	55,73,73	0.95	4 (7%)	61,113,113	1.17	6 (9%)
23	CLA	A	404	-	55,73,73	0.99	4 (7%)	61,113,113	1.22	8 (13%)
23	CLA	A	405	-	55,73,73	0.95	4 (7%)	61,113,113	1.15	6 (9%)
24	PHO	A	406	-	67,69,69	1.26	12 (17%)	84,99,99	1.13	8 (9%)
23	CLA	A	407	-	55,73,73	0.92	3 (5%)	61,113,113	1.21	4 (6%)
25	PL9	A	408	-	45,45,55	1.46	7 (15%)	56,57,69	1.73	13 (23%)
26	OEC	A	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	A	410	-	41,41,41	0.72	0	56,56,56	2.02	13 (23%)
28	DGD	A	411	-	57,57,67	1.22	8 (14%)	71,71,81	1.61	12 (16%)
29	LHG	A	412	-	38,38,48	1.03	2 (5%)	39,44,54	1.00	2 (5%)
30	SQD	A	413	-	50,51,54	0.98	3 (6%)	58,62,65	1.68	10 (17%)
31	LMG	A	414	-	51,51,55	1.15	6 (11%)	59,59,63	1.35	5 (8%)
29	LHG	A	415	-	36,36,48	1.04	2 (5%)	37,42,54	1.09	2 (5%)
30	SQD	A	417	-	53,54,54	1.01	5 (9%)	61,65,65	1.61	11 (18%)
31	LMG	A	418	-	42,42,55	1.22	6 (14%)	50,50,63	1.55	9 (18%)
23	CLA	B	601	-	55,73,73	0.98	4 (7%)	61,113,113	1.20	8 (13%)
23	CLA	B	602	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	B	603	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	7 (11%)
23	CLA	B	604	-	55,73,73	0.97	3 (5%)	61,113,113	1.15	7 (11%)
23	CLA	B	605	-	55,73,73	0.95	3 (5%)	61,113,113	1.25	8 (13%)
23	CLA	B	606	-	55,73,73	0.97	4 (7%)	61,113,113	1.22	8 (13%)
23	CLA	B	607	-	55,73,73	0.94	3 (5%)	61,113,113	1.23	7 (11%)
23	CLA	B	608	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
23	CLA	B	609	-	55,73,73	0.96	4 (7%)	61,113,113	1.25	7 (11%)
23	CLA	B	610	-	55,73,73	0.97	3 (5%)	61,113,113	1.28	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	611	-	55,73,73	0.95	4 (7%)	61,113,113	1.28	7 (11%)
23	CLA	B	612	-	55,73,73	0.96	4 (7%)	61,113,113	1.21	8 (13%)
23	CLA	B	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	8 (13%)
23	CLA	B	614	-	55,73,73	0.94	3 (5%)	61,113,113	1.16	7 (11%)
23	CLA	B	615	-	55,73,73	0.94	4 (7%)	61,113,113	1.21	8 (13%)
23	CLA	B	616	-	55,73,73	0.97	4 (7%)	61,113,113	1.22	8 (13%)
27	BCR	B	617	-	41,41,41	0.70	0	56,56,56	1.96	14 (25%)
27	BCR	B	618	-	41,41,41	0.68	0	56,56,56	2.32	13 (23%)
27	BCR	B	619	-	41,41,41	0.63	0	56,56,56	1.91	16 (28%)
27	BCR	B	620	-	41,41,41	0.69	0	56,56,56	2.17	17 (30%)
28	DGD	B	621	-	59,59,67	1.25	9 (15%)	73,73,81	1.16	6 (8%)
31	LMG	B	622	-	49,49,55	1.17	7 (14%)	57,57,63	1.41	8 (14%)
33	LMT	B	623	-	36,36,36	0.40	0	47,47,47	0.76	1 (2%)
33	LMT	B	624	-	36,36,36	0.43	0	47,47,47	0.71	1 (2%)
30	SQD	B	625	-	46,47,54	1.02	5 (10%)	54,58,65	1.74	8 (14%)
28	DGD	B	626	-	53,53,67	1.23	7 (13%)	67,67,81	1.42	10 (14%)
33	LMT	B	627	-	36,36,36	0.44	0	47,47,47	0.82	1 (2%)
33	LMT	B	628	-	36,36,36	0.45	0	47,47,47	0.64	0
23	CLA	C	501	-	55,73,73	0.96	4 (7%)	61,113,113	1.16	6 (9%)
23	CLA	C	502	-	55,73,73	0.96	4 (7%)	61,113,113	1.23	8 (13%)
23	CLA	C	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	C	504	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	7 (11%)
23	CLA	C	505	-	55,73,73	0.97	3 (5%)	61,113,113	1.19	7 (11%)
23	CLA	C	506	-	55,73,73	0.97	3 (5%)	61,113,113	1.31	8 (13%)
23	CLA	C	507	-	55,73,73	0.93	3 (5%)	61,113,113	1.25	8 (13%)
23	CLA	C	508	-	55,73,73	0.97	3 (5%)	61,113,113	1.22	7 (11%)
23	CLA	C	509	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	6 (9%)
23	CLA	C	510	-	55,73,73	0.99	3 (5%)	61,113,113	1.18	5 (8%)
23	CLA	C	511	3	55,73,73	0.95	4 (7%)	61,113,113	1.22	9 (14%)
23	CLA	C	512	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	8 (13%)
23	CLA	C	513	-	55,73,73	0.97	4 (7%)	61,113,113	1.21	8 (13%)
27	BCR	C	514	-	41,41,41	0.72	0	56,56,56	2.42	20 (35%)
27	BCR	C	515	-	41,41,41	0.66	0	56,56,56	2.01	16 (28%)
28	DGD	C	516	-	54,54,67	1.23	7 (12%)	68,68,81	1.33	10 (14%)
28	DGD	C	517	-	63,63,67	1.20	10 (15%)	77,77,81	1.26	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DGD	C	518	-	67,67,67	1.13	7 (10%)	81,81,81	1.48	9 (11%)
31	LMG	C	519	-	48,48,55	1.12	6 (12%)	56,56,63	1.37	7 (12%)
31	LMG	C	520	-	45,45,55	1.19	6 (13%)	53,53,63	1.48	8 (15%)
23	CLA	D	401	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	8 (13%)
24	PHO	D	402	-	67,69,69	1.22	11 (16%)	84,99,99	1.11	8 (9%)
23	CLA	D	403	-	55,73,73	0.94	4 (7%)	61,113,113	1.22	8 (13%)
25	PL9	D	404	-	55,55,55	1.44	8 (14%)	68,69,69	1.91	20 (29%)
27	BCR	D	405	-	41,41,41	0.66	0	56,56,56	2.26	19 (33%)
31	LMG	D	406	-	46,46,55	1.15	6 (13%)	54,54,63	1.36	6 (11%)
31	LMG	D	407	-	49,49,55	1.16	7 (14%)	57,57,63	1.28	8 (14%)
31	LMG	D	408	-	48,48,55	1.19	8 (16%)	56,56,63	1.45	8 (14%)
30	SQD	D	409	-	42,43,54	1.09	4 (9%)	50,54,65	2.24	9 (18%)
28	DGD	D	410	-	64,64,67	1.12	7 (10%)	78,78,81	1.48	8 (10%)
33	LMT	D	411	-	32,32,36	0.47	0	43,43,47	0.74	2 (4%)
31	LMG	E	101	-	44,44,55	1.20	8 (18%)	52,52,63	1.38	7 (13%)
34	HEM	F	101	5,6	30,50,50	2.09	7 (23%)	24,82,82	2.32	10 (41%)
30	SQD	F	102	-	44,45,54	1.03	4 (9%)	52,56,65	1.84	10 (19%)
27	BCR	H	101	-	41,41,41	0.69	0	56,56,56	1.75	14 (25%)
31	LMG	I	101	-	43,43,55	1.25	8 (18%)	51,51,63	1.37	7 (13%)
33	LMT	I	102	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
25	PL9	J	101	-	35,35,55	1.35	5 (14%)	44,45,69	1.70	8 (18%)
27	BCR	J	102	-	41,41,41	0.68	0	56,56,56	3.40	23 (41%)
27	BCR	K	102	-	41,41,41	0.69	0	56,56,56	1.89	12 (21%)
31	LMG	M	101	-	42,42,55	1.29	7 (16%)	50,50,63	1.54	9 (18%)
31	LMG	M	102	-	42,42,55	1.27	6 (14%)	50,50,63	1.51	9 (18%)
33	LMT	M	103	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
33	LMT	T	101	-	36,36,36	0.40	0	47,47,47	0.88	1 (2%)
27	BCR	T	102	-	41,41,41	0.71	0	56,56,56	1.94	13 (23%)
27	BCR	T	103	-	41,41,41	0.66	0	56,56,56	2.31	17 (30%)
34	HEM	V	201	16	30,50,50	2.23	8 (26%)	24,82,82	2.14	5 (20%)
27	BCR	Z	101	-	41,41,41	0.64	0	56,56,56	1.89	15 (26%)
30	SQD	a	401	-	53,54,54	0.96	4 (7%)	61,65,65	1.64	11 (18%)
31	LMG	a	402	-	42,42,55	1.21	6 (14%)	50,50,63	1.51	8 (16%)
23	CLA	a	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
23	CLA	a	405	-	55,73,73	0.94	4 (7%)	61,113,113	1.22	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	a	406	-	55,73,73	0.96	3 (5%)	61,113,113	1.21	10 (16%)
24	PHO	a	407	-	67,69,69	1.19	11 (16%)	84,99,99	1.07	6 (7%)
24	PHO	a	408	-	67,69,69	1.22	10 (14%)	84,99,99	1.04	5 (5%)
23	CLA	a	409	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	9 (14%)
25	PL9	a	410	-	45,45,55	1.41	7 (15%)	56,57,69	1.84	12 (21%)
26	OEC	a	411	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	a	412	-	41,41,41	0.68	0	56,56,56	1.93	16 (28%)
28	DGD	a	413	-	57,57,67	1.21	8 (14%)	71,71,81	1.58	12 (16%)
29	LHG	a	414	-	38,38,48	1.05	2 (5%)	39,44,54	1.00	3 (7%)
30	SQD	a	415	-	50,51,54	0.99	5 (10%)	58,62,65	1.66	9 (15%)
31	LMG	a	416	-	51,51,55	1.12	6 (11%)	59,59,63	1.42	5 (8%)
29	LHG	a	417	-	36,36,48	1.04	2 (5%)	37,42,54	1.10	2 (5%)
30	SQD	b	601	-	46,47,54	1.02	5 (10%)	54,58,65	1.81	9 (16%)
28	DGD	b	602	-	53,53,67	1.23	7 (13%)	67,67,81	1.44	9 (13%)
33	LMT	b	603	-	36,36,36	0.39	0	47,47,47	0.63	0
23	CLA	b	604	-	55,73,73	0.97	4 (7%)	61,113,113	1.23	8 (13%)
23	CLA	b	605	-	55,73,73	0.98	3 (5%)	61,113,113	1.18	6 (9%)
23	CLA	b	606	-	55,73,73	0.93	4 (7%)	61,113,113	1.21	7 (11%)
23	CLA	b	607	-	55,73,73	0.94	3 (5%)	61,113,113	1.18	9 (14%)
23	CLA	b	608	-	55,73,73	0.95	4 (7%)	61,113,113	1.19	7 (11%)
23	CLA	b	609	-	55,73,73	0.96	3 (5%)	61,113,113	1.26	7 (11%)
23	CLA	b	610	-	55,73,73	0.95	4 (7%)	61,113,113	1.21	8 (13%)
23	CLA	b	611	-	55,73,73	0.96	3 (5%)	61,113,113	1.30	8 (13%)
23	CLA	b	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	b	613	-	55,73,73	0.97	3 (5%)	61,113,113	1.23	7 (11%)
23	CLA	b	614	-	55,73,73	0.99	4 (7%)	61,113,113	1.23	6 (9%)
23	CLA	b	615	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
23	CLA	b	616	-	55,73,73	0.96	3 (5%)	61,113,113	1.23	8 (13%)
23	CLA	b	617	-	55,73,73	0.97	3 (5%)	61,113,113	1.17	6 (9%)
23	CLA	b	618	-	55,73,73	0.93	3 (5%)	61,113,113	1.24	8 (13%)
23	CLA	b	619	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	8 (13%)
27	BCR	b	620	-	41,41,41	0.63	0	56,56,56	1.96	16 (28%)
27	BCR	b	621	-	41,41,41	0.71	0	56,56,56	2.22	17 (30%)
28	DGD	b	622	-	59,59,67	1.23	9 (15%)	73,73,81	1.19	6 (8%)
31	LMG	b	623	-	49,49,55	1.20	7 (14%)	57,57,63	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LMG	b	624	-	49,49,55	1.15	7 (14%)	57,57,63	1.42	7 (12%)
33	LMT	b	625	-	36,36,36	0.39	0	47,47,47	0.77	1 (2%)
33	LMT	b	626	-	36,36,36	0.43	0	47,47,47	0.69	1 (2%)
23	CLA	c	501	-	55,73,73	0.95	3 (5%)	61,113,113	1.25	9 (14%)
23	CLA	c	502	-	55,73,73	0.97	3 (5%)	61,113,113	1.21	7 (11%)
23	CLA	c	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	6 (9%)
23	CLA	c	504	-	55,73,73	0.93	3 (5%)	61,113,113	1.27	8 (13%)
23	CLA	c	505	-	55,73,73	0.96	3 (5%)	61,113,113	1.26	7 (11%)
23	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.27	7 (11%)
23	CLA	c	507	-	55,73,73	0.94	3 (5%)	61,113,113	1.23	8 (13%)
23	CLA	c	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	8 (13%)
23	CLA	c	509	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	c	510	-	55,73,73	0.97	3 (5%)	61,113,113	1.15	7 (11%)
23	CLA	c	511	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	6 (9%)
23	CLA	c	512	-	55,73,73	0.93	3 (5%)	61,113,113	1.27	9 (14%)
23	CLA	c	513	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
27	BCR	c	514	-	41,41,41	0.68	0	56,56,56	2.45	17 (30%)
27	BCR	c	515	-	41,41,41	0.63	0	56,56,56	1.81	11 (19%)
27	BCR	c	516	-	41,41,41	0.66	0	56,56,56	1.97	16 (28%)
28	DGD	c	517	-	54,54,67	1.24	7 (12%)	68,68,81	1.34	8 (11%)
28	DGD	c	518	-	63,63,67	1.20	9 (14%)	77,77,81	1.30	7 (9%)
28	DGD	c	519	-	67,67,67	1.13	7 (10%)	81,81,81	1.46	10 (12%)
31	LMG	c	520	-	45,45,55	1.19	7 (15%)	53,53,63	1.43	8 (15%)
22	BCT	d	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	402	-	55,73,73	0.94	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	d	403	-	55,73,73	0.96	3 (5%)	61,113,113	1.21	7 (11%)
25	PL9	d	404	-	55,55,55	1.47	8 (14%)	68,69,69	1.87	19 (27%)
31	LMG	d	405	-	46,46,55	1.17	6 (13%)	54,54,63	1.37	5 (9%)
31	LMG	d	406	-	48,48,55	1.14	6 (12%)	56,56,63	1.44	7 (12%)
30	SQD	d	407	-	42,43,54	1.11	4 (9%)	50,54,65	2.25	9 (18%)
28	DGD	d	408	-	64,64,67	1.11	7 (10%)	78,78,81	1.52	9 (11%)
31	LMG	e	101	-	44,44,55	1.20	7 (15%)	52,52,63	1.32	8 (15%)
34	HEM	f	101	5,6	30,50,50	2.08	10 (33%)	24,82,82	2.33	10 (41%)
27	BCR	f	102	-	41,41,41	0.66	0	56,56,56	2.21	18 (32%)
30	SQD	f	103	-	44,45,54	1.03	5 (11%)	52,56,65	1.79	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LMG	i	101	-	43,43,55	1.26	7 (16%)	51,51,63	1.32	8 (15%)
33	LMT	i	102	-	36,36,36	0.50	1 (2%)	47,47,47	0.68	1 (2%)
25	PL9	j	101	-	35,35,55	1.34	5 (14%)	44,45,69	1.72	9 (20%)
27	BCR	j	102	-	41,41,41	0.69	0	56,56,56	3.41	24 (42%)
27	BCR	k	102	-	41,41,41	0.68	0	56,56,56	1.92	14 (25%)
31	LMG	k	103	-	48,48,55	1.13	6 (12%)	56,56,63	1.29	7 (12%)
33	LMT	m	101	-	36,36,36	0.38	0	47,47,47	0.72	1 (2%)
34	HEM	v	201	16	30,50,50	2.19	9 (30%)	24,82,82	2.18	7 (29%)
27	BCR	x	101	-	41,41,41	0.68	0	56,56,56	1.74	14 (25%)
33	LMT	x	102	-	32,32,36	0.47	0	43,43,47	0.67	1 (2%)

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	BCT	A	402	21	-	0/0/0/0	0/0/0/0
23	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	406	-	-	0/53/103/103	0/1/6/6
23	CLA	A	407	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	A	408	-	-	0/41/61/73	0/1/1/1
26	OEC	A	409	1,3	-	0/0/0/54	0/0/0/5
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
28	DGD	A	411	-	-	0/45/85/95	0/2/2/2
29	LHG	A	412	-	-	0/43/43/53	0/0/0/0
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
31	LMG	A	414	-	-	0/46/66/70	0/1/1/1
29	LHG	A	415	-	-	0/41/41/53	0/0/0/0
30	SQD	A	417	-	-	0/49/69/69	0/1/1/1
31	LMG	A	418	-	-	0/37/57/70	0/1/1/1
23	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	DGD	B	621	-	-	0/47/87/95	0/2/2/2
31	LMG	B	622	-	-	0/44/64/70	0/1/1/1
33	LMT	B	623	-	-	0/21/61/61	0/2/2/2
33	LMT	B	624	-	-	0/21/61/61	0/2/2/2
30	SQD	B	625	-	-	0/42/62/69	0/1/1/1
28	DGD	B	626	-	-	0/41/81/95	0/2/2/2
33	LMT	B	627	-	-	0/21/61/61	0/2/2/2
33	LMT	B	628	-	-	0/21/61/61	0/2/2/2
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
28	DGD	C	516	-	-	0/42/82/95	0/2/2/2
28	DGD	C	517	-	-	2/51/91/95	0/2/2/2
28	DGD	C	518	-	-	0/55/95/95	0/2/2/2
31	LMG	C	519	-	-	0/43/63/70	0/1/1/1
31	LMG	C	520	-	-	0/40/60/70	0/1/1/1
23	CLA	D	401	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	D	404	-	-	0/53/73/73	0/1/1/1
27	BCR	D	405	-	-	0/29/63/63	0/2/2/2
31	LMG	D	406	-	-	0/41/61/70	0/1/1/1
31	LMG	D	407	-	-	0/44/64/70	0/1/1/1
31	LMG	D	408	-	-	0/43/63/70	0/1/1/1
30	SQD	D	409	-	-	2/38/58/69	0/1/1/1
28	DGD	D	410	-	-	1/52/92/95	0/2/2/2
33	LMT	D	411	-	-	0/17/57/61	0/2/2/2
31	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
30	SQD	F	102	-	-	0/40/60/69	0/1/1/1
27	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	LMG	I	101	-	-	0/38/58/70	0/1/1/1
33	LMT	I	102	-	-	0/21/61/61	0/2/2/2
25	PL9	J	101	-	-	0/29/49/73	0/1/1/1
27	BCR	J	102	-	-	0/29/63/63	0/2/2/2
27	BCR	K	102	-	-	0/29/63/63	0/2/2/2
31	LMG	M	101	-	-	1/37/57/70	0/1/1/1
31	LMG	M	102	-	-	1/37/57/70	0/1/1/1
33	LMT	M	103	-	-	0/21/61/61	0/2/2/2
33	LMT	T	101	-	-	0/21/61/61	0/2/2/2
27	BCR	T	102	-	-	0/29/63/63	0/2/2/2
27	BCR	T	103	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/10/54/54	0/0/8/8
27	BCR	Z	101	-	-	0/29/63/63	0/2/2/2
30	SQD	a	401	-	-	0/49/69/69	0/1/1/1
31	LMG	a	402	-	-	0/37/57/70	0/1/1/1
23	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	a	409	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	a	410	-	-	0/41/61/73	0/1/1/1
26	OEC	a	411	1,3	-	0/0/0/54	0/0/0/5
27	BCR	a	412	-	-	0/29/63/63	0/2/2/2
28	DGD	a	413	-	-	0/45/85/95	0/2/2/2
29	LHG	a	414	-	-	0/43/43/53	0/0/0/0
30	SQD	a	415	-	-	0/46/66/69	0/1/1/1
31	LMG	a	416	-	-	0/46/66/70	0/1/1/1
29	LHG	a	417	-	-	0/41/41/53	0/0/0/0
30	SQD	b	601	-	-	0/42/62/69	0/1/1/1
28	DGD	b	602	-	-	0/41/81/95	0/2/2/2
33	LMT	b	603	-	-	0/21/61/61	0/2/2/2
23	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	b	620	-	-	0/29/63/63	0/2/2/2
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
28	DGD	b	622	-	-	0/47/87/95	0/2/2/2
31	LMG	b	623	-	-	0/44/64/70	0/1/1/1
31	LMG	b	624	-	-	0/44/64/70	0/1/1/1
33	LMT	b	625	-	-	0/21/61/61	0/2/2/2
33	LMT	b	626	-	-	0/21/61/61	0/2/2/2
23	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	BCR	c	516	-	-	0/29/63/63	0/2/2/2
28	DGD	c	517	-	-	0/42/82/95	0/2/2/2
28	DGD	c	518	-	-	2/51/91/95	0/2/2/2
28	DGD	c	519	-	-	0/55/95/95	0/2/2/2
31	LMG	c	520	-	-	0/40/60/70	0/1/1/1
22	BCT	d	401	21	-	0/0/0/0	0/0/0/0
23	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	d	404	-	-	0/53/73/73	0/1/1/1
31	LMG	d	405	-	-	0/41/61/70	0/1/1/1
31	LMG	d	406	-	-	0/43/63/70	0/1/1/1
30	SQD	d	407	-	-	2/38/58/69	0/1/1/1
28	DGD	d	408	-	-	1/52/92/95	0/2/2/2
31	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
27	BCR	f	102	-	-	0/29/63/63	0/2/2/2
30	SQD	f	103	-	-	0/40/60/69	0/1/1/1
31	LMG	i	101	-	-	0/38/58/70	0/1/1/1
33	LMT	i	102	-	-	0/21/61/61	0/2/2/2
25	PL9	j	101	-	-	0/29/49/73	0/1/1/1
27	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
31	LMG	k	103	-	-	0/43/63/70	0/1/1/1
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
34	HEM	v	201	16	-	0/10/54/54	0/0/8/8
27	BCR	x	101	-	-	0/29/63/63	0/2/2/2
33	LMT	x	102	-	-	0/17/57/61	0/2/2/2

All (659) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-8.15	1.44	1.51
34	v	201	HEM	C3B-C4B	-7.24	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.50	1.46	1.51
34	f	101	HEM	C3B-C4B	-6.20	1.46	1.51
34	F	101	HEM	C3D-C4D	-5.40	1.44	1.51
34	f	101	HEM	C3D-C4D	-5.32	1.44	1.51
34	V	201	HEM	C3D-C4D	-4.65	1.45	1.51
34	v	201	HEM	C3D-C4D	-4.41	1.45	1.51
34	V	201	HEM	C2C-C1C	-4.08	1.44	1.52
34	F	101	HEM	C2C-C1C	-3.86	1.45	1.52
34	v	201	HEM	C2C-C1C	-3.71	1.45	1.52
34	f	101	HEM	C2C-C1C	-3.42	1.46	1.52
31	D	406	LMG	O7-C8	-3.38	1.38	1.46
28	C	516	DGD	O2G-C2G	-3.31	1.38	1.46
31	D	407	LMG	O7-C8	-3.31	1.38	1.46
28	B	621	DGD	O2G-C2G	-3.25	1.38	1.46
28	b	622	DGD	O2G-C2G	-3.18	1.38	1.46
31	d	405	LMG	O7-C8	-3.17	1.38	1.46
31	M	102	LMG	O1-C7	-3.10	1.38	1.43
28	c	517	DGD	O2G-C2G	-3.09	1.38	1.46
31	b	624	LMG	O7-C8	-3.07	1.38	1.46
31	b	623	LMG	O7-C8	-3.07	1.38	1.46
31	M	101	LMG	O1-C7	-3.07	1.38	1.43
31	k	103	LMG	O7-C8	-3.06	1.38	1.46
31	I	101	LMG	O7-C8	-3.04	1.38	1.46
31	C	519	LMG	O7-C8	-3.04	1.38	1.46
31	A	418	LMG	O7-C8	-3.03	1.38	1.46
31	D	408	LMG	O7-C8	-3.01	1.38	1.46
23	b	614	CLA	CMB-C2B	-3.00	1.45	1.51
31	M	102	LMG	O7-C8	-2.98	1.39	1.46
31	a	402	LMG	O7-C8	-2.97	1.39	1.46
28	C	517	DGD	O2G-C2G	-2.95	1.39	1.46
31	i	101	LMG	O7-C8	-2.94	1.39	1.46
31	M	101	LMG	O7-C8	-2.91	1.39	1.46
28	D	410	DGD	O2G-C2G	-2.87	1.39	1.46
31	D	408	LMG	O3-C3	-2.86	1.36	1.43
31	d	406	LMG	O3-C3	-2.85	1.36	1.43
31	d	406	LMG	O7-C8	-2.83	1.39	1.46
31	a	416	LMG	O3-C3	-2.82	1.36	1.43
28	d	408	DGD	O2G-C2G	-2.81	1.39	1.46
23	B	611	CLA	CMB-C2B	-2.81	1.45	1.51
28	b	602	DGD	O2G-C2G	-2.80	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	518	DGD	O2G-C2G	-2.80	1.39	1.46
28	a	413	DGD	O2G-C2G	-2.79	1.39	1.46
31	A	414	LMG	O7-C8	-2.78	1.39	1.46
31	M	101	LMG	O8-C9	-2.77	1.38	1.45
28	C	518	DGD	O2G-C2G	-2.77	1.39	1.46
31	i	101	LMG	O1-C7	-2.76	1.38	1.43
31	B	622	LMG	O7-C8	-2.76	1.39	1.46
31	A	414	LMG	O3-C3	-2.75	1.36	1.43
31	D	407	LMG	O8-C9	-2.74	1.39	1.45
31	B	622	LMG	O3-C3	-2.72	1.36	1.43
31	i	101	LMG	O3-C3	-2.71	1.36	1.43
31	I	101	LMG	O3-C3	-2.70	1.36	1.43
31	b	624	LMG	O8-C9	-2.70	1.39	1.45
31	D	406	LMG	O3-C3	-2.69	1.36	1.43
31	b	623	LMG	O3-C3	-2.69	1.36	1.43
31	a	416	LMG	O7-C8	-2.69	1.39	1.46
23	C	510	CLA	CMB-C2B	-2.68	1.46	1.51
31	b	624	LMG	O3-C3	-2.67	1.36	1.43
31	d	405	LMG	O3-C3	-2.67	1.36	1.43
28	c	519	DGD	O2G-C2G	-2.66	1.39	1.46
31	b	623	LMG	O6-C5	-2.66	1.37	1.44
23	b	604	CLA	CMB-C2B	-2.65	1.46	1.51
23	B	604	CLA	CMB-C2B	-2.64	1.46	1.51
23	c	508	CLA	CMB-C2B	-2.64	1.46	1.51
31	e	101	LMG	O7-C8	-2.64	1.39	1.46
31	e	101	LMG	O8-C9	-2.63	1.39	1.45
31	A	418	LMG	O8-C9	-2.63	1.39	1.45
28	B	621	DGD	O3G-C3G	-2.63	1.38	1.43
28	A	411	DGD	O2G-C2G	-2.63	1.39	1.46
31	M	101	LMG	O3-C3	-2.63	1.36	1.43
31	E	101	LMG	O3-C3	-2.62	1.36	1.43
31	M	102	LMG	O8-C9	-2.62	1.39	1.45
23	B	608	CLA	CMB-C2B	-2.62	1.46	1.51
31	A	414	LMG	O1-C7	-2.61	1.38	1.43
31	a	402	LMG	O3-C3	-2.61	1.36	1.43
28	b	622	DGD	O3G-C3G	-2.61	1.38	1.43
31	i	101	LMG	O8-C9	-2.61	1.39	1.45
23	A	404	CLA	CMB-C2B	-2.61	1.46	1.51
28	B	626	DGD	O2G-C2G	-2.61	1.39	1.46
31	c	520	LMG	O3-C3	-2.60	1.36	1.43
28	b	602	DGD	O6E-C5E	-2.60	1.37	1.44
23	b	611	CLA	CMB-C2B	-2.58	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	519	LMG	O3-C3	-2.58	1.36	1.43
31	A	418	LMG	O3-C3	-2.58	1.36	1.43
23	C	508	CLA	CMB-C2B	-2.58	1.46	1.51
23	b	616	CLA	CMB-C2B	-2.58	1.46	1.51
31	C	520	LMG	O3-C3	-2.58	1.36	1.43
23	B	601	CLA	CMB-C2B	-2.58	1.46	1.51
23	B	610	CLA	CMB-C2B	-2.58	1.46	1.51
31	b	623	LMG	O8-C9	-2.57	1.39	1.45
23	b	605	CLA	CMB-C2B	-2.57	1.46	1.51
31	B	622	LMG	O1-C7	-2.57	1.39	1.43
31	D	408	LMG	O8-C9	-2.57	1.39	1.45
31	A	414	LMG	O8-C9	-2.57	1.39	1.45
31	D	406	LMG	O8-C9	-2.57	1.39	1.45
31	D	407	LMG	O1-C7	-2.56	1.39	1.43
23	B	606	CLA	CMB-C2B	-2.56	1.46	1.51
28	B	626	DGD	O6E-C5E	-2.56	1.37	1.44
28	c	518	DGD	O4D-C4D	-2.56	1.36	1.43
23	A	405	CLA	CMB-C2B	-2.55	1.46	1.51
31	e	101	LMG	O3-C3	-2.55	1.36	1.43
23	c	501	CLA	CMB-C2B	-2.55	1.46	1.51
23	b	609	CLA	CMB-C2B	-2.55	1.46	1.51
31	D	407	LMG	O3-C3	-2.55	1.36	1.43
31	I	101	LMG	O8-C9	-2.55	1.39	1.45
23	c	510	CLA	CMB-C2B	-2.54	1.46	1.51
31	a	416	LMG	O8-C9	-2.54	1.39	1.45
23	a	406	CLA	CMB-C2B	-2.54	1.46	1.51
23	C	513	CLA	CMB-C2B	-2.54	1.46	1.51
31	k	103	LMG	O3-C3	-2.53	1.36	1.43
31	c	520	LMG	O7-C8	-2.53	1.40	1.46
23	a	404	CLA	CMB-C2B	-2.53	1.46	1.51
31	E	101	LMG	O8-C9	-2.53	1.39	1.45
30	A	417	SQD	C4-C5	-2.53	1.47	1.53
31	M	102	LMG	O3-C3	-2.53	1.36	1.43
23	C	505	CLA	CMB-C2B	-2.53	1.46	1.51
23	B	616	CLA	CMB-C2B	-2.52	1.46	1.51
23	c	502	CLA	CMB-C2B	-2.52	1.46	1.51
31	k	103	LMG	O8-C9	-2.52	1.39	1.45
23	b	607	CLA	CMB-C2B	-2.52	1.46	1.51
28	A	411	DGD	O1G-C1G	-2.52	1.39	1.45
23	B	613	CLA	CMB-C2B	-2.51	1.46	1.51
28	C	516	DGD	O6E-C5E	-2.50	1.38	1.44
31	B	622	LMG	O8-C9	-2.50	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	CMB-C2B	-2.49	1.46	1.51
31	a	402	LMG	O8-C9	-2.49	1.39	1.45
23	C	501	CLA	CMB-C2B	-2.49	1.46	1.51
31	c	520	LMG	O8-C9	-2.49	1.39	1.45
23	B	612	CLA	CMD-C2D	-2.49	1.46	1.51
23	c	505	CLA	CMD-C2D	-2.49	1.46	1.51
23	a	409	CLA	CMB-C2B	-2.48	1.46	1.51
31	C	520	LMG	O7-C8	-2.48	1.40	1.46
23	a	405	CLA	CMB-C2B	-2.48	1.46	1.51
23	b	619	CLA	CMB-C2B	-2.48	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.48	1.46	1.51
23	b	613	CLA	CMB-C2B	-2.48	1.46	1.51
23	B	602	CLA	CMB-C2B	-2.48	1.46	1.51
28	B	626	DGD	O5D-C6D	-2.48	1.39	1.43
31	k	103	LMG	O1-C7	-2.47	1.39	1.43
23	C	502	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	403	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	512	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	504	CLA	CMB-C2B	-2.47	1.46	1.51
23	b	606	CLA	CMB-C2B	-2.47	1.46	1.51
23	c	513	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	509	CLA	CMB-C2B	-2.47	1.46	1.51
23	c	510	CLA	CMD-C2D	-2.46	1.46	1.51
31	E	101	LMG	O7-C8	-2.46	1.40	1.46
23	B	603	CLA	CMB-C2B	-2.46	1.46	1.51
23	c	506	CLA	CMB-C2B	-2.46	1.46	1.51
31	C	520	LMG	O8-C9	-2.46	1.39	1.45
31	b	624	LMG	O1-C7	-2.46	1.39	1.43
23	c	504	CLA	CMB-C2B	-2.45	1.46	1.51
31	d	405	LMG	O1-C7	-2.45	1.39	1.43
28	C	517	DGD	O4D-C4D	-2.45	1.37	1.43
23	C	503	CLA	CMB-C2B	-2.45	1.46	1.51
31	d	405	LMG	O8-C9	-2.45	1.39	1.45
23	B	609	CLA	CMB-C2B	-2.45	1.46	1.51
23	D	401	CLA	CMB-C2B	-2.45	1.46	1.51
23	b	617	CLA	CMD-C2D	-2.45	1.46	1.51
23	a	404	CLA	CMD-C2D	-2.45	1.46	1.51
23	C	505	CLA	CMD-C2D	-2.45	1.46	1.51
23	B	614	CLA	CMB-C2B	-2.45	1.46	1.51
30	A	417	SQD	O2-C2	-2.45	1.37	1.43
23	c	503	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	610	CLA	CMB-C2B	-2.44	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	CMB-C2B	-2.44	1.46	1.51
23	D	403	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	618	CLA	CMB-C2B	-2.44	1.46	1.51
31	a	402	LMG	O1-C7	-2.44	1.39	1.43
23	B	605	CLA	CMB-C2B	-2.44	1.46	1.51
23	d	403	CLA	CMB-C2B	-2.43	1.46	1.51
28	c	517	DGD	O6E-C5E	-2.43	1.38	1.44
23	b	617	CLA	CMB-C2B	-2.43	1.46	1.51
28	B	621	DGD	O6D-C5D	-2.43	1.38	1.44
23	c	512	CLA	CMB-C2B	-2.43	1.46	1.51
28	C	517	DGD	C4D-C5D	-2.43	1.47	1.53
23	B	615	CLA	CMB-C2B	-2.42	1.46	1.51
31	C	519	LMG	O8-C9	-2.42	1.39	1.45
23	c	511	CLA	CMB-C2B	-2.42	1.46	1.51
23	C	506	CLA	CMB-C2B	-2.42	1.46	1.51
23	C	507	CLA	CMB-C2B	-2.42	1.46	1.51
31	b	623	LMG	O1-C7	-2.42	1.39	1.43
23	b	615	CLA	CMB-C2B	-2.42	1.46	1.51
23	B	604	CLA	CMD-C2D	-2.42	1.46	1.51
23	b	615	CLA	CMD-C2D	-2.42	1.46	1.51
23	b	614	CLA	CMD-C2D	-2.41	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.41	1.46	1.51
28	c	518	DGD	O6E-C5E	-2.41	1.38	1.44
23	b	612	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	406	CLA	CMD-C2D	-2.39	1.46	1.51
31	I	101	LMG	O1-C7	-2.39	1.39	1.43
23	c	504	CLA	CMD-C2D	-2.39	1.46	1.51
23	c	509	CLA	CMB-C2B	-2.39	1.46	1.51
23	B	608	CLA	CMD-C2D	-2.39	1.46	1.51
23	B	607	CLA	CMB-C2B	-2.39	1.46	1.51
23	A	407	CLA	CMB-C2B	-2.39	1.46	1.51
23	A	403	CLA	CMD-C2D	-2.38	1.46	1.51
23	A	404	CLA	C3B-C2B	-2.38	1.37	1.40
23	B	605	CLA	CMD-C2D	-2.38	1.46	1.51
23	C	510	CLA	CMD-C2D	-2.38	1.46	1.51
23	C	502	CLA	CMD-C2D	-2.36	1.46	1.51
28	a	413	DGD	O1G-C1G	-2.36	1.39	1.45
28	C	518	DGD	O3G-C3G	-2.36	1.39	1.43
28	b	622	DGD	O6D-C5D	-2.36	1.38	1.44
28	C	517	DGD	O6E-C5E	-2.35	1.38	1.44
31	A	418	LMG	O1-C7	-2.35	1.39	1.43
28	c	518	DGD	O5D-C6D	-2.35	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	CMD-C2D	-2.34	1.46	1.51
23	d	402	CLA	CMB-C2B	-2.34	1.46	1.51
28	C	516	DGD	C4E-C5E	-2.34	1.48	1.53
28	B	621	DGD	O5D-C6D	-2.34	1.39	1.43
23	b	607	CLA	CMD-C2D	-2.34	1.46	1.51
23	C	503	CLA	CMD-C2D	-2.34	1.46	1.51
28	c	519	DGD	O3G-C3G	-2.34	1.39	1.43
23	C	508	CLA	CMD-C2D	-2.33	1.46	1.51
31	D	408	LMG	O1-C7	-2.33	1.39	1.43
28	c	518	DGD	O6D-C5D	-2.33	1.38	1.44
23	B	603	CLA	CMD-C2D	-2.33	1.46	1.51
23	c	502	CLA	CMD-C2D	-2.33	1.46	1.51
23	B	615	CLA	CMD-C2D	-2.33	1.46	1.51
23	B	611	CLA	CMD-C2D	-2.32	1.46	1.51
23	b	608	CLA	CMD-C2D	-2.32	1.46	1.51
23	D	401	CLA	CMD-C2D	-2.32	1.46	1.51
23	B	602	CLA	CMD-C2D	-2.32	1.46	1.51
23	c	505	CLA	CMB-C2B	-2.32	1.46	1.51
23	b	611	CLA	CMD-C2D	-2.32	1.46	1.51
23	C	509	CLA	CMD-C2D	-2.31	1.46	1.51
28	c	517	DGD	O4D-C4D	-2.31	1.37	1.43
23	b	610	CLA	CMD-C2D	-2.31	1.46	1.51
23	B	614	CLA	CMD-C2D	-2.31	1.46	1.51
23	d	402	CLA	CMD-C2D	-2.30	1.46	1.51
23	a	405	CLA	CMD-C2D	-2.30	1.46	1.51
23	A	407	CLA	CMD-C2D	-2.30	1.46	1.51
28	c	518	DGD	C4D-C5D	-2.30	1.48	1.53
23	b	605	CLA	CMD-C2D	-2.30	1.46	1.51
23	B	613	CLA	CMD-C2D	-2.30	1.46	1.51
23	a	409	CLA	CMD-C2D	-2.29	1.46	1.51
23	B	616	CLA	CMD-C2D	-2.28	1.46	1.51
28	D	410	DGD	O5D-C6D	-2.28	1.39	1.43
31	D	407	LMG	O6-C5	-2.28	1.38	1.44
31	a	416	LMG	O1-C7	-2.28	1.39	1.43
23	C	504	CLA	CMD-C2D	-2.27	1.46	1.51
31	d	406	LMG	O8-C9	-2.27	1.40	1.45
23	b	612	CLA	CMD-C2D	-2.27	1.46	1.51
23	A	404	CLA	CMD-C2D	-2.27	1.46	1.51
28	a	413	DGD	O4D-C4D	-2.26	1.37	1.43
23	A	405	CLA	CMD-C2D	-2.26	1.46	1.51
31	d	406	LMG	O1-C7	-2.26	1.39	1.43
23	C	513	CLA	CMD-C2D	-2.26	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	501	CLA	CMD-C2D	-2.26	1.46	1.51
23	c	507	CLA	CMD-C2D	-2.25	1.46	1.51
28	b	602	DGD	O5D-C6D	-2.25	1.39	1.43
23	c	513	CLA	CMD-C2D	-2.25	1.46	1.51
23	b	616	CLA	CMD-C2D	-2.25	1.46	1.51
30	a	401	SQD	O2-C2	-2.25	1.37	1.43
23	D	403	CLA	CMD-C2D	-2.24	1.46	1.51
24	a	407	PHO	C1C-NC	-2.24	1.33	1.38
23	c	508	CLA	CMD-C2D	-2.24	1.46	1.51
23	b	609	CLA	CMD-C2D	-2.24	1.46	1.51
23	c	511	CLA	CMD-C2D	-2.24	1.46	1.51
23	B	609	CLA	CMD-C2D	-2.24	1.46	1.51
28	c	519	DGD	O4D-C4D	-2.24	1.37	1.43
23	B	601	CLA	CMD-C2D	-2.24	1.46	1.51
31	C	519	LMG	O1-C7	-2.24	1.39	1.43
31	D	408	LMG	O6-C5	-2.23	1.38	1.44
23	b	604	CLA	CMD-C2D	-2.23	1.46	1.51
23	c	509	CLA	CMD-C2D	-2.23	1.46	1.51
23	C	506	CLA	CMD-C2D	-2.23	1.46	1.51
24	D	402	PHO	C1C-NC	-2.23	1.33	1.38
23	b	619	CLA	CMD-C2D	-2.22	1.46	1.51
23	B	606	CLA	CMD-C2D	-2.22	1.46	1.51
30	B	625	SQD	O2-C2	-2.22	1.37	1.43
23	d	403	CLA	CMD-C2D	-2.21	1.46	1.51
23	C	512	CLA	CMD-C2D	-2.21	1.46	1.51
31	I	101	LMG	O6-C5	-2.21	1.38	1.44
31	B	622	LMG	O6-C5	-2.21	1.38	1.44
28	C	518	DGD	O4D-C4D	-2.20	1.37	1.43
28	c	518	DGD	O1G-C1G	-2.20	1.40	1.45
28	A	411	DGD	O4D-C4D	-2.20	1.37	1.43
23	c	512	CLA	CMD-C2D	-2.20	1.46	1.51
23	C	511	CLA	CMD-C2D	-2.20	1.46	1.51
23	b	606	CLA	CMD-C2D	-2.20	1.46	1.51
28	C	517	DGD	O6D-C5D	-2.20	1.38	1.44
23	c	503	CLA	CMD-C2D	-2.20	1.46	1.51
31	e	101	LMG	O6-C5	-2.19	1.38	1.44
28	C	518	DGD	O6E-C5E	-2.19	1.38	1.44
31	c	520	LMG	O1-C7	-2.19	1.39	1.43
30	b	601	SQD	O2-C2	-2.19	1.37	1.43
28	B	621	DGD	O6E-C5E	-2.18	1.38	1.44
28	C	517	DGD	O5D-C6D	-2.18	1.39	1.43
23	b	618	CLA	CMD-C2D	-2.18	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	622	DGD	O6E-C5E	-2.18	1.38	1.44
23	b	613	CLA	CMD-C2D	-2.17	1.46	1.51
24	A	406	PHO	C1C-NC	-2.17	1.33	1.38
28	C	518	DGD	O1G-C1G	-2.17	1.40	1.45
34	V	201	HEM	C2D-C1D	-2.17	1.44	1.51
28	A	411	DGD	O3G-C3G	-2.16	1.39	1.43
31	I	101	LMG	C4-C5	-2.16	1.48	1.53
23	C	501	CLA	CMD-C2D	-2.16	1.46	1.51
24	a	407	PHO	CMD-C2D	-2.16	1.46	1.50
23	B	616	CLA	CMC-C2C	-2.16	1.46	1.50
23	C	507	CLA	CMD-C2D	-2.16	1.46	1.51
28	b	602	DGD	O4D-C4D	-2.16	1.37	1.43
23	B	610	CLA	CMD-C2D	-2.16	1.46	1.51
28	c	519	DGD	O6E-C5E	-2.15	1.39	1.44
28	a	413	DGD	O6E-C5E	-2.15	1.39	1.44
28	A	411	DGD	C4D-C5D	-2.15	1.48	1.53
28	a	413	DGD	O3G-C3G	-2.14	1.39	1.43
28	B	621	DGD	O4D-C4D	-2.14	1.37	1.43
24	a	408	PHO	C1C-NC	-2.14	1.33	1.38
23	b	608	CLA	CMC-C2C	-2.13	1.46	1.50
23	c	506	CLA	CMD-C2D	-2.13	1.47	1.51
31	e	101	LMG	O1-C7	-2.11	1.39	1.43
28	A	411	DGD	O6E-C5E	-2.11	1.39	1.44
31	c	520	LMG	O6-C5	-2.11	1.39	1.44
28	b	622	DGD	O5D-C6D	-2.11	1.39	1.43
28	D	410	DGD	O6E-C5E	-2.11	1.39	1.44
28	C	516	DGD	O4D-C4D	-2.11	1.37	1.43
31	C	520	LMG	O6-C5	-2.11	1.39	1.44
30	D	409	SQD	O3-C3	-2.10	1.37	1.43
30	A	413	SQD	O2-C2	-2.10	1.37	1.43
24	a	407	PHO	CMC-C2C	-2.09	1.46	1.50
23	C	502	CLA	CMC-C2C	-2.09	1.46	1.50
30	a	401	SQD	C4-C5	-2.09	1.48	1.53
24	D	402	PHO	CMC-C2C	-2.09	1.46	1.50
23	b	604	CLA	CMC-C2C	-2.09	1.46	1.50
28	B	621	DGD	O1G-C1G	-2.08	1.40	1.45
30	B	625	SQD	O4-C4	-2.08	1.38	1.43
31	D	406	LMG	O1-C7	-2.08	1.39	1.43
28	B	626	DGD	C4E-C5E	-2.08	1.48	1.53
24	D	402	PHO	CMD-C2D	-2.08	1.46	1.50
28	c	519	DGD	O1G-C1G	-2.08	1.40	1.45
31	i	101	LMG	O6-C5	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	626	DGD	O1G-C1G	-2.07	1.40	1.45
23	b	619	CLA	CMC-C2C	-2.07	1.46	1.50
34	f	101	HEM	C2B-C1B	-2.07	1.45	1.51
30	a	415	SQD	O3-C3	-2.07	1.38	1.43
28	b	622	DGD	O4D-C4D	-2.07	1.38	1.43
30	d	407	SQD	O4-C4	-2.07	1.38	1.43
28	b	622	DGD	O1G-C1G	-2.07	1.40	1.45
30	b	601	SQD	O3-C3	-2.07	1.38	1.43
31	D	408	LMG	O2-C2	-2.07	1.38	1.43
30	f	103	SQD	O2-C2	-2.06	1.38	1.43
23	B	601	CLA	CMC-C2C	-2.06	1.46	1.50
34	F	101	HEM	C2B-C1B	-2.06	1.45	1.51
24	A	406	PHO	CMB-C2B	-2.06	1.46	1.50
28	c	517	DGD	C4D-C5D	-2.06	1.48	1.53
28	C	517	DGD	O1G-C1G	-2.06	1.40	1.45
24	a	407	PHO	CMB-C2B	-2.06	1.46	1.50
31	E	101	LMG	O6-C5	-2.05	1.39	1.44
30	d	407	SQD	O3-C3	-2.05	1.38	1.43
23	a	405	CLA	CMC-C2C	-2.05	1.46	1.50
31	M	101	LMG	O6-C5	-2.05	1.39	1.44
28	D	410	DGD	O4D-C4D	-2.05	1.38	1.43
28	c	517	DGD	C4E-C5E	-2.05	1.48	1.53
23	A	403	CLA	CMC-C2C	-2.05	1.46	1.50
28	d	408	DGD	O4D-C4D	-2.05	1.38	1.43
30	A	417	SQD	O4-C4	-2.04	1.38	1.43
23	B	615	CLA	CMC-C2C	-2.04	1.46	1.50
24	a	408	PHO	CMD-C2D	-2.04	1.46	1.50
28	d	408	DGD	O5D-C6D	-2.04	1.39	1.43
28	D	410	DGD	C4D-C5D	-2.04	1.48	1.53
30	b	601	SQD	O4-C4	-2.04	1.38	1.43
23	D	403	CLA	CMC-C2C	-2.04	1.46	1.50
28	a	413	DGD	C4D-C5D	-2.04	1.48	1.53
23	A	405	CLA	CMC-C2C	-2.04	1.46	1.50
28	C	517	DGD	C4E-C5E	-2.04	1.48	1.53
30	F	102	SQD	O3-C3	-2.03	1.38	1.43
23	C	501	CLA	C3B-C2B	-2.03	1.37	1.40
23	c	511	CLA	CMC-C2C	-2.03	1.46	1.50
28	d	408	DGD	O6E-C5E	-2.03	1.39	1.44
24	A	406	PHO	CMD-C2D	-2.03	1.46	1.50
23	C	511	CLA	CMC-C2C	-2.03	1.46	1.50
30	F	102	SQD	O2-C2	-2.03	1.38	1.43
28	b	602	DGD	C4E-C5E	-2.02	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	625	SQD	O3-C3	-2.02	1.38	1.43
30	f	103	SQD	O3-C3	-2.02	1.38	1.43
31	b	624	LMG	O6-C5	-2.02	1.39	1.44
30	D	409	SQD	O4-C4	-2.02	1.38	1.43
24	a	408	PHO	CMC-C2C	-2.02	1.46	1.50
28	C	516	DGD	O1G-C1G	-2.02	1.40	1.45
30	a	415	SQD	O4-C4	-2.02	1.38	1.43
30	a	415	SQD	O2-C2	-2.02	1.38	1.43
23	b	614	CLA	CMC-C2C	-2.01	1.46	1.50
34	f	101	HEM	C2D-C1D	-2.01	1.45	1.51
30	f	103	SQD	O4-C4	-2.01	1.38	1.43
23	B	609	CLA	CMC-C2C	-2.01	1.46	1.50
23	b	610	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	611	CLA	CMC-C2C	-2.01	1.46	1.50
31	E	101	LMG	O1-C7	-2.01	1.40	1.43
23	B	612	CLA	CMC-C2C	-2.01	1.46	1.50
31	E	101	LMG	O4-C4	-2.01	1.38	1.43
23	b	606	CLA	CMC-C2C	-2.00	1.46	1.50
28	d	408	DGD	O1G-C1G	-2.00	1.40	1.45
34	V	201	HEM	C2B-C1B	-2.00	1.45	1.51
23	C	513	CLA	C3B-C2B	-2.00	1.37	1.40
23	B	606	CLA	CMC-C2C	-2.00	1.46	1.50
34	F	101	HEM	FE-ND	2.00	2.08	1.97
24	a	408	PHO	C1C-C2C	2.01	1.50	1.45
24	a	407	PHO	C1B-C2B	2.01	1.50	1.45
34	f	101	HEM	C1C-NC	2.02	1.38	1.36
24	A	406	PHO	C4B-NB	2.03	1.41	1.37
34	F	101	HEM	C3C-CAC	2.09	1.55	1.51
34	v	201	HEM	C3B-CAB	2.09	1.55	1.51
33	i	102	LMT	O1'-C1'	2.11	1.43	1.40
34	f	101	HEM	C3B-CAB	2.11	1.55	1.51
24	A	406	PHO	CHB-C4A	2.12	1.44	1.40
34	V	201	HEM	C4C-NC	2.12	1.38	1.36
24	A	406	PHO	C1C-C2C	2.13	1.50	1.45
34	v	201	HEM	C1C-NC	2.14	1.38	1.36
34	f	101	HEM	FE-NC	2.14	2.04	1.95
34	F	101	HEM	C3B-CAB	2.17	1.55	1.51
25	j	101	PL9	C28-C29	2.17	1.38	1.32
34	V	201	HEM	C3C-CAC	2.18	1.55	1.51
24	D	402	PHO	CHB-C4A	2.19	1.44	1.40
24	A	406	PHO	C4C-C3C	2.19	1.49	1.45
28	B	621	DGD	O2G-C1B	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	101	PL9	C28-C29	2.22	1.39	1.32
24	a	408	PHO	C1A-NA	2.22	1.42	1.37
24	D	402	PHO	C1B-C2B	2.22	1.50	1.45
34	v	201	HEM	C3C-CAC	2.23	1.55	1.51
34	V	201	HEM	FE-ND	2.24	2.09	1.97
24	a	407	PHO	C1A-NA	2.26	1.42	1.37
23	B	604	CLA	CHC-C1C	2.26	1.42	1.35
34	f	101	HEM	FE-ND	2.26	2.09	1.97
23	c	507	CLA	CHC-C1C	2.26	1.42	1.35
24	a	407	PHO	CHD-C1D	2.27	1.43	1.38
31	D	406	LMG	O7-C10	2.28	1.41	1.34
23	b	604	CLA	CHC-C1C	2.28	1.42	1.35
24	D	402	PHO	C1A-NA	2.29	1.42	1.37
23	a	405	CLA	CHC-C1C	2.29	1.42	1.35
28	D	410	DGD	O2G-C1B	2.31	1.41	1.34
24	a	407	PHO	C4C-C3C	2.31	1.49	1.45
23	b	619	CLA	CHC-C1C	2.32	1.42	1.35
34	v	201	HEM	C4C-NC	2.32	1.38	1.36
24	A	406	PHO	C1A-NA	2.33	1.42	1.37
34	v	201	HEM	FE-ND	2.34	2.09	1.97
28	b	622	DGD	O2G-C1B	2.34	1.41	1.34
24	D	402	PHO	CHD-C1D	2.34	1.43	1.38
23	d	402	CLA	CHC-C1C	2.35	1.42	1.35
23	c	501	CLA	CHC-C1C	2.35	1.42	1.35
24	A	406	PHO	CHD-C1D	2.35	1.43	1.38
23	b	607	CLA	CHC-C1C	2.36	1.42	1.35
23	c	503	CLA	CHC-C1C	2.37	1.42	1.35
23	b	610	CLA	CHC-C1C	2.37	1.42	1.35
23	C	509	CLA	CHC-C1C	2.37	1.42	1.35
23	A	407	CLA	CHC-C1C	2.38	1.42	1.35
23	C	501	CLA	CHC-C1C	2.38	1.42	1.35
23	C	508	CLA	CHC-C1C	2.38	1.42	1.35
23	A	405	CLA	CHC-C1C	2.39	1.42	1.35
23	B	616	CLA	CHC-C1C	2.39	1.42	1.35
24	D	402	PHO	C4C-C3C	2.39	1.49	1.45
24	a	408	PHO	C4C-C3C	2.39	1.49	1.45
23	c	512	CLA	CHC-C1C	2.39	1.42	1.35
23	B	611	CLA	CHC-C1C	2.39	1.42	1.35
34	f	101	HEM	C3C-CAC	2.40	1.55	1.51
28	C	516	DGD	O2G-C1B	2.40	1.41	1.34
23	D	403	CLA	CHC-C1C	2.40	1.42	1.35
23	B	613	CLA	CHC-C1C	2.41	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CHC-C1C	2.41	1.42	1.35
23	B	612	CLA	CHC-C1C	2.41	1.42	1.35
31	D	406	LMG	O8-C28	2.41	1.40	1.33
23	A	403	CLA	CHC-C1C	2.41	1.42	1.35
31	D	407	LMG	O7-C10	2.42	1.41	1.34
23	C	510	CLA	CHC-C1C	2.42	1.42	1.35
23	C	505	CLA	CHC-C1C	2.42	1.42	1.35
24	a	407	PHO	CHC-C1C	2.42	1.43	1.38
23	c	513	CLA	CHC-C1C	2.42	1.42	1.35
23	B	609	CLA	CHC-C1C	2.42	1.42	1.35
23	B	605	CLA	CHC-C1C	2.43	1.42	1.35
23	D	401	CLA	CHC-C1C	2.43	1.42	1.35
23	c	511	CLA	CHC-C1C	2.43	1.42	1.35
23	C	507	CLA	CHC-C1C	2.43	1.42	1.35
24	a	407	PHO	C4C-NC	2.43	1.42	1.37
24	a	408	PHO	CHD-C1D	2.43	1.43	1.38
23	a	406	CLA	CHC-C1C	2.45	1.43	1.35
23	c	505	CLA	CHC-C1C	2.45	1.43	1.35
23	C	511	CLA	CHC-C1C	2.46	1.43	1.35
23	B	601	CLA	CHC-C1C	2.46	1.43	1.35
23	B	608	CLA	CHC-C1C	2.46	1.43	1.35
23	c	510	CLA	CHC-C1C	2.46	1.43	1.35
23	b	616	CLA	CHC-C1C	2.46	1.43	1.35
23	b	609	CLA	CHC-C1C	2.47	1.43	1.35
23	C	512	CLA	CHC-C1C	2.47	1.43	1.35
23	B	603	CLA	CHC-C1C	2.47	1.43	1.35
23	b	615	CLA	CHC-C1C	2.48	1.43	1.35
28	C	517	DGD	O2G-C1B	2.48	1.41	1.34
23	a	404	CLA	CHC-C1C	2.48	1.43	1.35
31	A	418	LMG	O8-C28	2.48	1.40	1.33
24	D	402	PHO	C4C-NC	2.48	1.42	1.37
23	C	513	CLA	CHC-C1C	2.49	1.43	1.35
23	c	509	CLA	CHC-C1C	2.49	1.43	1.35
31	C	519	LMG	O7-C10	2.50	1.41	1.34
23	b	612	CLA	CHC-C1C	2.50	1.43	1.35
23	B	607	CLA	CHC-C1C	2.50	1.43	1.35
31	i	101	LMG	O8-C28	2.50	1.40	1.33
23	b	606	CLA	CHC-C1C	2.50	1.43	1.35
23	c	504	CLA	CHC-C1C	2.50	1.43	1.35
23	b	614	CLA	CHC-C1C	2.50	1.43	1.35
23	C	502	CLA	CHC-C1C	2.50	1.43	1.35
31	k	103	LMG	O7-C10	2.50	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	101	LMG	O7-C10	2.51	1.41	1.34
23	B	606	CLA	CHC-C1C	2.51	1.43	1.35
28	d	408	DGD	O2G-C1B	2.51	1.41	1.34
31	b	624	LMG	O8-C28	2.51	1.40	1.33
31	D	407	LMG	O8-C28	2.51	1.40	1.33
23	c	502	CLA	CHC-C1C	2.51	1.43	1.35
31	d	405	LMG	O8-C28	2.52	1.40	1.33
23	B	615	CLA	CHC-C1C	2.52	1.43	1.35
23	C	503	CLA	CHC-C1C	2.52	1.43	1.35
23	d	403	CLA	CHC-C1C	2.52	1.43	1.35
30	A	413	SQD	O47-C7	2.53	1.41	1.34
31	b	623	LMG	O7-C10	2.53	1.41	1.34
23	B	610	CLA	CHC-C1C	2.53	1.43	1.35
31	b	623	LMG	O8-C28	2.54	1.40	1.33
31	D	408	LMG	O7-C10	2.54	1.41	1.34
23	C	504	CLA	CHC-C1C	2.54	1.43	1.35
31	d	405	LMG	O7-C10	2.54	1.41	1.34
23	c	506	CLA	CHC-C1C	2.54	1.43	1.35
23	b	617	CLA	CHC-C1C	2.54	1.43	1.35
31	D	408	LMG	O8-C28	2.55	1.41	1.33
31	b	624	LMG	O7-C10	2.56	1.41	1.34
31	B	622	LMG	O8-C28	2.56	1.41	1.33
31	M	101	LMG	O8-C28	2.56	1.41	1.33
28	A	411	DGD	O1G-C1A	2.56	1.41	1.33
23	b	613	CLA	CHC-C1C	2.56	1.43	1.35
23	b	618	CLA	CHC-C1C	2.57	1.43	1.35
24	A	406	PHO	C4C-NC	2.57	1.42	1.37
31	I	101	LMG	O8-C28	2.57	1.41	1.33
31	A	418	LMG	O7-C10	2.57	1.42	1.34
23	c	508	CLA	CHC-C1C	2.57	1.43	1.35
23	C	506	CLA	CHC-C1C	2.58	1.43	1.35
31	e	101	LMG	O8-C28	2.58	1.41	1.33
23	b	608	CLA	CHC-C1C	2.59	1.43	1.35
31	a	402	LMG	O8-C28	2.62	1.41	1.33
31	A	414	LMG	O8-C28	2.62	1.41	1.33
24	a	408	PHO	C4C-NC	2.62	1.43	1.37
28	a	413	DGD	O2G-C1B	2.63	1.42	1.34
31	M	102	LMG	O8-C28	2.64	1.41	1.33
23	b	611	CLA	CHC-C1C	2.64	1.43	1.35
31	a	402	LMG	O7-C10	2.64	1.42	1.34
31	d	406	LMG	O7-C10	2.64	1.42	1.34
31	e	101	LMG	O7-C10	2.64	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	k	103	LMG	O8-C28	2.65	1.41	1.33
30	f	103	SQD	O47-C7	2.65	1.42	1.34
23	B	602	CLA	CHC-C1C	2.66	1.43	1.35
23	A	404	CLA	CHC-C1C	2.66	1.43	1.35
23	b	605	CLA	CHC-C1C	2.66	1.43	1.35
28	a	413	DGD	O1G-C1A	2.66	1.41	1.33
28	c	517	DGD	O2G-C1B	2.66	1.42	1.34
28	b	602	DGD	O2G-C1B	2.66	1.42	1.34
30	B	625	SQD	O47-C7	2.66	1.42	1.34
30	a	415	SQD	O47-C7	2.67	1.42	1.34
30	a	401	SQD	O47-C7	2.67	1.42	1.34
24	a	407	PHO	C3B-C4B	2.67	1.49	1.43
24	D	402	PHO	CHC-C1C	2.67	1.44	1.38
31	a	416	LMG	O8-C28	2.68	1.41	1.33
31	i	101	LMG	O7-C10	2.68	1.42	1.34
28	c	518	DGD	O2G-C1B	2.69	1.42	1.34
31	C	519	LMG	O8-C28	2.69	1.41	1.33
28	c	518	DGD	O1G-C1A	2.70	1.41	1.33
28	B	621	DGD	O1G-C1A	2.71	1.41	1.33
31	d	406	LMG	O8-C28	2.71	1.41	1.33
31	C	520	LMG	O8-C28	2.71	1.41	1.33
23	a	409	CLA	CHC-C1C	2.72	1.43	1.35
28	C	518	DGD	O1G-C1A	2.74	1.41	1.33
28	A	411	DGD	O2G-C1B	2.74	1.42	1.34
30	D	409	SQD	O47-C7	2.75	1.42	1.34
28	b	622	DGD	O1G-C1A	2.75	1.41	1.33
31	M	102	LMG	O7-C10	2.75	1.42	1.34
31	c	520	LMG	O8-C28	2.76	1.41	1.33
28	c	519	DGD	O1G-C1A	2.77	1.41	1.33
31	E	101	LMG	O8-C28	2.77	1.41	1.33
28	C	517	DGD	O1G-C1A	2.78	1.41	1.33
28	C	516	DGD	O1G-C1A	2.78	1.41	1.33
28	d	408	DGD	O1G-C1A	2.78	1.41	1.33
30	F	102	SQD	O47-C7	2.79	1.42	1.34
30	A	417	SQD	O47-C7	2.80	1.42	1.34
31	B	622	LMG	O7-C10	2.80	1.42	1.34
31	M	101	LMG	O7-C10	2.82	1.42	1.34
31	E	101	LMG	O7-C10	2.82	1.42	1.34
28	B	626	DGD	O1G-C1A	2.84	1.41	1.33
25	A	408	PL9	C38-C39	2.84	1.41	1.32
30	b	601	SQD	O47-C7	2.84	1.42	1.34
25	a	410	PL9	C38-C39	2.84	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	414	LMG	O7-C10	2.85	1.42	1.34
28	B	626	DGD	O2G-C1B	2.87	1.42	1.34
31	c	520	LMG	O7-C10	2.87	1.42	1.34
28	D	410	DGD	O1G-C1A	2.88	1.42	1.33
25	D	404	PL9	C28-C29	2.89	1.38	1.33
30	d	407	SQD	O47-C7	2.89	1.42	1.34
24	D	402	PHO	C3B-C4B	2.90	1.49	1.43
28	C	518	DGD	O2G-C1B	2.90	1.43	1.34
28	c	519	DGD	O2G-C1B	2.94	1.43	1.34
25	D	404	PL9	C8-C9	2.96	1.38	1.33
31	C	520	LMG	O7-C10	2.96	1.43	1.34
25	d	404	PL9	C28-C29	2.97	1.38	1.33
25	A	408	PL9	C28-C29	2.99	1.38	1.33
30	D	409	SQD	O48-C23	2.99	1.42	1.33
34	v	201	HEM	FE-NC	3.00	2.07	1.95
28	c	517	DGD	O1G-C1A	3.00	1.42	1.33
24	a	408	PHO	CHC-C1C	3.01	1.44	1.38
30	f	103	SQD	O48-C23	3.02	1.42	1.33
30	A	417	SQD	O48-C23	3.02	1.42	1.33
31	a	416	LMG	O7-C10	3.03	1.43	1.34
30	a	401	SQD	O48-C23	3.05	1.42	1.33
30	a	415	SQD	O48-C23	3.06	1.42	1.33
30	F	102	SQD	O48-C23	3.06	1.42	1.33
24	a	408	PHO	C3B-C4B	3.07	1.50	1.43
25	a	410	PL9	C8-C9	3.08	1.39	1.33
30	A	413	SQD	O48-C23	3.09	1.42	1.33
25	a	410	PL9	C28-C29	3.10	1.39	1.33
30	b	601	SQD	O48-C23	3.11	1.42	1.33
30	B	625	SQD	O48-C23	3.11	1.42	1.33
28	b	602	DGD	O1G-C1A	3.12	1.42	1.33
25	a	410	PL9	C13-C14	3.12	1.39	1.33
24	A	406	PHO	C3B-C4B	3.14	1.50	1.43
25	d	404	PL9	C8-C9	3.18	1.39	1.33
25	a	410	PL9	C18-C19	3.20	1.39	1.33
30	d	407	SQD	O48-C23	3.20	1.43	1.33
25	d	404	PL9	C13-C14	3.21	1.39	1.33
25	D	404	PL9	C13-C14	3.22	1.39	1.33
25	D	404	PL9	C23-C24	3.22	1.39	1.33
25	A	408	PL9	C8-C9	3.27	1.39	1.33
25	A	408	PL9	C18-C19	3.28	1.39	1.33
24	A	406	PHO	CHC-C1C	3.29	1.45	1.38
25	J	101	PL9	C13-C14	3.29	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PL9	C23-C24	3.32	1.39	1.33
25	j	101	PL9	C8-C9	3.33	1.39	1.33
25	D	404	PL9	C18-C19	3.33	1.39	1.33
25	j	101	PL9	C18-C19	3.33	1.39	1.33
25	J	101	PL9	C18-C19	3.35	1.39	1.33
25	a	410	PL9	C23-C24	3.36	1.39	1.33
25	d	404	PL9	C23-C24	3.36	1.39	1.33
25	j	101	PL9	C13-C14	3.40	1.39	1.33
25	d	404	PL9	C18-C19	3.41	1.39	1.33
25	J	101	PL9	C8-C9	3.41	1.39	1.33
25	j	101	PL9	C23-C24	3.43	1.39	1.33
25	A	408	PL9	C13-C14	3.46	1.39	1.33
25	J	101	PL9	C23-C24	3.48	1.39	1.33
25	D	404	PL9	C43-C44	3.64	1.40	1.33
29	a	417	LHG	O7-C7	3.89	1.45	1.34
25	d	404	PL9	C33-C34	3.91	1.40	1.33
25	d	404	PL9	C43-C44	3.93	1.40	1.33
29	A	415	LHG	O7-C7	3.94	1.46	1.34
25	D	404	PL9	C33-C34	3.98	1.40	1.33
25	a	410	PL9	C33-C34	3.99	1.40	1.33
25	d	404	PL9	C38-C39	4.02	1.40	1.33
25	D	404	PL9	C38-C39	4.03	1.40	1.33
29	A	412	LHG	O8-C23	4.04	1.45	1.33
29	a	417	LHG	O8-C23	4.06	1.45	1.33
29	A	412	LHG	O7-C7	4.07	1.46	1.34
29	A	415	LHG	O8-C23	4.12	1.45	1.33
29	a	414	LHG	O7-C7	4.12	1.46	1.34
25	A	408	PL9	C33-C34	4.15	1.41	1.33
29	a	414	LHG	O8-C23	4.24	1.46	1.33

All (1442) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	102	BCR	C32-C1-C6	-14.07	88.24	110.30
27	j	102	BCR	C32-C1-C6	-13.99	88.37	110.30
27	B	618	BCR	C7-C8-C9	-8.49	113.28	126.22
27	j	102	BCR	C32-C1-C31	-8.19	82.13	108.37
27	T	103	BCR	C7-C8-C9	-8.15	113.79	126.22
27	J	102	BCR	C32-C1-C31	-8.11	82.39	108.37
27	D	405	BCR	C7-C8-C9	-6.24	116.70	126.22
27	f	102	BCR	C7-C8-C9	-6.10	116.92	126.22
27	c	514	BCR	C15-C14-C13	-6.04	118.48	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	620	BCR	C3-C4-C5	-5.99	104.36	113.87
27	J	102	BCR	C32-C1-C2	-5.93	87.56	108.79
27	A	410	BCR	C33-C5-C6	-5.90	118.81	124.61
27	j	102	BCR	C32-C1-C2	-5.83	87.91	108.79
27	c	514	BCR	C33-C5-C6	-5.72	118.99	124.61
27	D	405	BCR	C28-C27-C26	-5.67	104.87	113.87
27	J	102	BCR	C28-C27-C26	-5.65	104.91	113.87
25	D	404	PL9	C3-C2-C1	-5.64	119.53	122.97
27	J	102	BCR	C15-C14-C13	-5.62	119.08	127.20
27	B	618	BCR	C11-C10-C9	-5.58	119.14	127.20
27	j	102	BCR	C28-C27-C26	-5.57	105.03	113.87
27	B	618	BCR	C3-C4-C5	-5.52	105.11	113.87
27	C	514	BCR	C33-C5-C6	-5.38	119.32	124.61
27	j	102	BCR	C15-C14-C13	-5.37	119.44	127.20
27	b	621	BCR	C3-C4-C5	-5.32	105.43	113.87
27	f	102	BCR	C28-C27-C26	-5.26	105.52	113.87
25	d	404	PL9	C3-C2-C1	-5.25	119.77	122.97
25	d	404	PL9	C7-C3-C2	-5.23	119.08	123.42
25	a	410	PL9	C3-C2-C1	-5.22	119.79	122.97
27	j	102	BCR	C20-C21-C22	-5.17	119.73	127.20
27	f	102	BCR	C15-C14-C13	-5.15	119.77	127.20
27	T	103	BCR	C11-C10-C9	-5.11	119.81	127.20
27	c	515	BCR	C15-C14-C13	-5.07	119.88	127.20
27	T	103	BCR	C3-C4-C5	-5.07	105.82	113.87
27	a	412	BCR	C33-C5-C6	-5.00	119.69	124.61
27	D	405	BCR	C11-C10-C9	-4.99	119.99	127.20
27	f	102	BCR	C33-C5-C6	-4.96	119.73	124.61
25	j	101	PL9	C7-C3-C2	-4.94	119.32	123.42
27	B	618	BCR	C28-C27-C26	-4.93	106.05	113.87
27	B	619	BCR	C28-C27-C26	-4.93	106.05	113.87
27	b	621	BCR	C24-C23-C22	-4.92	118.71	126.22
27	C	514	BCR	C15-C14-C13	-4.91	120.11	127.20
27	j	102	BCR	C24-C23-C22	-4.88	118.78	126.22
27	H	101	BCR	C33-C5-C6	-4.86	119.83	124.61
27	k	102	BCR	C38-C26-C25	-4.85	119.85	124.61
25	J	101	PL9	C7-C3-C2	-4.84	119.41	123.42
27	A	410	BCR	C16-C17-C18	-4.80	120.27	127.20
27	J	102	BCR	C11-C10-C9	-4.78	120.29	127.20
25	a	410	PL9	C7-C3-C2	-4.74	119.49	123.42
25	D	404	PL9	C7-C3-C2	-4.72	119.51	123.42
27	J	102	BCR	C20-C21-C22	-4.71	120.40	127.20
27	T	103	BCR	C28-C27-C26	-4.67	106.46	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	102	BCR	C15-C14-C13	-4.66	120.47	127.20
27	B	617	BCR	C33-C5-C6	-4.65	120.04	124.61
27	C	515	BCR	C28-C27-C26	-4.64	106.51	113.87
27	x	101	BCR	C33-C5-C6	-4.63	120.06	124.61
27	a	412	BCR	C38-C26-C25	-4.63	120.06	124.61
25	A	408	PL9	C3-C2-C1	-4.63	120.15	122.97
27	B	620	BCR	C38-C26-C25	-4.61	120.08	124.61
27	T	103	BCR	C38-C26-C25	-4.61	120.08	124.61
27	K	102	BCR	C38-C26-C25	-4.60	120.09	124.61
27	C	514	BCR	C3-C4-C5	-4.60	106.57	113.87
27	Z	101	BCR	C15-C14-C13	-4.58	120.59	127.20
27	B	620	BCR	C24-C23-C22	-4.57	119.25	126.22
25	j	101	PL9	C3-C2-C1	-4.57	120.19	122.97
28	C	518	DGD	C1D-O6D-C5D	-4.55	104.91	113.75
28	c	519	DGD	C1D-O6D-C5D	-4.55	104.91	113.75
27	b	621	BCR	C38-C26-C25	-4.54	120.15	124.61
27	J	102	BCR	C24-C23-C22	-4.52	119.33	126.22
27	K	102	BCR	C3-C4-C5	-4.51	106.71	113.87
27	c	516	BCR	C28-C27-C26	-4.51	106.71	113.87
27	b	620	BCR	C28-C27-C26	-4.50	106.73	113.87
27	T	102	BCR	C15-C14-C13	-4.48	120.73	127.20
27	T	102	BCR	C33-C5-C6	-4.48	120.21	124.61
27	b	620	BCR	C7-C8-C9	-4.47	119.40	126.22
27	B	617	BCR	C15-C14-C13	-4.47	120.75	127.20
27	A	410	BCR	C15-C14-C13	-4.46	120.75	127.20
27	D	405	BCR	C33-C5-C6	-4.42	120.26	124.61
25	J	101	PL9	C3-C2-C1	-4.42	120.28	122.97
27	j	102	BCR	C11-C10-C9	-4.41	120.83	127.20
27	T	102	BCR	C16-C17-C18	-4.40	120.84	127.20
27	A	410	BCR	C3-C4-C5	-4.39	106.91	113.87
27	f	102	BCR	C16-C17-C18	-4.35	120.91	127.20
27	B	618	BCR	C38-C26-C25	-4.34	120.34	124.61
27	B	620	BCR	C7-C8-C9	-4.31	119.65	126.22
27	C	515	BCR	C38-C26-C25	-4.30	120.38	124.61
27	j	102	BCR	C7-C8-C9	-4.30	119.66	126.22
27	C	515	BCR	C7-C8-C9	-4.29	119.67	126.22
27	A	410	BCR	C38-C26-C25	-4.28	120.40	124.61
27	J	102	BCR	C16-C17-C18	-4.26	121.04	127.20
27	C	515	BCR	C15-C14-C13	-4.22	121.11	127.20
27	b	621	BCR	C4-C5-C6	-4.22	117.41	122.78
27	B	620	BCR	C4-C5-C6	-4.21	117.42	122.78
27	b	621	BCR	C7-C8-C9	-4.21	119.80	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	617	BCR	C38-C26-C25	-4.20	120.48	124.61
27	k	102	BCR	C16-C17-C18	-4.19	121.14	127.20
27	b	621	BCR	C11-C10-C9	-4.18	121.16	127.20
27	B	617	BCR	C16-C17-C18	-4.17	121.18	127.20
27	k	102	BCR	C3-C4-C5	-4.17	107.26	113.87
27	D	405	BCR	C24-C23-C22	-4.14	119.91	126.22
27	T	102	BCR	C38-C26-C25	-4.12	120.56	124.61
27	T	102	BCR	C24-C23-C22	-4.12	119.94	126.22
27	b	620	BCR	C15-C14-C13	-4.10	121.28	127.20
27	c	516	BCR	C7-C8-C9	-4.09	119.98	126.22
27	B	617	BCR	C7-C8-C9	-4.08	119.99	126.22
27	a	412	BCR	C16-C17-C18	-4.08	121.31	127.20
27	c	515	BCR	C33-C5-C6	-4.07	120.61	124.61
27	c	514	BCR	C16-C17-C18	-4.05	121.34	127.20
27	Z	101	BCR	C24-C23-C22	-4.03	120.07	126.22
27	c	514	BCR	C11-C10-C9	-4.03	121.38	127.20
27	a	412	BCR	C15-C14-C13	-4.02	121.39	127.20
27	c	516	BCR	C15-C14-C13	-4.02	121.40	127.20
27	c	516	BCR	C16-C17-C18	-4.00	121.42	127.20
27	c	516	BCR	C33-C5-C6	-4.00	120.68	124.61
27	Z	101	BCR	C3-C4-C5	-3.99	107.53	113.87
27	B	617	BCR	C24-C23-C22	-3.99	120.14	126.22
27	B	619	BCR	C15-C14-C13	-3.97	121.46	127.20
27	K	102	BCR	C7-C8-C9	-3.97	120.16	126.22
27	b	620	BCR	C24-C23-C22	-3.96	120.17	126.22
27	Z	101	BCR	C16-C17-C18	-3.96	121.48	127.20
27	c	515	BCR	C3-C4-C5	-3.96	107.59	113.87
27	b	621	BCR	C16-C17-C18	-3.95	121.50	127.20
27	Z	101	BCR	C33-C5-C6	-3.94	120.73	124.61
27	B	620	BCR	C16-C17-C18	-3.93	121.51	127.20
27	x	101	BCR	C24-C23-C22	-3.93	120.22	126.22
27	b	621	BCR	C15-C14-C13	-3.93	121.52	127.20
27	D	405	BCR	C15-C14-C13	-3.92	121.54	127.20
27	a	412	BCR	C3-C4-C5	-3.92	107.65	113.87
25	D	404	PL9	C22-C23-C24	-3.85	119.39	127.76
27	c	514	BCR	C3-C4-C5	-3.85	107.76	113.87
27	C	515	BCR	C33-C5-C6	-3.84	120.83	124.61
27	J	102	BCR	C7-C8-C9	-3.82	120.40	126.22
28	A	411	DGD	C1D-O6D-C5D	-3.80	106.38	113.75
27	b	621	BCR	C20-C21-C22	-3.79	121.72	127.20
28	b	622	DGD	C1D-O6D-C5D	-3.77	106.42	113.75
28	B	621	DGD	C1D-O6D-C5D	-3.75	106.46	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	516	BCR	C38-C26-C25	-3.74	120.93	124.61
27	b	620	BCR	C33-C5-C6	-3.72	120.95	124.61
23	A	407	CLA	CMB-C2B-C1B	-3.71	122.22	128.36
27	D	405	BCR	C16-C17-C18	-3.69	121.87	127.20
27	c	516	BCR	C11-C10-C9	-3.69	121.87	127.20
23	B	613	CLA	CMB-C2B-C1B	-3.68	122.28	128.36
27	k	102	BCR	C20-C21-C22	-3.65	121.92	127.20
27	B	618	BCR	C4-C5-C6	-3.65	118.13	122.78
27	B	620	BCR	C15-C14-C13	-3.64	121.94	127.20
23	b	611	CLA	CMB-C2B-C1B	-3.63	122.35	128.36
27	j	102	BCR	C27-C26-C25	-3.62	118.17	122.78
27	B	619	BCR	C3-C4-C5	-3.61	108.14	113.87
23	c	508	CLA	CMB-C2B-C1B	-3.60	122.41	128.36
27	B	620	BCR	C11-C10-C9	-3.59	122.01	127.20
27	K	102	BCR	C16-C17-C18	-3.59	122.02	127.20
23	B	611	CLA	CMB-C2B-C1B	-3.58	122.44	128.36
27	b	620	BCR	C3-C4-C5	-3.57	108.19	113.87
23	B	612	CLA	CMB-C2B-C1B	-3.56	122.48	128.36
27	C	515	BCR	C3-C4-C5	-3.55	108.23	113.87
23	B	608	CLA	CMB-C2B-C1B	-3.54	122.50	128.36
27	T	103	BCR	C4-C5-C6	-3.54	118.27	122.78
27	C	514	BCR	C28-C27-C26	-3.53	108.27	113.87
27	B	620	BCR	C20-C21-C22	-3.53	122.10	127.20
25	d	404	PL9	C37-C38-C39	-3.53	120.09	127.76
27	c	514	BCR	C7-C6-C5	-3.53	113.30	121.37
23	C	508	CLA	CMB-C2B-C1B	-3.52	122.53	128.36
27	c	515	BCR	C20-C21-C22	-3.51	122.12	127.20
27	j	102	BCR	C16-C17-C18	-3.50	122.15	127.20
27	B	619	BCR	C20-C21-C22	-3.49	122.16	127.20
27	C	515	BCR	C20-C21-C22	-3.49	122.16	127.20
27	f	102	BCR	C24-C23-C22	-3.48	120.91	126.22
27	a	412	BCR	C24-C23-C22	-3.48	120.91	126.22
25	A	408	PL9	C7-C3-C2	-3.47	120.54	123.42
30	A	413	SQD	O9-S-O7	-3.47	100.83	113.48
23	b	618	CLA	CMB-C2B-C1B	-3.46	122.64	128.36
23	b	606	CLA	CMB-C2B-C1B	-3.45	122.65	128.36
27	K	102	BCR	C33-C5-C6	-3.45	121.22	124.61
25	D	404	PL9	C7-C8-C9	-3.45	120.86	126.70
30	f	103	SQD	O9-S-O7	-3.44	100.94	113.48
30	F	102	SQD	O9-S-O7	-3.43	100.97	113.48
23	b	611	CLA	O2D-CGD-O1D	-3.43	116.71	123.79
27	B	619	BCR	C33-C5-C6	-3.42	121.24	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	407	SQD	O9-S-O7	-3.42	101.03	113.48
23	B	603	CLA	CMB-C2B-C1B	-3.41	122.72	128.36
27	T	102	BCR	C20-C21-C22	-3.40	122.28	127.20
23	b	616	CLA	CMB-C2B-C1B	-3.40	122.74	128.36
27	C	514	BCR	C38-C26-C25	-3.40	121.27	124.61
30	D	409	SQD	O9-S-O7	-3.39	101.13	113.48
28	C	517	DGD	O5D-C6D-C5D	-3.38	102.95	109.08
27	c	516	BCR	C3-C4-C5	-3.38	108.50	113.87
23	a	405	CLA	CMB-C2B-C1B	-3.38	122.77	128.36
31	M	101	LMG	C1-O6-C5	-3.38	107.18	113.75
27	J	102	BCR	C27-C26-C25	-3.38	118.47	122.78
27	C	515	BCR	C11-C10-C9	-3.37	122.32	127.20
27	j	102	BCR	C33-C5-C6	-3.37	121.29	124.61
31	A	414	LMG	C1-O6-C5	-3.37	107.20	113.75
23	b	609	CLA	CMB-C2B-C1B	-3.37	122.79	128.36
27	k	102	BCR	C7-C8-C9	-3.35	121.10	126.22
27	B	617	BCR	C20-C21-C22	-3.35	122.36	127.20
27	K	102	BCR	C15-C14-C13	-3.34	122.37	127.20
23	C	507	CLA	CMB-C2B-C1B	-3.34	122.83	128.36
30	a	415	SQD	O9-S-O7	-3.34	101.31	113.48
27	T	102	BCR	C11-C10-C9	-3.34	122.38	127.20
27	C	515	BCR	C16-C17-C18	-3.33	122.39	127.20
27	b	620	BCR	C11-C10-C9	-3.32	122.39	127.20
27	b	620	BCR	C20-C21-C22	-3.32	122.40	127.20
27	B	619	BCR	C24-C23-C22	-3.32	121.16	126.22
27	B	617	BCR	C11-C10-C9	-3.31	122.41	127.20
27	H	101	BCR	C16-C17-C18	-3.31	122.42	127.20
23	b	613	CLA	CMB-C2B-C1B	-3.31	122.89	128.36
28	a	413	DGD	C1D-O6D-C5D	-3.31	107.33	113.75
27	B	619	BCR	C16-C17-C18	-3.30	122.42	127.20
23	B	606	CLA	O2D-CGD-O1D	-3.30	116.97	123.79
25	a	410	PL9	C22-C23-C24	-3.29	120.60	127.76
31	M	101	LMG	C6-C5-C4	-3.29	104.89	113.02
31	C	519	LMG	C1-O6-C5	-3.29	107.36	113.75
27	C	514	BCR	C11-C10-C9	-3.29	122.45	127.20
27	J	102	BCR	C33-C5-C6	-3.28	121.38	124.61
27	c	515	BCR	C16-C17-C18	-3.28	122.46	127.20
23	c	504	CLA	O2D-CGD-O1D	-3.28	117.02	123.79
27	c	514	BCR	C35-C13-C14	-3.28	118.06	122.90
23	b	615	CLA	CMB-C2B-C1B	-3.28	122.94	128.36
23	B	606	CLA	CMB-C2B-C1B	-3.27	122.95	128.36
23	c	507	CLA	CMB-C2B-C1B	-3.27	122.95	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	CMB-C2B-C1B	-3.27	122.96	128.36
27	f	102	BCR	C38-C26-C25	-3.26	121.40	124.61
27	x	101	BCR	C10-C11-C12	-3.26	113.20	123.13
31	D	408	LMG	C1-O6-C5	-3.26	107.42	113.75
23	B	610	CLA	CMB-C2B-C1B	-3.25	122.98	128.36
27	c	514	BCR	C28-C27-C26	-3.25	108.71	113.87
30	B	625	SQD	O9-S-O7	-3.25	101.64	113.48
23	b	617	CLA	CMB-C2B-C1B	-3.25	122.99	128.36
27	A	410	BCR	C24-C23-C22	-3.25	121.27	126.22
30	b	601	SQD	O9-S-O7	-3.25	101.66	113.48
27	H	101	BCR	C38-C26-C25	-3.24	121.42	124.61
23	B	614	CLA	CMB-C2B-C1B	-3.24	123.00	128.36
24	A	406	PHO	O2D-CGD-O1D	-3.23	117.11	123.79
31	M	102	LMG	C1-O6-C5	-3.22	107.50	113.75
27	f	102	BCR	C11-C10-C9	-3.22	122.55	127.20
27	H	101	BCR	C24-C23-C22	-3.21	121.32	126.22
27	D	405	BCR	C3-C4-C5	-3.21	108.78	113.87
27	T	102	BCR	C7-C8-C9	-3.21	121.33	126.22
27	k	102	BCR	C33-C5-C6	-3.21	121.46	124.61
23	B	616	CLA	CMB-C2B-C1B	-3.21	123.06	128.36
28	A	411	DGD	C3G-C2G-C1G	-3.20	104.58	112.07
27	x	101	BCR	C20-C21-C22	-3.19	122.58	127.20
28	c	518	DGD	O5D-C6D-C5D	-3.19	103.29	109.08
31	c	520	LMG	C1-O6-C5	-3.19	107.55	113.75
23	c	503	CLA	CMB-C2B-C1B	-3.19	123.09	128.36
25	d	404	PL9	C22-C23-C24	-3.19	120.83	127.76
23	C	506	CLA	CMB-C2B-C1B	-3.18	123.10	128.36
23	b	610	CLA	O2D-CGD-O1D	-3.18	117.22	123.79
27	a	412	BCR	C11-C10-C9	-3.18	122.61	127.20
23	c	512	CLA	O2D-CGD-O1D	-3.17	117.24	123.79
23	C	504	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
23	a	409	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
24	A	406	PHO	CBD-CHA-C4D	-3.16	104.92	108.46
23	b	609	CLA	O2D-CGD-O1D	-3.16	117.26	123.79
23	c	512	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
27	x	101	BCR	C15-C14-C13	-3.15	122.64	127.20
27	C	514	BCR	C7-C6-C5	-3.13	114.21	121.37
27	C	514	BCR	C20-C21-C22	-3.12	122.69	127.20
30	a	401	SQD	O9-S-O7	-3.12	102.13	113.48
23	b	614	CLA	CMB-C2B-C1B	-3.12	123.21	128.36
25	A	408	PL9	C22-C23-C24	-3.11	120.99	127.76
23	c	504	CLA	CMB-C2B-C1B	-3.11	123.22	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	CMB-C2B-C1B	-3.11	123.22	128.36
25	d	404	PL9	C7-C8-C9	-3.10	121.44	126.70
23	B	615	CLA	CMB-C2B-C1B	-3.10	123.24	128.36
23	D	403	CLA	CMB-C2B-C1B	-3.09	123.25	128.36
27	b	620	BCR	C16-C17-C18	-3.09	122.73	127.20
27	Z	101	BCR	C20-C21-C22	-3.09	122.73	127.20
27	B	619	BCR	C11-C10-C9	-3.07	122.76	127.20
28	a	413	DGD	C3G-C2G-C1G	-3.07	104.89	112.07
23	B	602	CLA	CMB-C2B-C1B	-3.07	123.29	128.36
23	b	619	CLA	CMB-C2B-C1B	-3.07	123.29	128.36
23	C	502	CLA	CMB-C2B-C1B	-3.06	123.30	128.36
23	b	614	CLA	O2D-CGD-O1D	-3.06	117.48	123.79
23	B	609	CLA	CMB-C2B-C1B	-3.06	123.31	128.36
31	A	418	LMG	C6-C5-C4	-3.05	105.48	113.02
23	B	607	CLA	O2D-CGD-O1D	-3.05	117.49	123.79
27	B	617	BCR	C3-C4-C5	-3.04	109.05	113.87
30	A	417	SQD	O9-S-O7	-3.04	102.41	113.48
23	a	404	CLA	CMB-C2B-C1B	-3.04	123.34	128.36
31	d	406	LMG	C1-O6-C5	-3.03	107.86	113.75
31	b	623	LMG	O4-C4-C3	-3.02	103.53	110.34
23	C	506	CLA	O2D-CGD-O1D	-3.02	117.56	123.79
27	K	102	BCR	C24-C23-C22	-3.02	121.62	126.22
27	a	412	BCR	C20-C21-C22	-3.02	122.84	127.20
31	M	102	LMG	C6-C5-C4	-3.01	105.58	113.02
23	B	605	CLA	CMB-C2B-C1B	-3.01	123.38	128.36
23	b	604	CLA	O2D-CGD-O1D	-3.00	117.59	123.79
23	d	402	CLA	CMB-C2B-C1B	-3.00	123.40	128.36
25	a	410	PL9	C12-C13-C14	-3.00	121.24	127.76
23	C	510	CLA	O2D-CGD-O1D	-2.99	117.62	123.79
23	A	403	CLA	CMB-C2B-C1B	-2.99	123.42	128.36
23	c	503	CLA	O2D-CGD-O1D	-2.99	117.62	123.79
23	D	401	CLA	CMB-C2B-C1B	-2.99	123.42	128.36
23	b	605	CLA	CMB-C2B-C1B	-2.98	123.43	128.36
23	B	607	CLA	CMB-C2B-C1B	-2.98	123.44	128.36
27	C	514	BCR	C34-C9-C10	-2.98	118.50	122.90
23	C	512	CLA	CMB-C2B-C1B	-2.98	123.44	128.36
25	D	404	PL9	C37-C38-C39	-2.97	121.30	127.76
27	B	619	BCR	C7-C8-C9	-2.97	121.69	126.22
25	D	404	PL9	C12-C13-C14	-2.97	121.31	127.76
23	b	610	CLA	CMB-C2B-C1B	-2.97	123.46	128.36
27	C	514	BCR	C35-C13-C14	-2.96	118.52	122.90
23	C	509	CLA	CMB-C2B-C1B	-2.96	123.47	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	514	BCR	C24-C23-C22	-2.96	121.70	126.22
31	k	103	LMG	C1-O6-C5	-2.96	108.00	113.75
23	d	403	CLA	CMB-C2B-C1B	-2.96	123.47	128.36
23	a	406	CLA	O2D-CGD-O1D	-2.96	117.68	123.79
27	c	514	BCR	C34-C9-C10	-2.95	118.54	122.90
27	D	405	BCR	C27-C26-C25	-2.94	119.04	122.78
27	Z	101	BCR	C11-C10-C9	-2.93	122.96	127.20
31	a	416	LMG	C1-O6-C5	-2.92	108.07	113.75
28	a	413	DGD	C4D-C3D-C2D	-2.91	105.36	110.79
27	C	514	BCR	C16-C17-C18	-2.91	122.99	127.20
23	C	513	CLA	CMB-C2B-C1B	-2.90	123.56	128.36
27	Z	101	BCR	C28-C27-C26	-2.90	109.26	113.87
31	a	402	LMG	C6-C5-C4	-2.90	105.85	113.02
23	B	614	CLA	O2D-CGD-O1D	-2.90	117.80	123.79
23	c	506	CLA	O2D-CGD-O1D	-2.90	117.81	123.79
23	b	616	CLA	O2D-CGD-O1D	-2.89	117.82	123.79
23	A	404	CLA	CMB-C2B-C1B	-2.89	123.59	128.36
23	b	608	CLA	CMB-C2B-C1B	-2.88	123.59	128.36
27	D	405	BCR	C38-C26-C25	-2.88	121.77	124.61
28	c	517	DGD	C1D-O6D-C5D	-2.87	108.17	113.75
23	C	503	CLA	O2D-CGD-O1D	-2.87	117.86	123.79
23	a	406	CLA	CMB-C2B-C1B	-2.87	123.62	128.36
31	b	623	LMG	C1-O6-C5	-2.87	108.18	113.75
24	D	402	PHO	CBD-CHA-C4D	-2.87	105.25	108.46
23	c	501	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
25	J	101	PL9	C12-C13-C14	-2.86	121.54	127.76
23	C	503	CLA	CMB-C2B-C1B	-2.86	123.63	128.36
25	D	404	PL9	C42-C43-C44	-2.85	121.56	127.76
27	B	619	BCR	C27-C26-C25	-2.85	119.15	122.78
23	b	619	CLA	O2D-CGD-O1D	-2.85	117.90	123.79
23	C	511	CLA	O2D-CGD-O1D	-2.84	117.92	123.79
23	c	511	CLA	CMB-C2B-C1B	-2.84	123.67	128.36
31	b	624	LMG	C1-O6-C5	-2.84	108.24	113.75
23	b	607	CLA	CMB-C2B-C1B	-2.83	123.68	128.36
23	c	509	CLA	CMB-C2B-C1B	-2.83	123.69	128.36
23	c	505	CLA	O2D-CGD-O1D	-2.82	117.96	123.79
23	b	612	CLA	CMB-C2B-C1B	-2.82	123.70	128.36
23	c	513	CLA	CMB-C2B-C1B	-2.81	123.71	128.36
24	a	408	PHO	O2D-CGD-O1D	-2.81	118.00	123.79
27	c	514	BCR	C20-C21-C22	-2.81	123.14	127.20
23	c	501	CLA	CMB-C2B-C1B	-2.80	123.73	128.36
27	c	514	BCR	C38-C26-C25	-2.80	121.86	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405	CLA	CMB-C2B-C1B	-2.79	123.74	128.36
23	C	511	CLA	CMB-C2B-C1B	-2.79	123.74	128.36
27	c	515	BCR	C38-C26-C25	-2.79	121.87	124.61
23	b	613	CLA	O2D-CGD-O1D	-2.79	118.04	123.79
23	b	606	CLA	O2D-CGD-O1D	-2.79	118.04	123.79
24	a	407	PHO	O2D-CGD-O1D	-2.78	118.04	123.79
31	d	406	LMG	C1-C2-C3	-2.78	104.48	109.97
27	c	516	BCR	C20-C21-C22	-2.78	123.18	127.20
31	C	520	LMG	C1-O6-C5	-2.78	108.34	113.75
23	C	510	CLA	CMB-C2B-C1B	-2.78	123.76	128.36
23	C	502	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
25	D	404	PL9	C45-C44-C43	-2.78	118.04	123.50
31	A	418	LMG	C1-O6-C5	-2.78	108.36	113.75
31	D	406	LMG	O8-C28-O10	-2.78	116.33	123.49
23	C	505	CLA	O2D-CGD-O1D	-2.77	118.06	123.79
25	d	404	PL9	C32-C33-C34	-2.77	121.73	127.76
27	x	101	BCR	C3-C4-C5	-2.77	109.47	113.87
27	T	102	BCR	C3-C4-C5	-2.77	109.47	113.87
27	b	620	BCR	C27-C26-C25	-2.77	119.26	122.78
24	D	402	PHO	O2D-CGD-O1D	-2.76	118.08	123.79
23	B	605	CLA	O2D-CGD-O1D	-2.76	118.09	123.79
25	j	101	PL9	C12-C13-C14	-2.76	121.76	127.76
27	D	405	BCR	C16-C15-C14	-2.76	117.29	123.39
27	c	515	BCR	C24-C23-C22	-2.75	122.02	126.22
27	K	102	BCR	C11-C10-C9	-2.75	123.22	127.20
27	x	101	BCR	C38-C26-C25	-2.75	121.91	124.61
27	H	101	BCR	C15-C14-C13	-2.74	123.23	127.20
23	B	601	CLA	CMB-C2B-C1B	-2.74	123.83	128.36
23	D	401	CLA	O2D-CGD-O1D	-2.74	118.13	123.79
34	f	101	HEM	CAA-C2A-C1A	-2.74	124.04	127.01
23	B	611	CLA	O2D-CGD-O1D	-2.73	118.14	123.79
23	D	403	CLA	O2D-CGD-O1D	-2.73	118.14	123.79
31	a	402	LMG	C1-O6-C5	-2.73	108.45	113.75
23	B	604	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
28	B	626	DGD	C6D-C5D-C4D	-2.72	105.86	112.03
25	D	404	PL9	C32-C33-C34	-2.72	121.85	127.76
27	H	101	BCR	C10-C11-C12	-2.72	114.85	123.13
23	B	604	CLA	CMB-C2B-C1B	-2.71	123.87	128.36
23	B	601	CLA	O2D-CGD-O1D	-2.71	118.19	123.79
27	j	102	BCR	C39-C30-C25	-2.71	106.05	110.30
23	c	502	CLA	CMB-C2B-C1B	-2.71	123.88	128.36
27	B	618	BCR	C21-C20-C19	-2.71	114.87	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	502	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
31	D	408	LMG	C1-C2-C3	-2.70	104.65	109.97
23	c	511	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
23	b	604	CLA	CMB-C2B-C1B	-2.69	123.91	128.36
25	j	101	PL9	C22-C23-C24	-2.69	121.91	127.76
28	A	411	DGD	O4D-C4D-C5D	-2.69	102.11	109.24
27	K	102	BCR	C20-C21-C22	-2.69	123.31	127.20
27	A	410	BCR	C11-C10-C9	-2.68	123.32	127.20
31	A	418	LMG	O3-C3-C4	-2.68	104.31	110.34
25	a	410	PL9	C32-C33-C34	-2.67	121.96	127.76
27	f	102	BCR	C27-C26-C25	-2.67	119.38	122.78
23	d	402	CLA	O2D-CGD-O1D	-2.66	118.29	123.79
27	T	103	BCR	C23-C24-C25	-2.66	119.32	127.32
23	B	615	CLA	O2D-CGD-O1D	-2.66	118.29	123.79
23	c	509	CLA	O2D-CGD-O1D	-2.66	118.30	123.79
27	H	101	BCR	C20-C21-C22	-2.64	123.38	127.20
27	H	101	BCR	C3-C4-C5	-2.64	109.68	113.87
23	A	404	CLA	O2D-CGD-O1D	-2.64	118.34	123.79
23	a	409	CLA	O2D-CGD-O1D	-2.64	118.34	123.79
27	x	101	BCR	C16-C17-C18	-2.64	123.39	127.20
27	A	410	BCR	C20-C21-C22	-2.63	123.40	127.20
23	C	507	CLA	O2D-CGD-O1D	-2.63	118.36	123.79
23	C	501	CLA	O2D-CGD-O1D	-2.62	118.38	123.79
28	c	519	DGD	C4D-C3D-C2D	-2.62	105.91	110.79
23	c	508	CLA	O2D-CGD-O1D	-2.62	118.39	123.79
27	T	103	BCR	C21-C20-C19	-2.61	115.16	123.13
27	Z	101	BCR	C38-C26-C25	-2.61	122.04	124.61
31	d	405	LMG	O8-C28-O10	-2.61	116.75	123.49
23	b	617	CLA	O2D-CGD-O1D	-2.61	118.40	123.79
23	C	505	CLA	CMB-C2B-C1B	-2.61	124.05	128.36
25	d	404	PL9	C12-C13-C14	-2.60	122.10	127.76
23	B	602	CLA	O2D-CGD-O1D	-2.60	118.43	123.79
27	D	405	BCR	C23-C24-C25	-2.60	119.52	127.32
23	c	513	CLA	O2D-CGD-O1D	-2.60	118.43	123.79
23	c	507	CLA	O2D-CGD-O1D	-2.59	118.44	123.79
27	J	102	BCR	C35-C13-C14	-2.59	119.08	122.90
28	C	518	DGD	C4D-C3D-C2D	-2.59	105.96	110.79
23	c	510	CLA	O2D-CGD-O1D	-2.59	118.45	123.79
31	C	520	LMG	C6-C5-C4	-2.58	106.64	113.02
27	f	102	BCR	C3-C4-C5	-2.58	109.77	113.87
31	I	101	LMG	C1-O6-C5	-2.58	108.75	113.75
23	B	610	CLA	O2D-CGD-O1D	-2.57	118.48	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	612	CLA	O2D-CGD-O1D	-2.56	118.50	123.79
33	D	411	LMT	C1B-O1B-C4'	-2.55	111.33	118.01
27	H	101	BCR	C8-C7-C6	-2.55	119.66	127.32
27	J	102	BCR	C1-C6-C5	-2.55	118.92	122.66
27	D	405	BCR	C21-C20-C19	-2.54	115.39	123.13
28	a	413	DGD	O4D-C4D-C5D	-2.54	102.52	109.24
28	c	518	DGD	C4D-C3D-C2D	-2.54	106.06	110.79
23	a	404	CLA	O2D-CGD-O1D	-2.53	118.56	123.79
23	b	618	CLA	O2D-CGD-O1D	-2.53	118.57	123.79
31	B	622	LMG	C1-O6-C5	-2.52	108.85	113.75
27	c	515	BCR	C7-C8-C9	-2.52	122.38	126.22
23	B	616	CLA	O2D-CGD-O1D	-2.52	118.59	123.79
27	a	412	BCR	C28-C27-C26	-2.52	109.88	113.87
23	B	609	CLA	O2D-CGD-O1D	-2.51	118.60	123.79
23	d	403	CLA	O2D-CGD-O1D	-2.51	118.61	123.79
25	A	408	PL9	C12-C13-C14	-2.51	122.32	127.76
25	A	408	PL9	C32-C33-C34	-2.49	122.35	127.76
27	T	102	BCR	C28-C27-C26	-2.49	109.92	113.87
27	T	102	BCR	C36-C18-C17	-2.49	119.23	122.90
27	c	514	BCR	C24-C23-C22	-2.49	122.43	126.22
28	a	413	DGD	C6E-C5E-C4E	-2.48	106.89	113.02
27	b	621	BCR	C28-C27-C26	-2.48	109.93	113.87
27	B	617	BCR	C23-C24-C25	-2.48	119.88	127.32
23	C	513	CLA	O2D-CGD-O1D	-2.48	118.68	123.79
25	J	101	PL9	C22-C23-C24	-2.47	122.38	127.76
31	i	101	LMG	C1-O6-C5	-2.47	108.94	113.75
23	C	506	CLA	CAA-CBA-CGA	-2.47	106.08	113.32
27	Z	101	BCR	C8-C7-C6	-2.47	119.89	127.32
27	c	515	BCR	C28-C27-C26	-2.46	109.96	113.87
27	f	102	BCR	C16-C15-C14	-2.46	117.95	123.39
25	d	404	PL9	C36-C34-C33	-2.44	116.41	121.05
27	C	514	BCR	C39-C30-C25	-2.44	106.47	110.30
23	b	618	CLA	O2A-CGA-O1A	-2.44	117.19	123.49
27	c	515	BCR	C8-C7-C6	-2.43	120.01	127.32
28	A	411	DGD	C4D-C3D-C2D	-2.43	106.25	110.79
23	A	404	CLA	O2A-CGA-O1A	-2.43	117.23	123.49
34	F	101	HEM	CAA-C2A-C1A	-2.43	124.37	127.01
23	A	405	CLA	O2D-CGD-O1D	-2.42	118.78	123.79
27	J	102	BCR	C39-C30-C25	-2.42	106.50	110.30
23	a	404	CLA	O2A-CGA-O1A	-2.42	117.25	123.49
31	D	407	LMG	C1-O6-C5	-2.42	109.06	113.75
25	D	404	PL9	C27-C28-C29	-2.41	122.52	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	O2D-CGD-O1D	-2.41	118.82	123.79
27	T	103	BCR	C24-C23-C22	-2.41	122.55	126.22
23	b	608	CLA	O2D-CGD-O1D	-2.41	118.82	123.79
27	B	618	BCR	C23-C24-C25	-2.40	120.10	127.32
27	B	620	BCR	C32-C1-C6	-2.40	106.53	110.30
23	C	512	CLA	O2A-CGA-O1A	-2.40	117.30	123.49
25	d	404	PL9	C45-C44-C43	-2.40	118.80	123.50
34	v	201	HEM	CAA-CBA-CGA	-2.39	108.36	112.75
31	k	103	LMG	O8-C28-O10	-2.39	117.31	123.49
27	j	102	BCR	C11-C12-C13	-2.38	119.31	126.32
31	C	519	LMG	C6-C5-C4	-2.38	107.14	113.02
34	F	101	HEM	CBA-CAA-C2A	-2.38	108.27	112.53
31	M	101	LMG	O8-C9-C8	-2.38	102.30	108.69
23	C	508	CLA	O2D-CGD-O1D	-2.37	118.89	123.79
27	j	102	BCR	C37-C22-C21	-2.37	119.40	122.90
27	j	102	BCR	C1-C6-C5	-2.37	119.18	122.66
28	C	517	DGD	C1D-O6D-C5D	-2.37	109.15	113.75
28	C	516	DGD	C6E-C5E-C4E	-2.36	107.19	113.02
28	A	411	DGD	C6D-C5D-C4D	-2.36	106.67	112.03
23	C	509	CLA	O2D-CGD-O1D	-2.36	118.92	123.79
23	b	607	CLA	O2D-CGD-O1D	-2.36	118.92	123.79
27	k	102	BCR	C24-C23-C22	-2.35	122.63	126.22
23	C	504	CLA	O2D-CGD-O1D	-2.35	118.93	123.79
24	A	406	PHO	C2B-C1B-NB	-2.35	106.20	109.73
23	c	512	CLA	O2A-CGA-O1A	-2.35	117.44	123.49
23	b	605	CLA	O2D-CGD-O1D	-2.34	118.96	123.79
27	A	410	BCR	C32-C1-C6	-2.34	106.64	110.30
27	B	617	BCR	C28-C27-C26	-2.34	110.16	113.87
25	D	404	PL9	C36-C34-C33	-2.34	116.62	121.05
25	A	408	PL9	C11-C9-C8	-2.33	116.62	121.05
23	a	409	CLA	O2A-CGA-O1A	-2.33	117.48	123.49
27	f	102	BCR	C21-C20-C19	-2.32	116.06	123.13
31	D	408	LMG	O8-C28-O10	-2.32	117.51	123.49
31	E	101	LMG	O9-C10-C11	-2.32	114.45	123.72
33	b	625	LMT	C1B-O1B-C4'	-2.32	111.96	118.01
27	J	102	BCR	C36-C18-C17	-2.32	119.48	122.90
27	T	103	BCR	C33-C5-C6	-2.31	122.34	124.61
23	B	605	CLA	O2A-CGA-O1A	-2.31	117.54	123.49
31	c	520	LMG	C6-C5-C4	-2.30	107.33	113.02
33	B	624	LMT	C1B-O1B-C4'	-2.30	111.99	118.01
23	B	612	CLA	O2D-CGD-O1D	-2.30	119.04	123.79
27	J	102	BCR	C11-C12-C13	-2.29	119.57	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	403	CLA	O2D-CGD-O1D	-2.29	119.06	123.79
27	C	515	BCR	C23-C24-C25	-2.29	120.44	127.32
31	C	519	LMG	O8-C28-O10	-2.28	117.60	123.49
34	f	101	HEM	CBA-CAA-C2A	-2.28	108.44	112.53
27	Z	101	BCR	C7-C8-C9	-2.28	122.75	126.22
23	B	609	CLA	CAA-CBA-CGA	-2.28	106.66	113.32
27	C	514	BCR	C23-C24-C25	-2.27	120.49	127.32
27	c	516	BCR	C23-C24-C25	-2.27	120.50	127.32
31	a	402	LMG	O3-C3-C4	-2.27	105.24	110.34
27	b	621	BCR	C40-C30-C25	-2.26	106.75	110.30
30	A	417	SQD	O2-C2-C3	-2.26	105.25	110.34
23	B	613	CLA	O2D-CGD-O1D	-2.26	119.13	123.79
23	b	607	CLA	CAA-CBA-CGA	-2.26	106.71	113.32
27	K	102	BCR	C32-C1-C6	-2.26	106.77	110.30
25	d	404	PL9	C27-C28-C29	-2.26	122.86	127.76
24	a	407	PHO	CBD-CHA-C4D	-2.25	105.94	108.46
31	i	101	LMG	O8-C28-O10	-2.25	117.67	123.49
28	c	517	DGD	C6E-C5E-C4E	-2.25	107.46	113.02
25	a	410	PL9	C17-C18-C19	-2.25	122.87	127.76
31	e	101	LMG	C1-O6-C5	-2.25	109.38	113.75
28	C	516	DGD	C1D-O6D-C5D	-2.25	109.38	113.75
27	B	617	BCR	C36-C18-C17	-2.25	119.58	122.90
27	J	102	BCR	C37-C22-C21	-2.25	119.58	122.90
27	f	102	BCR	C23-C24-C25	-2.24	120.58	127.32
23	C	511	CLA	O2A-CGA-O1A	-2.24	117.71	123.49
31	I	101	LMG	O3-C3-C4	-2.24	105.30	110.34
25	A	408	PL9	C26-C24-C23	-2.24	116.81	121.05
24	D	402	PHO	C2B-C1B-NB	-2.23	106.38	109.73
23	C	507	CLA	O2A-CGA-O1A	-2.23	117.73	123.49
27	C	515	BCR	C21-C20-C19	-2.23	116.33	123.13
31	I	101	LMG	C6-C5-C4	-2.23	107.52	113.02
27	k	102	BCR	C37-C22-C21	-2.23	119.61	122.90
27	j	102	BCR	C35-C13-C14	-2.23	119.61	122.90
23	B	603	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
23	d	402	CLA	O2A-CGA-O1A	-2.22	117.76	123.49
23	B	604	CLA	O2A-CGA-O1A	-2.22	117.76	123.49
23	C	501	CLA	CMB-C2B-C1B	-2.22	124.69	128.36
28	c	518	DGD	C1D-O6D-C5D	-2.21	109.45	113.75
27	Z	101	BCR	C23-C24-C25	-2.21	120.67	127.32
23	b	611	CLA	O2A-CGA-O1A	-2.21	117.79	123.49
27	Z	101	BCR	C15-C16-C17	-2.21	118.51	123.39
23	B	608	CLA	O2D-CGD-O1D	-2.21	119.23	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	k	103	LMG	C6-C5-C4	-2.21	107.57	113.02
23	c	505	CLA	CMB-C2B-C1B	-2.21	124.72	128.36
27	B	620	BCR	C40-C30-C25	-2.20	106.85	110.30
27	T	102	BCR	C23-C24-C25	-2.20	120.71	127.32
23	b	607	CLA	O2A-CGA-O1A	-2.19	117.84	123.49
27	H	101	BCR	C16-C15-C14	-2.19	118.56	123.39
31	E	101	LMG	C1-O6-C5	-2.19	109.50	113.75
23	a	405	CLA	O2D-CGD-O1D	-2.18	119.28	123.79
31	C	520	LMG	O3-C3-C4	-2.18	105.42	110.34
34	f	101	HEM	C3B-C4B-NB	-2.18	107.46	111.63
31	M	101	LMG	O4-C4-C3	-2.18	105.42	110.34
31	c	520	LMG	O3-C3-C4	-2.18	105.43	110.34
28	c	519	DGD	O1G-C1A-O1A	-2.18	117.86	123.49
27	A	410	BCR	C34-C9-C10	-2.18	119.68	122.90
27	x	101	BCR	C8-C7-C6	-2.18	120.77	127.32
23	D	401	CLA	O2A-CGA-O1A	-2.18	117.87	123.49
24	a	408	PHO	CMB-C2B-C1B	-2.18	121.51	125.06
27	Z	101	BCR	C10-C11-C12	-2.17	116.50	123.13
31	A	418	LMG	O8-C28-O10	-2.17	117.88	123.49
25	A	408	PL9	C17-C18-C19	-2.17	123.05	127.76
27	T	103	BCR	C15-C16-C17	-2.17	118.60	123.39
27	c	516	BCR	C15-C16-C17	-2.16	118.61	123.39
27	T	103	BCR	C16-C17-C18	-2.16	124.07	127.20
27	C	515	BCR	C15-C16-C17	-2.16	118.61	123.39
25	a	410	PL9	C7-C8-C9	-2.16	123.04	126.70
23	B	601	CLA	O2A-CGA-O1A	-2.16	117.92	123.49
24	A	406	PHO	CMB-C2B-C1B	-2.16	121.55	125.06
33	M	103	LMT	C1B-O1B-C4'	-2.16	112.37	118.01
27	a	412	BCR	C23-C24-C25	-2.15	120.85	127.32
27	b	621	BCR	C34-C9-C10	-2.15	119.72	122.90
27	j	102	BCR	C38-C26-C25	-2.14	122.50	124.61
25	D	404	PL9	C17-C18-C19	-2.14	123.12	127.76
27	a	412	BCR	C8-C7-C6	-2.13	120.92	127.32
27	b	621	BCR	C33-C5-C6	-2.13	122.51	124.61
23	C	513	CLA	O2A-CGA-O1A	-2.13	118.01	123.49
27	k	102	BCR	C15-C16-C17	-2.12	118.69	123.39
27	f	102	BCR	C36-C18-C17	-2.12	119.77	122.90
31	e	101	LMG	O7-C10-O9	-2.12	117.99	123.67
27	B	620	BCR	C8-C7-C6	-2.11	120.97	127.32
23	B	612	CLA	CAA-CBA-CGA	-2.11	107.13	113.32
28	C	518	DGD	O1G-C1A-O1A	-2.11	118.04	123.49
28	A	411	DGD	C6E-C5E-C4E	-2.11	107.81	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	m	101	LMT	C1B-O1B-C4'	-2.11	112.50	118.01
27	T	103	BCR	C32-C1-C6	-2.11	107.00	110.30
24	a	408	PHO	CBD-CHA-C4D	-2.10	106.11	108.46
23	b	619	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
27	c	516	BCR	C21-C20-C19	-2.10	116.73	123.13
27	H	101	BCR	C21-C20-C19	-2.10	116.73	123.13
23	a	405	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
28	b	602	DGD	C6D-C5D-C4D	-2.10	107.27	112.03
27	B	620	BCR	C33-C5-C6	-2.10	122.55	124.61
31	D	407	LMG	O4-C4-C3	-2.10	105.62	110.34
25	d	404	PL9	C26-C24-C23	-2.10	117.08	121.05
24	A	406	PHO	C2A-C1A-NA	-2.09	109.40	112.08
31	A	414	LMG	O8-C28-O10	-2.09	118.09	123.49
24	D	402	PHO	O2A-CGA-O1A	-2.09	118.10	123.49
23	A	405	CLA	O2A-CGA-O1A	-2.09	118.10	123.49
27	a	412	BCR	C21-C20-C19	-2.09	116.77	123.13
31	b	624	LMG	O8-C28-O10	-2.08	118.11	123.49
25	d	404	PL9	C17-C18-C19	-2.08	123.23	127.76
31	e	101	LMG	O9-C10-C11	-2.08	115.39	123.72
27	A	410	BCR	C23-C24-C25	-2.08	121.06	127.32
31	M	102	LMG	O4-C4-C3	-2.08	105.65	110.34
27	b	620	BCR	C39-C30-C25	-2.08	107.05	110.30
25	a	410	PL9	C11-C9-C8	-2.07	117.12	121.05
27	b	621	BCR	C32-C1-C6	-2.07	107.05	110.30
23	c	501	CLA	OBD-CAD-CBD	-2.07	122.81	125.94
23	D	403	CLA	O2A-CGA-O1A	-2.07	118.15	123.49
33	x	102	LMT	C1B-O1B-C4'	-2.07	112.61	118.01
23	b	610	CLA	O2A-CGA-O1A	-2.06	118.17	123.49
27	B	617	BCR	C8-C7-C6	-2.06	121.12	127.32
23	c	513	CLA	O2A-CGA-O1A	-2.06	118.17	123.49
27	B	620	BCR	C28-C27-C26	-2.05	110.61	113.87
24	a	407	PHO	O2A-CGA-O1A	-2.05	118.20	123.49
27	k	102	BCR	C35-C13-C14	-2.05	119.87	122.90
23	B	610	CLA	OBD-CAD-CBD	-2.05	122.84	125.94
31	M	101	LMG	O3-C3-C4	-2.05	105.73	110.34
28	d	408	DGD	O2G-C1B-O1B	-2.05	118.18	123.67
23	B	613	CLA	O2A-CGA-O1A	-2.05	118.21	123.49
27	x	101	BCR	C40-C30-C25	-2.04	107.10	110.30
23	a	406	CLA	OBD-CAD-CBD	-2.04	122.85	125.94
33	b	626	LMT	C1B-O1B-C4'	-2.04	112.67	118.01
27	D	405	BCR	C34-C9-C10	-2.04	119.89	122.90
28	B	621	DGD	C4D-C3D-C2D	-2.04	106.98	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	x	101	BCR	C28-C27-C26	-2.04	110.63	113.87
27	A	410	BCR	C21-C20-C19	-2.04	116.91	123.13
27	a	412	BCR	C40-C30-C25	-2.04	107.10	110.30
23	c	507	CLA	O2A-CGA-O1A	-2.04	118.23	123.49
27	B	619	BCR	C23-C24-C25	-2.04	121.19	127.32
31	d	406	LMG	O8-C28-O10	-2.04	118.23	123.49
24	a	407	PHO	C2B-C1B-NB	-2.04	106.67	109.73
31	B	622	LMG	C6-C5-C4	-2.04	107.99	113.02
34	F	101	HEM	C3B-C4B-NB	-2.04	107.73	111.63
27	B	619	BCR	C15-C16-C17	-2.04	118.89	123.39
25	j	101	PL9	C21-C19-C18	-2.04	117.19	121.05
23	b	615	CLA	O2D-CGD-O1D	-2.04	119.59	123.79
31	i	101	LMG	O3-C3-C4	-2.03	105.77	110.34
31	B	622	LMG	O8-C28-O10	-2.03	118.26	123.49
31	b	623	LMG	O3-C3-C4	-2.03	105.78	110.34
31	B	622	LMG	O4-C4-C3	-2.02	105.78	110.34
31	D	406	LMG	C6-C5-C4	-2.02	108.03	113.02
28	B	626	DGD	O4D-C4D-C5D	-2.02	103.88	109.24
27	k	102	BCR	C28-C27-C26	-2.02	110.67	113.87
23	d	403	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
23	B	607	CLA	O2A-CGA-O1A	-2.01	118.29	123.49
27	a	412	BCR	C34-C9-C10	-2.01	119.93	122.90
27	b	620	BCR	C38-C26-C25	-2.01	122.63	124.61
28	C	517	DGD	O4D-C4D-C5D	-2.01	103.91	109.24
31	D	407	LMG	O8-C28-O10	-2.01	118.31	123.49
28	D	410	DGD	O2G-C1B-O1B	-2.01	118.28	123.67
27	D	405	BCR	C39-C30-C25	-2.01	107.16	110.30
27	a	412	BCR	C16-C15-C14	-2.00	118.96	123.39
27	B	618	BCR	C31-C1-C6	-2.00	107.16	110.30
23	B	616	CLA	OBD-CAD-CBD	-2.00	122.92	125.94
23	a	406	CLA	O2A-CGA-O1A	-2.00	118.32	123.49
31	M	102	LMG	O3-C3-C4	-2.00	105.83	110.34
23	c	508	CLA	O2D-CGD-CBD	2.00	114.05	111.30
31	D	408	LMG	O2-C2-C1	2.00	114.41	110.02
23	c	501	CLA	C1D-CHD-C4C	2.01	125.64	122.60
34	F	101	HEM	C2D-C3D-C4D	2.01	104.91	101.50
27	H	101	BCR	C36-C18-C19	2.01	121.45	118.10
23	A	404	CLA	O2D-CGD-CBD	2.01	114.06	111.30
29	a	414	LHG	O8-C23-C24	2.02	118.05	111.90
23	c	504	CLA	C1D-CHD-C4C	2.02	125.66	122.60
23	b	607	CLA	CMD-C2D-C3D	2.02	129.04	125.09
28	c	517	DGD	O3D-C3D-C4D	2.02	114.88	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	413	DGD	O5D-C1E-C2E	2.02	110.59	108.04
30	b	601	SQD	C1-O5-C5	2.02	117.67	113.75
23	D	401	CLA	CMD-C2D-C3D	2.02	129.05	125.09
23	B	615	CLA	O2D-CGD-CBD	2.03	114.08	111.30
24	a	407	PHO	CBD-CHA-C1A	2.03	131.14	126.36
23	D	401	CLA	CHB-C4A-NA	2.03	127.32	124.51
28	C	518	DGD	O2G-C1B-C2B	2.03	115.94	111.53
25	D	404	PL9	C51-C49-C50	2.03	119.64	114.64
33	B	623	LMT	O1'-C1'-C2'	2.04	110.61	108.04
27	c	516	BCR	C2-C1-C6	2.04	113.59	110.36
23	a	406	CLA	O1D-CGD-CBD	2.04	127.54	124.62
24	D	402	PHO	CBD-CHA-C1A	2.04	131.16	126.36
23	a	409	CLA	O1D-CGD-CBD	2.04	127.54	124.62
23	a	404	CLA	O1D-CGD-CBD	2.04	127.54	124.62
23	b	608	CLA	CMD-C2D-C3D	2.04	129.08	125.09
23	b	619	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	b	604	CLA	CMB-C2B-C3B	2.05	129.09	125.09
31	k	103	LMG	C7-O1-C1	2.05	118.12	113.82
24	a	408	PHO	C1B-NB-C4B	2.05	110.56	106.51
23	a	409	CLA	O2D-CGD-CBD	2.05	114.11	111.30
27	B	619	BCR	C33-C5-C4	2.05	117.31	113.43
27	c	516	BCR	C33-C5-C4	2.05	117.31	113.43
31	i	101	LMG	C8-O7-C10	2.05	122.81	117.89
27	b	620	BCR	C2-C1-C6	2.05	113.61	110.36
23	c	508	CLA	O1D-CGD-CBD	2.05	127.57	124.62
23	c	509	CLA	CMD-C2D-C3D	2.05	129.11	125.09
23	B	610	CLA	CMD-C2D-C3D	2.06	129.11	125.09
31	c	520	LMG	C3-C4-C5	2.06	113.79	110.20
27	c	514	BCR	C29-C30-C25	2.06	113.63	110.36
23	B	616	CLA	CMD-C2D-C3D	2.06	129.13	125.09
23	C	511	CLA	O2D-CGD-CBD	2.07	114.13	111.30
23	B	613	CLA	O1D-CGD-CBD	2.07	127.58	124.62
23	c	505	CLA	CMD-C2D-C3D	2.07	129.14	125.09
23	C	508	CLA	C1D-CHD-C4C	2.07	125.73	122.60
23	B	602	CLA	O1D-CGD-CBD	2.07	127.60	124.62
23	B	606	CLA	CMD-C2D-C3D	2.08	129.15	125.09
23	A	404	CLA	O1D-CGD-CBD	2.08	127.60	124.62
23	B	612	CLA	CMD-C2D-C3D	2.08	129.16	125.09
23	b	618	CLA	CMD-C2D-C3D	2.08	129.16	125.09
23	B	601	CLA	O2D-CGD-CBD	2.09	114.16	111.30
30	A	413	SQD	O5-C1-C2	2.09	114.56	110.28
23	C	504	CLA	O2D-CGD-CBD	2.09	114.17	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	404	PL9	C10-C9-C11	2.09	118.60	115.41
23	c	507	CLA	O1D-CGD-CBD	2.09	127.62	124.62
31	b	623	LMG	C4-C3-C2	2.09	114.70	110.79
23	B	615	CLA	O1D-CGD-CBD	2.10	127.62	124.62
23	C	502	CLA	O2D-CGD-CBD	2.10	114.17	111.30
34	v	201	HEM	C2D-C3D-C4D	2.10	105.06	101.50
23	B	610	CLA	C1D-CHD-C4C	2.10	125.78	122.60
28	c	519	DGD	O2G-C1B-C2B	2.10	116.09	111.53
23	c	513	CLA	O1D-CGD-CBD	2.10	127.63	124.62
23	C	501	CLA	O1D-CGD-CBD	2.10	127.63	124.62
27	C	514	BCR	C38-C26-C27	2.10	117.41	113.43
27	a	412	BCR	C38-C26-C27	2.11	117.42	113.43
23	c	510	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	b	612	CLA	CMD-C2D-C3D	2.11	129.22	125.09
30	a	401	SQD	O9-S-C6	2.11	108.72	106.94
23	B	610	CLA	O1D-CGD-CBD	2.11	127.65	124.62
23	B	601	CLA	O1D-CGD-CBD	2.11	127.65	124.62
27	j	102	BCR	C33-C5-C4	2.11	117.44	113.43
23	B	614	CLA	CHB-C4A-NA	2.11	127.44	124.51
23	B	614	CLA	O1D-CGD-CBD	2.12	127.65	124.62
28	C	516	DGD	C1G-O1G-C1A	2.12	122.77	116.85
23	b	614	CLA	CMB-C2B-C3B	2.12	129.23	125.09
23	B	611	CLA	CMD-C2D-C3D	2.12	129.24	125.09
23	B	616	CLA	O2D-CGD-CBD	2.12	114.21	111.30
28	c	517	DGD	O3G-C1D-C2D	2.12	110.72	108.04
25	d	404	PL9	C30-C29-C31	2.12	118.65	115.41
23	C	503	CLA	CMB-C2B-C3B	2.13	129.25	125.09
23	C	501	CLA	C1D-CHD-C4C	2.13	125.82	122.60
23	C	502	CLA	CMD-C2D-C3D	2.13	129.25	125.09
23	B	602	CLA	CMD-C2D-C3D	2.13	129.26	125.09
25	J	101	PL9	C10-C9-C11	2.13	118.66	115.41
23	C	513	CLA	C1D-CHD-C4C	2.13	125.83	122.60
24	D	402	PHO	C1B-NB-C4B	2.13	110.73	106.51
23	b	616	CLA	CMD-C2D-C3D	2.14	129.27	125.09
23	b	614	CLA	CHB-C4A-NA	2.14	127.47	124.51
23	c	501	CLA	CMD-C2D-C3D	2.14	129.28	125.09
31	b	624	LMG	C7-O1-C1	2.14	118.32	113.82
23	B	604	CLA	CMB-C2B-C3B	2.14	129.28	125.09
23	C	508	CLA	O1D-CGD-CBD	2.15	127.70	124.62
28	b	622	DGD	O5D-C6D-C5D	2.15	112.97	109.08
31	M	102	LMG	O6-C5-C4	2.15	113.72	109.68
27	c	515	BCR	C33-C5-C4	2.15	117.50	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	O2D-CGD-CBD	2.15	114.25	111.30
23	a	404	CLA	CMB-C2B-C3B	2.15	129.30	125.09
23	a	406	CLA	CHB-C4A-NA	2.15	127.49	124.51
23	C	511	CLA	CMD-C2D-C3D	2.15	129.30	125.09
27	f	102	BCR	C36-C18-C19	2.16	121.68	118.10
23	A	405	CLA	CMD-C2D-C3D	2.16	129.31	125.09
31	C	520	LMG	C9-O8-C28	2.16	122.88	116.85
27	C	515	BCR	C33-C5-C4	2.16	117.52	113.43
23	A	405	CLA	C4A-NA-C1A	2.16	109.15	106.36
23	a	406	CLA	CMB-C2B-C3B	2.16	129.31	125.09
25	D	404	PL9	C45-C44-C46	2.16	118.71	115.41
27	C	514	BCR	C29-C30-C25	2.16	113.79	110.36
23	c	507	CLA	CMD-C2D-C3D	2.16	129.32	125.09
23	c	505	CLA	CBA-CAA-C2A	2.16	119.84	113.73
27	K	102	BCR	C38-C26-C27	2.17	117.54	113.43
24	D	402	PHO	C4A-NA-C1A	2.17	110.15	108.21
23	b	604	CLA	CMD-C2D-C3D	2.17	129.33	125.09
23	c	510	CLA	O1D-CGD-CBD	2.17	127.74	124.62
23	b	605	CLA	CMD-C2D-C3D	2.17	129.34	125.09
23	A	403	CLA	CMB-C2B-C3B	2.18	129.34	125.09
31	B	622	LMG	C3-C4-C5	2.18	113.99	110.20
23	b	616	CLA	O1D-CGD-CBD	2.18	127.75	124.62
23	b	612	CLA	O2D-CGD-CBD	2.18	114.29	111.30
27	C	515	BCR	C2-C1-C6	2.18	113.82	110.36
27	D	405	BCR	C36-C18-C19	2.18	121.73	118.10
23	b	607	CLA	O1D-CGD-CBD	2.19	127.75	124.62
30	d	407	SQD	O48-C23-C24	2.19	118.56	111.90
23	C	505	CLA	CHB-C4A-NA	2.19	127.53	124.51
23	C	512	CLA	O1D-CGD-CBD	2.19	127.76	124.62
28	B	626	DGD	C1E-C2E-C3E	2.19	114.28	109.97
23	A	405	CLA	CMB-C2B-C3B	2.19	129.37	125.09
23	c	510	CLA	CMD-C2D-C3D	2.19	129.37	125.09
23	b	607	CLA	CMB-C2B-C3B	2.20	129.39	125.09
27	k	102	BCR	C38-C26-C27	2.20	117.60	113.43
27	b	621	BCR	C38-C26-C27	2.20	117.60	113.43
23	C	502	CLA	O1D-CGD-CBD	2.20	127.78	124.62
23	d	402	CLA	CHB-C4A-NA	2.20	127.56	124.51
23	b	610	CLA	O1D-CGD-CBD	2.21	127.78	124.62
27	Z	101	BCR	C33-C5-C4	2.21	117.61	113.43
33	I	102	LMT	O1B-C4'-C3'	2.21	112.87	107.17
27	x	101	BCR	C35-C13-C12	2.22	121.79	118.10
23	C	510	CLA	O1D-CGD-CBD	2.22	127.80	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	103	SQD	O5-C1-C2	2.22	114.83	110.28
34	f	101	HEM	C2D-C3D-C4D	2.22	105.27	101.50
23	B	616	CLA	C4A-NA-C1A	2.22	109.23	106.36
27	B	619	BCR	C2-C1-C6	2.22	113.89	110.36
31	i	101	LMG	C3-C4-C5	2.23	114.08	110.20
23	D	403	CLA	CMD-C2D-C3D	2.23	129.44	125.09
23	B	603	CLA	C1D-CHD-C4C	2.23	125.97	122.60
28	C	516	DGD	O3G-C3G-C2G	2.23	116.30	110.99
23	C	503	CLA	CHB-C4A-NA	2.23	127.60	124.51
33	D	411	LMT	O1'-C1'-C2'	2.23	110.86	108.04
23	b	604	CLA	CHB-C4A-NA	2.24	127.60	124.51
23	b	619	CLA	CMD-C2D-C3D	2.24	129.46	125.09
23	C	511	CLA	CMB-C2B-C3B	2.24	129.46	125.09
28	C	516	DGD	O3D-C3D-C4D	2.24	115.38	110.34
23	B	611	CLA	O1D-CGD-CBD	2.24	127.83	124.62
23	B	613	CLA	CMD-C2D-C3D	2.24	129.47	125.09
23	c	501	CLA	CMB-C2B-C3B	2.24	129.48	125.09
27	B	617	BCR	C33-C5-C4	2.24	117.68	113.43
31	a	416	LMG	O1-C7-C8	2.24	116.33	110.99
23	c	502	CLA	CMB-C2B-C3B	2.24	129.48	125.09
23	b	608	CLA	O1D-CGD-CBD	2.25	127.84	124.62
27	x	101	BCR	C34-C9-C8	2.25	121.84	118.10
28	c	519	DGD	O3D-C3D-C4D	2.25	115.40	110.34
28	b	602	DGD	C1E-C2E-C3E	2.25	114.40	109.97
27	B	620	BCR	C38-C26-C27	2.25	117.69	113.43
23	b	604	CLA	O2D-CGD-CBD	2.25	114.39	111.30
28	d	408	DGD	C2G-O2G-C1B	2.25	123.30	117.89
31	b	623	LMG	C7-O1-C1	2.26	118.56	113.82
23	b	617	CLA	O2D-CGD-CBD	2.26	114.40	111.30
23	B	604	CLA	CHB-C4A-NA	2.26	127.64	124.51
28	C	516	DGD	O3G-C1D-C2D	2.26	110.89	108.04
28	c	518	DGD	O6E-C1E-C2E	2.26	114.92	110.28
23	b	612	CLA	C4A-NA-C1A	2.27	109.29	106.36
23	B	605	CLA	CMD-C2D-C3D	2.27	129.53	125.09
27	b	620	BCR	C33-C5-C4	2.27	117.73	113.43
23	C	513	CLA	O1D-CGD-CBD	2.27	127.88	124.62
25	D	404	PL9	C20-C19-C21	2.27	118.88	115.41
29	A	412	LHG	O8-C23-C24	2.28	118.83	111.90
23	c	511	CLA	CMB-C2B-C3B	2.28	129.54	125.09
23	d	402	CLA	CMD-C2D-C3D	2.29	129.56	125.09
31	e	101	LMG	O7-C10-C11	2.29	116.50	111.53
27	k	102	BCR	C33-C5-C4	2.29	117.76	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	O1D-CGD-CBD	2.29	127.90	124.62
23	c	510	CLA	C4A-NA-C1A	2.29	109.31	106.36
23	b	616	CLA	O2D-CGD-CBD	2.29	114.44	111.30
23	c	511	CLA	O1D-CGD-CBD	2.29	127.90	124.62
30	F	102	SQD	O6-C1-C2	2.29	110.94	108.04
30	A	417	SQD	O48-C23-C24	2.29	118.89	111.90
23	B	612	CLA	CHB-C4A-NA	2.30	127.69	124.51
28	A	411	DGD	C3D-C4D-C5D	2.30	114.20	110.20
23	B	612	CLA	C4A-NA-C1A	2.30	109.33	106.36
23	B	603	CLA	O1D-CGD-CBD	2.30	127.92	124.62
28	b	602	DGD	O6D-C1D-O3G	2.30	115.60	110.05
27	C	514	BCR	C33-C5-C4	2.30	117.80	113.43
23	B	609	CLA	CMD-C2D-C3D	2.30	129.59	125.09
23	c	504	CLA	CMB-C2B-C3B	2.30	129.60	125.09
23	C	507	CLA	O2D-CGD-CBD	2.31	114.46	111.30
23	B	616	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	C	506	CLA	O1D-CGD-CBD	2.31	127.93	124.62
23	c	509	CLA	CMB-C2B-C3B	2.31	129.61	125.09
23	b	613	CLA	C4A-NA-C1A	2.32	109.35	106.36
31	k	103	LMG	O1-C1-C2	2.32	110.97	108.04
23	C	511	CLA	O1D-CGD-CBD	2.32	127.95	124.62
28	D	410	DGD	O2G-C1B-C2B	2.32	116.57	111.53
23	b	619	CLA	CMB-C2B-C3B	2.32	129.63	125.09
23	c	502	CLA	O2D-CGD-CBD	2.32	114.48	111.30
28	B	621	DGD	C3G-O3G-C1D	2.32	118.70	113.82
23	B	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	b	614	CLA	C4A-NA-C1A	2.32	109.36	106.36
30	f	103	SQD	O48-C23-C24	2.33	118.99	111.90
27	D	405	BCR	C33-C5-C4	2.33	117.84	113.43
23	C	504	CLA	CMD-C2D-C3D	2.33	129.65	125.09
30	A	413	SQD	O6-C1-C2	2.33	110.99	108.04
23	B	608	CLA	C4A-NA-C1A	2.33	109.37	106.36
23	C	512	CLA	CMB-C2B-C3B	2.33	129.65	125.09
28	d	408	DGD	O2G-C1B-C2B	2.33	116.60	111.53
27	A	410	BCR	C33-C5-C4	2.34	117.86	113.43
23	B	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	C	506	CLA	O2D-CGD-CBD	2.34	114.51	111.30
28	C	516	DGD	C3G-O3G-C1D	2.34	118.74	113.82
27	B	619	BCR	C38-C26-C27	2.34	117.87	113.43
31	D	407	LMG	C4-C3-C2	2.34	115.17	110.79
23	b	615	CLA	O1D-CGD-CBD	2.35	127.98	124.62
23	c	507	CLA	CHB-C4A-NA	2.35	127.77	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	403	CLA	C4A-NA-C1A	2.36	109.40	106.36
25	A	408	PL9	C30-C29-C31	2.36	119.01	115.41
30	a	415	SQD	O48-C23-C24	2.36	119.08	111.90
28	B	626	DGD	O6D-C1D-O3G	2.36	115.73	110.05
23	d	403	CLA	CMB-C2B-C3B	2.36	129.71	125.09
27	T	102	BCR	C36-C18-C19	2.36	122.03	118.10
23	B	614	CLA	O2D-CGD-CBD	2.37	114.54	111.30
27	x	101	BCR	C33-C5-C4	2.37	117.91	113.43
23	b	607	CLA	CHB-C4A-NA	2.37	127.78	124.51
25	d	404	PL9	C20-C19-C21	2.37	119.02	115.41
23	b	606	CLA	C4A-NA-C1A	2.37	109.42	106.36
23	b	613	CLA	CHB-C4A-NA	2.37	127.79	124.51
28	C	516	DGD	O1G-C1A-C2A	2.37	119.12	111.90
23	b	604	CLA	O1D-CGD-CBD	2.37	128.02	124.62
23	C	510	CLA	C4A-NA-C1A	2.37	109.42	106.36
30	B	625	SQD	C1-O5-C5	2.37	118.35	113.75
23	a	405	CLA	C4A-NA-C1A	2.37	109.42	106.36
30	a	401	SQD	O48-C23-C24	2.37	119.13	111.90
25	j	101	PL9	C10-C9-C11	2.38	119.04	115.41
23	C	509	CLA	O1D-CGD-CBD	2.38	128.03	124.62
23	A	404	CLA	CMB-C2B-C3B	2.38	129.74	125.09
23	b	619	CLA	C4A-NA-C1A	2.38	109.44	106.36
28	b	622	DGD	C3G-O3G-C1D	2.38	118.82	113.82
30	A	417	SQD	O6-C1-C2	2.39	111.06	108.04
23	C	510	CLA	O2D-CGD-CBD	2.39	114.58	111.30
23	c	513	CLA	CMB-C2B-C3B	2.39	129.76	125.09
23	a	406	CLA	C4A-NA-C1A	2.39	109.45	106.36
23	C	513	CLA	CMB-C2B-C3B	2.39	129.76	125.09
23	C	512	CLA	CMD-C2D-C3D	2.39	129.76	125.09
30	A	413	SQD	C44-O6-C1	2.39	118.84	113.82
28	B	626	DGD	O1G-C1A-C2A	2.39	119.19	111.90
23	C	503	CLA	CMD-C2D-C3D	2.40	129.77	125.09
33	i	102	LMT	O1'-C1'-C2'	2.40	111.07	108.04
28	a	413	DGD	O3D-C3D-C4D	2.40	115.73	110.34
23	C	505	CLA	CMD-C2D-C3D	2.40	129.78	125.09
23	A	404	CLA	C4A-NA-C1A	2.40	109.46	106.36
30	F	102	SQD	O48-C23-C24	2.41	119.24	111.90
28	B	621	DGD	O2G-C1B-C2B	2.41	116.77	111.53
31	d	405	LMG	C3-C4-C5	2.41	114.40	110.20
23	b	606	CLA	CMD-C2D-C3D	2.41	129.80	125.09
23	C	507	CLA	CMD-C2D-C3D	2.41	129.80	125.09
23	B	614	CLA	C4A-NA-C1A	2.41	109.48	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	101	BCR	C35-C13-C12	2.41	122.11	118.10
28	B	621	DGD	O1G-C1A-C2A	2.42	119.27	111.90
23	c	512	CLA	CMD-C2D-C3D	2.42	129.82	125.09
23	c	507	CLA	C4A-NA-C1A	2.42	109.49	106.36
23	c	510	CLA	CMB-C2B-C3B	2.42	129.83	125.09
23	B	601	CLA	CMD-C2D-C3D	2.42	129.83	125.09
23	B	613	CLA	C4A-NA-C1A	2.42	109.49	106.36
28	B	626	DGD	C1G-O1G-C1A	2.43	123.64	116.85
27	c	514	BCR	C33-C5-C4	2.43	118.04	113.43
23	c	503	CLA	C4A-NA-C1A	2.43	109.50	106.36
23	B	615	CLA	CMB-C2B-C3B	2.44	129.86	125.09
23	c	512	CLA	O1D-CGD-CBD	2.44	128.12	124.62
23	c	512	CLA	O2D-CGD-CBD	2.44	114.64	111.30
23	C	505	CLA	O1D-CGD-CBD	2.44	128.12	124.62
25	a	410	PL9	C15-C14-C16	2.44	119.13	115.41
23	C	509	CLA	CMB-C2B-C3B	2.44	129.86	125.09
23	B	606	CLA	C4A-NA-C1A	2.44	109.51	106.36
30	D	409	SQD	O48-C23-C24	2.44	119.34	111.90
23	b	613	CLA	CMD-C2D-C3D	2.44	129.86	125.09
23	C	508	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	c	508	CLA	C4A-NA-C1A	2.44	109.52	106.36
31	b	624	LMG	C3-C4-C5	2.45	114.46	110.20
23	D	401	CLA	CMB-C2B-C3B	2.45	129.88	125.09
23	D	403	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	D	407	LMG	C7-O1-C1	2.45	118.97	113.82
27	f	102	BCR	C33-C5-C4	2.45	118.08	113.43
23	B	604	CLA	C4A-NA-C1A	2.45	109.53	106.36
23	C	505	CLA	CBA-CAA-C2A	2.46	120.66	113.73
25	J	101	PL9	C20-C19-C21	2.46	119.16	115.41
23	c	501	CLA	O1D-CGD-CBD	2.46	128.14	124.62
23	b	609	CLA	C4A-NA-C1A	2.46	109.54	106.36
23	B	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	A	407	CLA	C4A-NA-C1A	2.46	109.54	106.36
31	i	101	LMG	C7-O1-C1	2.46	118.99	113.82
23	B	603	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	D	404	PL9	C10-C9-C11	2.46	119.17	115.41
23	b	604	CLA	C4A-NA-C1A	2.46	109.55	106.36
27	c	516	BCR	C38-C26-C27	2.47	118.10	113.43
23	b	610	CLA	CMB-C2B-C3B	2.47	129.91	125.09
23	c	508	CLA	CMD-C2D-C3D	2.47	129.91	125.09
25	j	101	PL9	C20-C19-C21	2.47	119.18	115.41
23	c	511	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402	CLA	CMB-C2B-C3B	2.47	129.92	125.09
24	A	406	PHO	C1B-NB-C4B	2.47	111.40	106.51
23	c	506	CLA	CMD-C2D-C3D	2.47	129.92	125.09
27	b	620	BCR	C38-C26-C27	2.47	118.12	113.43
23	c	501	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	A	403	CLA	O1D-CGD-CBD	2.48	128.18	124.62
23	B	602	CLA	CMB-C2B-C3B	2.48	129.94	125.09
31	e	101	LMG	C8-O7-C10	2.48	123.84	117.89
30	F	102	SQD	O5-C1-C2	2.48	115.37	110.28
27	C	515	BCR	C29-C30-C25	2.48	114.30	110.36
30	A	413	SQD	O48-C23-C24	2.49	119.47	111.90
28	A	411	DGD	O3D-C3D-C4D	2.49	115.94	110.34
23	b	609	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	B	603	CLA	C4A-NA-C1A	2.49	109.58	106.36
23	B	602	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	c	502	CLA	CMD-C2D-C3D	2.49	129.96	125.09
23	c	509	CLA	O1D-CGD-CBD	2.49	128.19	124.62
25	A	408	PL9	C10-C9-C11	2.50	119.22	115.41
31	I	101	LMG	C7-O1-C1	2.50	119.06	113.82
23	C	502	CLA	CMB-C2B-C3B	2.50	129.97	125.09
23	b	617	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	D	401	CLA	C4A-NA-C1A	2.50	109.59	106.36
30	b	601	SQD	O48-C23-C24	2.50	119.51	111.90
28	c	518	DGD	O1G-C1A-C2A	2.50	119.52	111.90
23	c	503	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	B	615	CLA	CMD-C2D-C3D	2.50	129.98	125.09
23	B	615	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	612	CLA	CMB-C2B-C3B	2.50	129.99	125.09
23	A	404	CLA	CHB-C4A-NA	2.51	127.98	124.51
28	C	517	DGD	O6E-C1E-C2E	2.51	115.42	110.28
23	B	613	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	b	605	CLA	CMB-C2B-C3B	2.51	130.00	125.09
23	B	606	CLA	O2D-CGD-CBD	2.51	114.74	111.30
28	c	517	DGD	O1G-C1A-C2A	2.51	119.55	111.90
25	j	101	PL9	C15-C14-C16	2.51	119.24	115.41
23	B	604	CLA	O1D-CGD-CBD	2.51	128.22	124.62
27	B	619	BCR	C29-C30-C25	2.52	114.35	110.36
23	d	403	CLA	C4A-NA-C1A	2.52	109.61	106.36
29	a	417	LHG	O8-C23-C24	2.52	119.57	111.90
23	C	509	CLA	C4A-NA-C1A	2.52	109.61	106.36
23	C	506	CLA	C4A-NA-C1A	2.52	109.62	106.36
23	c	506	CLA	O2D-CGD-CBD	2.53	114.76	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	CMD-C2D-C3D	2.53	130.03	125.09
23	B	609	CLA	C4A-NA-C1A	2.53	109.63	106.36
23	b	611	CLA	C4A-NA-C1A	2.53	109.63	106.36
23	C	508	CLA	C4A-NA-C1A	2.53	109.63	106.36
23	B	612	CLA	O1D-CGD-CBD	2.53	128.25	124.62
28	a	413	DGD	C3D-C4D-C5D	2.53	114.61	110.20
23	B	614	CLA	CMB-C2B-C3B	2.53	130.04	125.09
23	a	406	CLA	O2D-CGD-CBD	2.53	114.77	111.30
23	B	605	CLA	O1D-CGD-CBD	2.53	128.25	124.62
23	c	512	CLA	C4A-NA-C1A	2.53	109.64	106.36
23	b	610	CLA	C4A-NA-C1A	2.54	109.64	106.36
23	B	601	CLA	C4A-NA-C1A	2.54	109.64	106.36
23	b	612	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	C	511	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	b	618	CLA	O1D-CGD-CBD	2.54	128.27	124.62
23	B	605	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	D	404	PL9	C15-C14-C16	2.55	119.30	115.41
30	A	413	SQD	O5-C5-C4	2.55	114.46	109.68
23	A	403	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	c	505	CLA	O1D-CGD-CBD	2.55	128.28	124.62
23	d	403	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	B	606	CLA	O1D-CGD-CBD	2.55	128.28	124.62
28	b	622	DGD	O1G-C1A-C2A	2.55	119.68	111.90
23	C	507	CLA	C4A-NA-C1A	2.55	109.66	106.36
23	b	606	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	B	607	CLA	CMB-C2B-C3B	2.56	130.09	125.09
23	B	605	CLA	C4A-NA-C1A	2.56	109.67	106.36
25	D	404	PL9	C40-C39-C41	2.56	119.31	115.41
23	b	611	CLA	O2D-CGD-CBD	2.56	114.81	111.30
23	d	403	CLA	CMD-C2D-C3D	2.56	130.10	125.09
28	a	413	DGD	O1G-C1A-C2A	2.57	119.72	111.90
23	b	616	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	D	405	BCR	C29-C30-C25	2.57	114.44	110.36
25	A	408	PL9	C20-C19-C21	2.57	119.34	115.41
23	a	404	CLA	C4A-NA-C1A	2.57	109.68	106.36
28	b	622	DGD	O2G-C1B-C2B	2.57	117.12	111.53
23	a	404	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	B	625	SQD	O47-C7-C8	2.57	117.12	111.53
23	B	605	CLA	CHB-C4A-NA	2.58	128.07	124.51
23	B	606	CLA	CHB-C4A-NA	2.58	128.07	124.51
24	A	406	PHO	C4A-NA-C1A	2.58	110.51	108.21
23	C	501	CLA	C4A-NA-C1A	2.58	109.69	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	501	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	c	512	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	c	512	CLA	CMB-C2B-C3B	2.59	130.15	125.09
23	a	409	CLA	C4A-NA-C1A	2.60	109.71	106.36
31	M	102	LMG	O1-C1-C2	2.60	111.32	108.04
29	A	415	LHG	O8-C23-C24	2.60	119.82	111.90
23	c	503	CLA	CMB-C2B-C3B	2.60	130.17	125.09
23	b	617	CLA	C4A-NA-C1A	2.60	109.72	106.36
23	B	608	CLA	O1D-CGD-CBD	2.60	128.35	124.62
31	E	101	LMG	O7-C10-C11	2.60	117.18	111.53
23	D	401	CLA	O1D-CGD-CBD	2.60	128.35	124.62
31	C	519	LMG	C7-O1-C1	2.60	119.29	113.82
27	C	515	BCR	C38-C26-C27	2.60	118.36	113.43
23	B	609	CLA	CMB-C2B-C3B	2.61	130.19	125.09
31	M	101	LMG	O8-C28-C29	2.61	119.86	111.90
31	M	102	LMG	O8-C28-C29	2.61	119.87	111.90
23	D	403	CLA	O2D-CGD-CBD	2.62	114.89	111.30
23	C	503	CLA	O2D-CGD-CBD	2.62	114.89	111.30
23	D	403	CLA	CMB-C2B-C3B	2.62	130.21	125.09
23	C	504	CLA	C4A-NA-C1A	2.62	109.74	106.36
23	c	506	CLA	CMB-C2B-C3B	2.62	130.21	125.09
23	B	616	CLA	CMB-C2B-C3B	2.63	130.22	125.09
28	A	411	DGD	O1G-C1A-C2A	2.63	119.90	111.90
23	b	608	CLA	C4A-NA-C1A	2.63	109.75	106.36
23	b	618	CLA	C4A-NA-C1A	2.63	109.76	106.36
23	C	503	CLA	C4A-NA-C1A	2.63	109.76	106.36
31	a	402	LMG	C7-O1-C1	2.63	119.34	113.82
31	E	101	LMG	C7-O1-C1	2.63	119.34	113.82
27	B	620	BCR	C2-C1-C6	2.63	114.53	110.36
30	B	625	SQD	O48-C23-C24	2.63	119.92	111.90
23	B	606	CLA	CMB-C2B-C3B	2.63	130.24	125.09
27	c	516	BCR	C29-C30-C25	2.63	114.53	110.36
23	B	611	CLA	C4A-NA-C1A	2.63	109.77	106.36
23	B	602	CLA	C4A-NA-C1A	2.64	109.77	106.36
23	B	615	CLA	C4A-NA-C1A	2.64	109.77	106.36
23	B	610	CLA	C4A-NA-C1A	2.64	109.77	106.36
31	D	406	LMG	C3-C4-C5	2.64	114.80	110.20
23	B	611	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	C	507	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	a	409	CLA	CMB-C2B-C3B	2.64	130.25	125.09
30	b	601	SQD	O5-C5-C4	2.64	114.64	109.68
23	a	406	CLA	CMD-C2D-C3D	2.64	130.26	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	508	CLA	CHB-C4A-NA	2.64	128.17	124.51
30	B	625	SQD	O5-C5-C4	2.65	114.66	109.68
23	b	607	CLA	C4A-NA-C1A	2.66	109.79	106.36
23	a	409	CLA	CMD-C2D-C3D	2.66	130.29	125.09
23	B	610	CLA	CMB-C2B-C3B	2.66	130.29	125.09
27	K	102	BCR	C33-C5-C4	2.66	118.47	113.43
31	d	406	LMG	O8-C28-C29	2.67	120.02	111.90
23	a	405	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	c	506	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	b	606	CLA	O2D-CGD-CBD	2.67	114.96	111.30
23	C	504	CLA	CMB-C2B-C3B	2.67	130.31	125.09
23	b	608	CLA	CMB-C2B-C3B	2.67	130.32	125.09
23	C	504	CLA	CHB-C4A-NA	2.68	128.21	124.51
27	T	103	BCR	C29-C30-C25	2.68	114.61	110.36
23	C	502	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	b	616	CLA	CMB-C2B-C3B	2.68	130.33	125.09
23	B	609	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	b	618	CLA	CHB-C4A-NA	2.68	128.22	124.51
28	b	602	DGD	C1G-O1G-C1A	2.68	124.36	116.85
23	c	501	CLA	C4A-NA-C1A	2.68	109.83	106.36
23	b	611	CLA	O1D-CGD-CBD	2.69	128.47	124.62
23	b	619	CLA	O1D-CGD-CBD	2.69	128.47	124.62
23	b	605	CLA	C4A-NA-C1A	2.69	109.83	106.36
28	D	410	DGD	O1G-C1A-C2A	2.69	120.09	111.90
28	b	602	DGD	O1G-C1A-C2A	2.69	120.09	111.90
23	b	610	CLA	O2D-CGD-CBD	2.69	114.99	111.30
23	a	409	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	c	506	CLA	C4A-NA-C1A	2.69	109.84	106.36
23	a	405	CLA	CMB-C2B-C3B	2.70	130.36	125.09
23	b	609	CLA	O1D-CGD-CBD	2.70	128.49	124.62
25	d	404	PL9	C15-C14-C16	2.70	119.53	115.41
23	B	611	CLA	CMB-C2B-C3B	2.71	130.38	125.09
27	H	101	BCR	C33-C5-C4	2.71	118.56	113.43
33	T	101	LMT	O1B-C4'-C3'	2.71	114.16	107.17
23	c	511	CLA	C4A-NA-C1A	2.71	109.86	106.36
30	b	601	SQD	O47-C7-C8	2.71	117.42	111.53
30	b	601	SQD	O6-C1-C2	2.71	111.47	108.04
27	B	618	BCR	C29-C30-C25	2.71	114.66	110.36
23	b	616	CLA	C4A-NA-C1A	2.72	109.87	106.36
23	b	617	CLA	CMB-C2B-C3B	2.72	130.41	125.09
23	C	513	CLA	C4A-NA-C1A	2.72	109.87	106.36
31	M	101	LMG	O1-C1-C2	2.72	111.47	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	C	502	CLA	C4A-NA-C1A	2.72	109.88	106.36
23	c	505	CLA	CHB-C4A-NA	2.72	128.28	124.51
25	a	410	PL9	C20-C19-C21	2.72	119.57	115.41
23	C	512	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	b	613	CLA	CMB-C2B-C3B	2.73	130.42	125.09
31	e	101	LMG	O8-C28-C29	2.73	120.21	111.90
23	b	609	CLA	CMB-C2B-C3B	2.74	130.44	125.09
31	D	408	LMG	O8-C28-C29	2.74	120.26	111.90
23	c	507	CLA	CMB-C2B-C3B	2.74	130.46	125.09
23	b	614	CLA	O2D-CGD-CBD	2.75	115.06	111.30
29	a	414	LHG	C6-O8-C23	2.75	124.53	116.85
23	b	615	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	B	608	CLA	CMB-C2B-C3B	2.75	130.47	125.09
23	c	504	CLA	O2D-CGD-CBD	2.75	115.08	111.30
31	i	101	LMG	O8-C28-C29	2.76	120.30	111.90
28	D	410	DGD	O5D-C6D-C5D	2.76	114.08	109.08
23	b	615	CLA	C4A-NA-C1A	2.76	109.93	106.36
23	c	509	CLA	C4A-NA-C1A	2.77	109.94	106.36
28	d	408	DGD	O1G-C1A-C2A	2.77	120.34	111.90
23	C	505	CLA	C4A-NA-C1A	2.77	109.94	106.36
31	c	520	LMG	C7-O1-C1	2.77	119.64	113.82
23	c	502	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	b	605	CLA	CHB-C4A-NA	2.78	128.35	124.51
31	b	623	LMG	O8-C28-C29	2.78	120.37	111.90
33	B	627	LMT	O1B-C4'-C3'	2.79	114.37	107.17
23	C	509	CLA	CHB-C4A-NA	2.79	128.37	124.51
28	c	519	DGD	O6D-C5D-C6D	2.79	112.32	106.61
31	C	519	LMG	O1-C1-C2	2.79	111.57	108.04
23	b	615	CLA	CMB-C2B-C3B	2.79	130.55	125.09
23	c	503	CLA	O2D-CGD-CBD	2.80	115.14	111.30
27	J	102	BCR	C38-C26-C27	2.80	118.73	113.43
23	C	508	CLA	CMB-C2B-C3B	2.80	130.56	125.09
23	C	513	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	B	603	CLA	CMB-C2B-C3B	2.80	130.57	125.09
23	A	403	CLA	C4A-NA-C1A	2.81	109.99	106.36
23	b	611	CLA	CHB-C4A-NA	2.81	128.39	124.51
23	C	507	CLA	CMB-C2B-C3B	2.81	130.58	125.09
23	c	513	CLA	C4A-NA-C1A	2.81	109.99	106.36
30	a	401	SQD	O6-C1-C2	2.81	111.59	108.04
27	B	618	BCR	C2-C1-C6	2.81	114.82	110.36
23	C	506	CLA	CMB-C2B-C3B	2.82	130.60	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	406	LMG	C7-O1-C1	2.82	119.75	113.82
31	e	101	LMG	C7-O1-C1	2.82	119.75	113.82
23	C	512	CLA	C4A-NA-C1A	2.83	110.01	106.36
30	f	103	SQD	O5-C5-C4	2.83	114.99	109.68
27	b	620	BCR	C29-C30-C25	2.83	114.84	110.36
31	I	101	LMG	O8-C28-C29	2.83	120.53	111.90
28	b	602	DGD	O2G-C1B-C2B	2.84	117.70	111.53
31	a	402	LMG	O8-C28-C29	2.85	120.57	111.90
23	d	402	CLA	O1D-CGD-CBD	2.85	128.71	124.62
34	f	101	HEM	CMD-C2D-C3D	2.85	126.96	114.35
25	J	101	PL9	C15-C14-C16	2.86	119.77	115.41
30	a	415	SQD	C44-O6-C1	2.86	119.82	113.82
30	f	103	SQD	O6-C1-C2	2.86	111.65	108.04
31	E	101	LMG	C8-O7-C10	2.86	124.75	117.89
23	c	504	CLA	CHB-C4A-NA	2.86	128.47	124.51
31	A	418	LMG	O1-C1-C2	2.86	111.66	108.04
27	B	618	BCR	C38-C26-C27	2.88	118.88	113.43
31	I	101	LMG	O7-C10-C11	2.88	117.78	111.53
23	c	509	CLA	CHB-C4A-NA	2.88	128.50	124.51
28	b	622	DGD	O3D-C3D-C4D	2.89	116.84	110.34
31	E	101	LMG	O1-C1-C2	2.89	111.69	108.04
28	C	517	DGD	O1G-C1A-C2A	2.89	120.72	111.90
31	D	408	LMG	O7-C10-C11	2.90	117.83	111.53
31	A	418	LMG	O8-C28-C29	2.90	120.75	111.90
23	b	613	CLA	O2D-CGD-CBD	2.90	115.28	111.30
23	c	502	CLA	C4A-NA-C1A	2.91	110.12	106.36
23	b	618	CLA	CMB-C2B-C3B	2.91	130.78	125.09
23	B	612	CLA	CMB-C2B-C3B	2.91	130.79	125.09
23	d	402	CLA	C4A-NA-C1A	2.91	110.13	106.36
23	c	508	CLA	CMB-C2B-C3B	2.92	130.79	125.09
27	f	102	BCR	C29-C30-C25	2.92	114.98	110.36
30	A	417	SQD	C1-C2-C3	2.92	115.73	109.97
31	A	418	LMG	C3-C4-C5	2.93	115.30	110.20
23	B	607	CLA	C4A-NA-C1A	2.93	110.14	106.36
28	C	518	DGD	O1G-C1A-C2A	2.94	120.87	111.90
34	F	101	HEM	CMD-C2D-C3D	2.95	127.38	114.35
31	a	402	LMG	O1-C1-C2	2.95	111.77	108.04
28	B	621	DGD	O3D-C3D-C4D	2.95	116.99	110.34
31	d	405	LMG	O8-C28-C29	2.96	120.91	111.90
25	d	404	PL9	C40-C39-C41	2.96	119.92	115.41
23	B	607	CLA	O2D-CGD-CBD	2.96	115.36	111.30
34	F	101	HEM	C3B-C4B-CHC	2.97	127.34	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	102	SQD	C44-O6-C1	2.97	120.05	113.82
27	B	618	BCR	C33-C5-C4	2.97	119.06	113.43
23	C	511	CLA	C4A-NA-C1A	2.97	110.20	106.36
30	D	409	SQD	O5-C5-C4	2.97	115.26	109.68
23	c	513	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	b	608	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	A	407	CLA	CHB-C4A-NA	2.98	128.63	124.51
30	a	401	SQD	C44-O6-C1	2.98	120.08	113.82
23	b	606	CLA	CMB-C2B-C3B	2.98	130.92	125.09
30	a	415	SQD	O5-C5-C4	2.99	115.30	109.68
28	c	517	DGD	C1G-O1G-C1A	2.99	125.21	116.85
34	v	201	HEM	CMD-C2D-C3D	3.00	127.60	114.35
23	B	613	CLA	CMB-C2B-C3B	3.00	130.95	125.09
31	a	416	LMG	O8-C28-C29	3.00	121.04	111.90
23	c	504	CLA	C4A-NA-C1A	3.00	110.24	106.36
31	D	407	LMG	O8-C28-C29	3.00	121.05	111.90
31	E	101	LMG	O8-C28-C29	3.00	121.05	111.90
31	D	408	LMG	C7-O1-C1	3.01	120.14	113.82
27	b	621	BCR	C2-C1-C6	3.01	115.12	110.36
31	A	414	LMG	C7-O1-C1	3.01	120.14	113.82
31	a	402	LMG	C3-C4-C5	3.01	115.45	110.20
30	f	103	SQD	C44-O6-C1	3.02	120.17	113.82
27	D	405	BCR	C38-C26-C27	3.03	119.17	113.43
31	b	624	LMG	O8-C28-C29	3.03	121.13	111.90
23	b	611	CLA	CMB-C2B-C3B	3.03	131.02	125.09
31	d	406	LMG	O7-C10-C11	3.03	118.12	111.53
31	D	407	LMG	O1-C1-C2	3.04	111.87	108.04
30	a	401	SQD	C1-C2-C3	3.04	115.95	109.97
27	f	102	BCR	C38-C26-C27	3.04	119.20	113.43
28	d	408	DGD	O5D-C6D-C5D	3.04	114.59	109.08
28	c	517	DGD	O2G-C1B-C2B	3.05	118.15	111.53
30	F	102	SQD	O5-C5-C4	3.06	115.42	109.68
23	B	607	CLA	CHB-C4A-NA	3.06	128.75	124.51
28	c	519	DGD	O1G-C1A-C2A	3.07	121.24	111.90
31	A	414	LMG	O8-C28-C29	3.07	121.25	111.90
25	D	404	PL9	C25-C24-C26	3.08	120.11	115.41
31	B	622	LMG	O8-C28-C29	3.09	121.31	111.90
27	j	102	BCR	C38-C26-C27	3.09	119.29	113.43
31	C	520	LMG	C7-O1-C1	3.09	120.32	113.82
23	A	407	CLA	CMB-C2B-C3B	3.11	131.17	125.09
27	C	514	BCR	C1-C6-C7	3.11	124.53	115.82
31	D	406	LMG	C7-O1-C1	3.12	120.37	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	CHB-C4A-NA	3.12	128.83	124.51
28	B	626	DGD	C3D-C4D-C5D	3.13	115.66	110.20
24	D	402	PHO	O1D-CGD-CBD	3.13	129.11	124.62
34	V	201	HEM	CMD-C2D-C3D	3.13	128.21	114.35
31	c	520	LMG	O8-C28-C29	3.14	121.46	111.90
30	A	417	SQD	O5-C5-C4	3.14	115.58	109.68
27	T	103	BCR	C33-C5-C4	3.14	119.39	113.43
28	C	517	DGD	O3G-C1D-C2D	3.15	112.01	108.04
23	c	505	CLA	C4A-NA-C1A	3.15	110.43	106.36
30	A	417	SQD	O5-C1-C2	3.15	116.74	110.28
34	v	201	HEM	CMC-C2C-C3C	3.16	124.41	116.53
31	A	418	LMG	C7-O1-C1	3.16	120.47	113.82
27	T	103	BCR	C2-C1-C6	3.17	115.38	110.36
31	M	101	LMG	C3-C4-C5	3.18	115.74	110.20
34	f	101	HEM	CMB-C2B-C3B	3.18	124.47	116.53
27	T	103	BCR	C38-C26-C27	3.20	119.50	113.43
28	c	519	DGD	O5D-C1E-C2E	3.21	112.09	108.04
31	C	520	LMG	O8-C28-C29	3.21	121.68	111.90
30	d	407	SQD	O5-C5-C4	3.22	115.73	109.68
27	j	102	BCR	C2-C1-C6	3.24	115.49	110.36
31	C	519	LMG	O8-C28-C29	3.24	121.78	111.90
31	I	101	LMG	O1-C1-C2	3.25	112.14	108.04
27	J	102	BCR	C29-C30-C25	3.25	115.52	110.36
28	b	602	DGD	C3G-O3G-C1D	3.28	120.71	113.82
31	c	520	LMG	O1-C1-C2	3.29	112.20	108.04
31	D	406	LMG	O8-C28-C29	3.29	121.94	111.90
28	C	518	DGD	C2G-O2G-C1B	3.29	125.79	117.89
31	e	101	LMG	O1-C1-C2	3.30	112.21	108.04
30	a	415	SQD	C1-O5-C5	3.30	120.16	113.75
31	i	101	LMG	O7-C10-C11	3.31	118.73	111.53
34	f	101	HEM	C3B-C4B-CHC	3.33	127.84	123.16
27	c	514	BCR	C1-C6-C7	3.33	125.14	115.82
28	a	413	DGD	O6D-C5D-C6D	3.33	113.42	106.61
31	M	102	LMG	C3-C4-C5	3.34	116.01	110.20
28	C	516	DGD	O2G-C1B-C2B	3.34	118.78	111.53
24	A	406	PHO	O1D-CGD-CBD	3.34	129.40	124.62
30	A	417	SQD	C44-O6-C1	3.34	120.83	113.82
28	B	626	DGD	C3G-O3G-C1D	3.34	120.84	113.82
30	b	601	SQD	C44-O6-C1	3.35	120.85	113.82
30	B	625	SQD	C44-O6-C1	3.35	120.86	113.82
30	D	409	SQD	C1-O5-C5	3.35	120.26	113.75
31	k	103	LMG	O8-C28-C29	3.36	122.13	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	404	PL9	C35-C34-C36	3.38	120.57	115.41
27	j	102	BCR	C29-C30-C25	3.38	115.72	110.36
30	a	401	SQD	O5-C5-C4	3.39	116.04	109.68
24	a	407	PHO	O1D-CGD-CBD	3.39	129.48	124.62
29	a	414	LHG	O7-C7-C8	3.40	118.92	111.53
28	B	626	DGD	O2G-C1B-C2B	3.41	118.94	111.53
28	D	410	DGD	C3G-O3G-C1D	3.44	121.05	113.82
34	F	101	HEM	CMB-C2B-C3B	3.45	125.15	116.53
25	D	404	PL9	C35-C34-C36	3.46	120.69	115.41
27	B	620	BCR	C33-C5-C4	3.47	120.01	113.43
27	J	102	BCR	C2-C1-C6	3.48	115.87	110.36
27	b	621	BCR	C33-C5-C4	3.49	120.05	113.43
28	c	519	DGD	C2G-O2G-C1B	3.51	126.32	117.89
31	k	103	LMG	O7-C10-C11	3.52	119.17	111.53
29	A	412	LHG	O7-C7-C8	3.52	119.17	111.53
25	j	101	PL9	C25-C24-C26	3.52	120.78	115.41
28	C	517	DGD	O2G-C1B-C2B	3.52	119.17	111.53
31	d	405	LMG	C7-O1-C1	3.52	121.22	113.82
30	A	417	SQD	C1-O5-C5	3.52	120.58	113.75
28	C	518	DGD	O6D-C5D-C6D	3.52	113.81	106.61
25	J	101	PL9	C25-C24-C26	3.53	120.80	115.41
30	A	413	SQD	C1-O5-C5	3.54	120.61	113.75
30	A	413	SQD	O47-C7-C8	3.55	119.23	111.53
31	a	402	LMG	O7-C10-C11	3.55	119.24	111.53
28	b	602	DGD	C3D-C4D-C5D	3.55	116.39	110.20
30	a	415	SQD	O47-C7-C8	3.55	119.25	111.53
31	D	407	LMG	O7-C10-C11	3.57	119.29	111.53
31	D	406	LMG	O7-C10-C11	3.60	119.35	111.53
31	A	418	LMG	O7-C10-C11	3.60	119.35	111.53
30	f	103	SQD	C1-O5-C5	3.62	120.77	113.75
31	B	622	LMG	O1-C1-C2	3.62	112.61	108.04
25	A	408	PL9	C35-C34-C36	3.62	120.94	115.41
28	d	408	DGD	C3G-O3G-C1D	3.63	121.44	113.82
25	a	410	PL9	C25-C24-C26	3.63	120.95	115.41
30	a	401	SQD	C1-O5-C5	3.65	120.84	113.75
27	J	102	BCR	C31-C1-C2	3.67	121.93	108.79
28	A	411	DGD	O6D-C5D-C6D	3.67	114.11	106.61
30	a	415	SQD	O6-C1-C2	3.67	112.68	108.04
24	a	408	PHO	O1D-CGD-CBD	3.68	129.90	124.62
31	C	519	LMG	O7-C10-C11	3.68	119.53	111.53
28	c	518	DGD	O2G-C1B-C2B	3.70	119.58	111.53
34	V	201	HEM	CMC-C2C-C3C	3.71	125.80	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	401	SQD	O5-C1-C2	3.72	117.92	110.28
27	j	102	BCR	C31-C1-C2	3.73	122.13	108.79
28	D	410	DGD	O5D-C1E-C2E	3.74	112.77	108.04
28	B	626	DGD	O5D-C1E-C2E	3.74	112.77	108.04
30	d	407	SQD	C1-O5-C5	3.75	121.02	113.75
28	C	516	DGD	O5D-C1E-C2E	3.76	112.78	108.04
29	A	415	LHG	O7-C7-C8	3.77	119.72	111.53
29	a	417	LHG	O7-C7-C8	3.79	119.77	111.53
30	f	103	SQD	O47-C7-C8	3.79	119.77	111.53
30	D	409	SQD	O7-S-C6	3.80	110.15	106.94
31	b	624	LMG	O1-C1-C2	3.81	112.85	108.04
31	b	623	LMG	O7-C10-C11	3.82	119.83	111.53
31	c	520	LMG	O7-C10-C11	3.85	119.90	111.53
30	F	102	SQD	C1-O5-C5	3.86	121.24	113.75
30	A	417	SQD	O47-C7-C8	3.87	119.93	111.53
31	C	520	LMG	O7-C10-C11	3.87	119.94	111.53
25	a	410	PL9	C35-C34-C36	3.89	121.36	115.41
30	F	102	SQD	O47-C7-C8	3.91	120.03	111.53
30	a	401	SQD	O47-C7-C8	3.93	120.06	111.53
31	b	623	LMG	O1-C1-C2	3.93	113.00	108.04
34	F	101	HEM	CAD-C3D-C4D	3.93	126.34	112.47
31	a	416	LMG	C7-O1-C1	3.93	122.08	113.82
31	M	102	LMG	O7-C10-C11	3.94	120.08	111.53
25	A	408	PL9	C25-C24-C26	3.94	121.43	115.41
25	d	404	PL9	C25-C24-C26	3.94	121.43	115.41
31	B	622	LMG	O7-C10-C11	3.94	120.10	111.53
30	D	409	SQD	O47-C7-C8	3.96	120.14	111.53
31	d	405	LMG	O7-C10-C11	3.96	120.14	111.53
31	M	101	LMG	O7-C10-C11	3.97	120.15	111.53
30	d	407	SQD	O7-S-C6	3.98	110.30	106.94
31	b	624	LMG	O7-C10-C11	4.04	120.31	111.53
27	c	514	BCR	C8-C7-C6	4.04	139.45	127.32
31	C	520	LMG	O1-C1-C2	4.06	113.16	108.04
28	c	517	DGD	O5D-C1E-C2E	4.08	113.19	108.04
34	v	201	HEM	CAD-C3D-C4D	4.08	126.88	112.47
28	a	413	DGD	O2G-C1B-C2B	4.09	120.41	111.53
31	A	414	LMG	O7-C10-C11	4.13	120.51	111.53
34	f	101	HEM	CAD-C3D-C4D	4.15	127.11	112.47
28	D	410	DGD	O2D-C2D-C1D	4.18	119.18	110.02
30	d	407	SQD	O47-C7-C8	4.18	120.61	111.53
28	c	518	DGD	O3G-C1D-C2D	4.19	113.33	108.04
34	V	201	HEM	CAD-C3D-C4D	4.21	127.33	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	514	BCR	C8-C7-C6	4.24	140.04	127.32
28	d	408	DGD	O2D-C2D-C1D	4.27	119.37	110.02
31	a	416	LMG	O7-C10-C11	4.37	121.02	111.53
28	A	411	DGD	O2G-C1B-C2B	4.40	121.08	111.53
30	A	417	SQD	O7-S-C6	4.42	110.67	106.94
31	d	406	LMG	O1-C1-C2	4.44	113.64	108.04
28	C	518	DGD	O5D-C1E-C2E	4.48	113.70	108.04
30	a	415	SQD	O9-S-C6	4.53	110.76	106.94
34	v	201	HEM	CMB-C2B-C3B	4.55	127.88	116.53
30	f	103	SQD	O9-S-C6	4.58	110.80	106.94
28	b	602	DGD	O5D-C1E-C2E	4.63	113.89	108.04
30	a	401	SQD	O7-S-C6	4.66	110.87	106.94
34	f	101	HEM	CMC-C2C-C3C	4.66	128.16	116.53
34	V	201	HEM	CMB-C2B-C3B	4.66	128.17	116.53
28	d	408	DGD	O5D-C1E-C2E	4.67	113.93	108.04
30	B	625	SQD	O9-S-C6	4.79	110.98	106.94
30	b	601	SQD	O9-S-C6	4.91	111.08	106.94
31	D	408	LMG	O1-C1-C2	4.99	114.34	108.04
34	f	101	HEM	CAD-C3D-C2D	5.01	127.62	113.22
34	F	101	HEM	CMC-C2C-C3C	5.05	129.12	116.53
34	V	201	HEM	CAD-C3D-C2D	5.12	127.94	113.22
34	v	201	HEM	CAD-C3D-C2D	5.16	128.06	113.22
30	d	407	SQD	C44-O6-C1	5.19	124.72	113.82
30	a	415	SQD	O7-S-C6	5.20	111.32	106.94
34	F	101	HEM	CAD-C3D-C2D	5.40	128.75	113.22
28	C	518	DGD	C3G-O3G-C1D	5.44	125.25	113.82
30	D	409	SQD	C44-O6-C1	5.48	125.33	113.82
30	A	413	SQD	O9-S-C6	5.53	111.60	106.94
30	F	102	SQD	O9-S-C6	5.64	111.70	106.94
30	F	102	SQD	O7-S-C6	5.71	111.75	106.94
28	D	410	DGD	O3G-C1D-C2D	5.73	115.28	108.04
28	c	519	DGD	C3G-O3G-C1D	5.83	126.08	113.82
30	A	413	SQD	O7-S-C6	5.89	111.91	106.94
28	a	413	DGD	C3G-O3G-C1D	5.92	126.26	113.82
28	A	411	DGD	C3G-O3G-C1D	6.11	126.66	113.82
30	f	103	SQD	O7-S-C6	6.34	112.29	106.94
28	d	408	DGD	O3G-C1D-C2D	6.37	116.08	108.04
30	D	409	SQD	O9-S-C6	6.44	112.37	106.94
27	J	102	BCR	C31-C1-C6	6.66	120.75	110.30
30	d	407	SQD	O9-S-C6	6.73	112.61	106.94
27	j	102	BCR	C31-C1-C6	6.80	120.96	110.30
30	B	625	SQD	O7-S-C6	6.84	112.70	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	601	SQD	O7-S-C6	7.41	113.19	106.94
27	c	514	BCR	C7-C8-C9	8.04	138.47	126.22
30	d	407	SQD	O6-C1-C2	8.16	118.35	108.04
27	C	514	BCR	C7-C8-C9	8.35	138.94	126.22
30	D	409	SQD	O6-C1-C2	8.59	118.89	108.04

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	617	CLA	NC
23	b	617	CLA	ND
23	b	617	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	ND
23	a	405	CLA	NA
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	c	501	CLA	NC
23	c	501	CLA	ND
23	c	501	CLA	NA
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	616	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	601	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	B	609	CLA	NC
23	B	609	CLA	ND
23	B	609	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	b	618	CLA	NC
23	b	618	CLA	ND
23	b	618	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	503	CLA	NA
23	D	401	CLA	NC
23	D	401	CLA	ND
23	D	401	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	c	509	CLA	NA
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	C	506	CLA	NC
23	C	506	CLA	ND
23	C	506	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	609	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	NA
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA
23	D	403	CLA	NC
23	D	403	CLA	ND
23	D	403	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	A	403	CLA	NC
23	A	403	CLA	ND
23	A	403	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	d	402	CLA	NC
23	d	402	CLA	ND
23	d	402	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	c	510	CLA	NC

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Mol	Chain	Res	Type	Atom
23	c	510	CLA	ND
23	c	510	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	ND
23	A	407	CLA	NA
23	a	404	CLA	NC
23	a	404	CLA	ND
23	a	404	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	ND
23	a	406	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	505	CLA	NA
23	c	502	CLA	NC
23	c	502	CLA	ND
23	c	502	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	C	501	CLA	NC
23	C	501	CLA	ND
23	C	501	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	C	507	CLA	NC

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Mol	Chain	Res	Type	Atom
23	C	507	CLA	ND
23	C	507	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	d	408	DGD	C3G-O3G-C1D-O6D
28	D	410	DGD	C3G-O3G-C1D-O6D
31	M	101	LMG	C8-O7-C10-C11
31	M	102	LMG	C8-O7-C10-C11
28	c	518	DGD	C2G-O2G-C1B-O1B
28	C	517	DGD	C2G-O2G-C1B-O1B
28	c	518	DGD	C2G-O2G-C1B-C2B
28	C	517	DGD	C2G-O2G-C1B-C2B
30	D	409	SQD	C45-O47-C7-C8
30	d	407	SQD	C45-O47-C7-O49
30	d	407	SQD	C45-O47-C7-C8
30	D	409	SQD	C45-O47-C7-O49

There are no ring outliers.

88 monomers are involved in 421 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	403	CLA	13	0
23	A	404	CLA	23	0
23	A	405	CLA	17	0
24	A	406	PHO	4	0
23	A	407	CLA	1	0
25	A	408	PL9	2	0
27	A	410	BCR	5	0
28	A	411	DGD	1	0
29	A	412	LHG	3	0
30	A	413	SQD	5	0
31	A	414	LMG	3	0
29	A	415	LHG	3	0
30	A	417	SQD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	418	LMG	2	0
23	B	601	CLA	2	0
23	B	602	CLA	8	0
23	B	603	CLA	12	0
23	B	604	CLA	9	0
23	B	605	CLA	17	0
23	B	606	CLA	18	0
23	B	607	CLA	12	0
23	B	608	CLA	20	0
23	B	609	CLA	13	0
23	B	610	CLA	9	0
23	B	611	CLA	13	0
23	B	612	CLA	10	0
23	B	613	CLA	4	0
23	B	614	CLA	8	0
23	B	615	CLA	9	0
23	B	616	CLA	10	0
27	B	617	BCR	7	0
27	B	618	BCR	9	0
27	B	619	BCR	5	0
27	B	620	BCR	10	0
28	B	621	DGD	1	0
31	B	622	LMG	4	0
33	B	623	LMT	1	0
30	B	625	SQD	1	0
28	B	626	DGD	4	0
33	B	627	LMT	1	0
33	B	628	LMT	2	0
23	C	501	CLA	8	0
23	C	502	CLA	2	0
23	C	503	CLA	5	0
23	C	504	CLA	7	0
23	C	505	CLA	5	0
23	C	506	CLA	3	0
23	C	507	CLA	7	0
23	C	508	CLA	3	0
23	C	509	CLA	3	0
23	C	510	CLA	5	0
23	C	511	CLA	9	0
23	C	512	CLA	4	0
23	C	513	CLA	5	0
27	C	514	BCR	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	515	BCR	9	0
28	C	516	DGD	4	0
28	C	517	DGD	11	0
28	C	518	DGD	6	0
31	C	519	LMG	2	0
31	C	520	LMG	2	0
23	D	401	CLA	7	0
24	D	402	PHO	7	0
23	D	403	CLA	5	0
25	D	404	PL9	11	0
27	D	405	BCR	3	0
31	D	406	LMG	7	0
31	D	407	LMG	3	0
31	D	408	LMG	7	0
30	D	409	SQD	3	0
28	D	410	DGD	3	0
33	D	411	LMT	2	0
31	E	101	LMG	1	0
34	F	101	HEM	4	0
30	F	102	SQD	2	0
27	H	101	BCR	4	0
31	I	101	LMG	3	0
33	I	102	LMT	2	0
25	J	101	PL9	1	0
27	J	102	BCR	5	0
27	K	102	BCR	10	0
31	M	101	LMG	2	0
31	M	102	LMG	4	0
33	T	101	LMT	2	0
27	T	102	BCR	5	0
27	T	103	BCR	7	0
34	V	201	HEM	4	0
27	Z	101	BCR	5	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	335/360 (93%)	0.08	8 (2%) 62 57	44, 65, 104, 152	0
1	a	335/360 (93%)	-0.14	2 (0%) 90 87	46, 65, 104, 153	0
2	B	490/510 (96%)	0.28	24 (4%) 33 32	46, 70, 103, 156	0
2	b	490/510 (96%)	0.26	18 (3%) 45 41	43, 70, 103, 160	0
3	C	447/461 (96%)	0.05	13 (2%) 55 49	52, 79, 105, 133	0
3	c	447/461 (96%)	0.19	25 (5%) 28 27	56, 81, 106, 135	0
4	D	340/352 (96%)	-0.09	1 (0%) 94 92	44, 66, 102, 139	0
4	d	340/352 (96%)	-0.05	3 (0%) 85 81	43, 66, 102, 135	0
5	E	82/84 (97%)	0.13	2 (2%) 62 57	68, 92, 123, 132	0
5	e	82/84 (97%)	-0.10	1 (1%) 81 75	70, 92, 123, 127	0
6	F	35/45 (77%)	-0.26	0 100 100	67, 84, 119, 143	0
6	f	35/45 (77%)	-0.18	1 (2%) 55 49	72, 83, 121, 141	0
7	H	65/66 (98%)	0.46	6 (9%) 11 15	74, 93, 119, 145	0
7	h	65/66 (98%)	0.71	7 (10%) 8 11	73, 94, 119, 148	0
8	I	35/38 (92%)	0.23	1 (2%) 55 49	65, 80, 106, 120	0
8	i	35/38 (92%)	-0.03	0 100 100	68, 80, 105, 120	0
9	J	34/40 (85%)	-0.20	0 100 100	72, 85, 95, 112	0
9	j	34/40 (85%)	-0.00	0 100 100	77, 87, 96, 115	0
10	K	37/46 (80%)	-0.11	0 100 100	76, 88, 99, 125	0
10	k	37/46 (80%)	0.49	2 (5%) 29 29	73, 89, 104, 126	0
11	L	37/37 (100%)	0.40	4 (10%) 8 11	50, 63, 126, 156	0
11	l	37/37 (100%)	0.10	0 100 100	51, 63, 127, 155	0
12	M	34/36 (94%)	0.18	2 (5%) 26 25	53, 69, 107, 165	0
12	m	34/36 (94%)	0.26	3 (8%) 12 15	55, 69, 109, 163	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.62	21 (8%) 13 16	49, 79, 122, 167	0
13	o	243/272 (89%)	0.50	13 (5%) 30 30	49, 79, 121, 167	0
14	T	32/32 (100%)	0.27	4 (12%) 5 10	57, 69, 159, 169	0
14	t	32/32 (100%)	-0.03	0 100 100	56, 67, 158, 170	0
15	U	97/134 (72%)	0.65	4 (4%) 41 38	56, 70, 90, 112	0
15	u	97/134 (72%)	0.60	2 (2%) 67 61	56, 70, 89, 111	0
16	V	137/163 (84%)	0.07	6 (4%) 38 35	55, 71, 85, 100	0
16	v	137/163 (84%)	0.50	4 (2%) 55 49	58, 71, 86, 96	0
17	g	28/46 (60%)	0.94	4 (14%) 4 8	96, 108, 125, 129	0
17	y	28/46 (60%)	0.09	1 (3%) 46 42	92, 108, 128, 129	0
18	X	37/41 (90%)	0.93	7 (18%) 2 6	77, 92, 120, 140	0
18	x	37/41 (90%)	0.85	5 (13%) 4 9	75, 90, 124, 145	0
19	Z	62/62 (100%)	0.92	6 (9%) 10 13	87, 103, 170, 186	0
19	z	62/62 (100%)	0.42	1 (1%) 74 68	88, 104, 169, 184	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.21	201 (3%) 43 40	43, 75, 115, 186	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.6
16	v	132	ASN	5.3
1	A	11	ALA	5.1
1	A	10	SER	4.9
7	h	66	GLY	4.5
5	E	84	LYS	4.1
13	o	55	ALA	4.1
3	c	180	MET	4.0
1	A	230	THR	4.0
2	B	129	GLY	4.0
3	c	200	THR	4.0
1	A	12	ASN	3.9
2	B	379	ALA	3.9
1	a	10	SER	3.8
13	O	51	THR	3.8
3	c	201	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	128	THR	3.8
7	h	2	ALA	3.6
2	B	477	ASP	3.6
15	U	38	GLU	3.6
2	B	127	ARG	3.6
4	d	13	GLY	3.6
7	h	23	PRO	3.5
7	h	27	THR	3.5
3	c	372	PRO	3.5
2	b	393	GLU	3.4
18	x	12	ILE	3.4
2	B	126	PRO	3.4
13	O	269	ILE	3.4
2	B	132	ALA	3.3
18	X	42	GLN	3.3
7	H	2	ALA	3.3
3	c	202	PRO	3.3
13	o	220	LYS	3.3
3	c	373	ASN	3.3
12	m	7	GLY	3.3
3	C	27	ASP	3.2
18	X	47	GLN	3.2
16	v	131	ARG	3.2
13	O	57	PRO	3.2
3	C	332	GLN	3.2
2	b	119	ASP	3.2
18	X	11	THR	3.1
2	b	303	SER	3.1
3	c	365	TRP	3.1
3	c	140	LEU	3.0
16	V	28	GLU	3.0
2	b	394	GLN	3.0
13	O	195	ASP	3.0
3	c	329	GLY	3.0
3	c	199	ILE	3.0
3	c	147	PHE	2.9
2	b	302	TRP	2.9
3	c	142	GLU	2.9
3	c	330	SER	2.9
19	z	1	MET	2.9
19	Z	57	LEU	2.9
3	c	203	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	c	27	ASP	2.9
13	O	54	GLY	2.9
13	O	58	ILE	2.9
3	C	473	ASP	2.8
1	A	229	GLU	2.8
2	B	2	GLY	2.8
2	B	3	LEU	2.8
2	b	402	TYR	2.7
13	O	55	ALA	2.7
2	b	195	PRO	2.7
12	M	2	GLU	2.7
14	T	27	PRO	2.7
2	B	476	ARG	2.7
14	T	28	ARG	2.7
13	O	88	GLU	2.7
13	O	89	ALA	2.7
2	B	397	VAL	2.7
2	B	162	PHE	2.7
7	h	3	ARG	2.7
18	X	12	ILE	2.6
5	e	84	LYS	2.6
13	O	87	GLN	2.6
13	O	56	TYR	2.6
1	a	224	ILE	2.6
12	m	5	GLN	2.6
3	c	204	LEU	2.6
3	c	148	GLY	2.6
1	A	15	GLU	2.6
13	O	90	GLU	2.6
3	C	28	GLN	2.6
2	B	347	ARG	2.6
3	C	262	ARG	2.5
13	O	52	ALA	2.5
1	A	251	ALA	2.5
3	c	191	PRO	2.5
2	b	219	VAL	2.5
2	b	228	ALA	2.5
3	C	266	TRP	2.5
3	C	261	ARG	2.5
3	c	192	GLY	2.5
18	x	42	GLN	2.5
5	E	83	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
15	U	54	LYS	2.5
13	o	54	GLY	2.5
6	f	12	SER	2.5
1	A	222	SER	2.5
12	m	4	ASN	2.5
17	g	31	ALA	2.5
2	B	295	GLY	2.5
3	C	137	PRO	2.4
19	Z	62	VAL	2.4
19	Z	56	VAL	2.4
13	O	59	ASP	2.4
18	X	45	LYS	2.4
11	L	7	ARG	2.4
2	b	217	ILE	2.4
7	H	66	GLY	2.4
7	h	26	GLY	2.4
2	B	84	THR	2.4
13	o	158	ASN	2.4
2	b	295	GLY	2.4
17	g	28	ILE	2.4
3	C	135	ARG	2.4
2	B	4	PRO	2.4
13	O	125	ASP	2.4
13	o	169	LYS	2.4
10	k	13	GLU	2.4
13	o	125	ASP	2.4
4	d	98	GLN	2.4
13	o	31	LEU	2.4
18	x	13	THR	2.4
19	Z	34	ASP	2.4
12	M	34	LYS	2.4
3	c	143	TYR	2.4
13	o	51	THR	2.4
3	C	147	PHE	2.4
19	Z	1	MET	2.4
13	O	53	ARG	2.3
11	L	5	PRO	2.3
2	B	214	LEU	2.3
2	b	70	GLY	2.3
2	b	403	GLY	2.3
3	c	371	GLY	2.3
2	B	370	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	294	SER	2.3
16	V	154	ASP	2.3
2	B	259	GLY	2.3
11	L	8	GLN	2.3
15	u	38	GLU	2.3
7	H	55	LEU	2.3
15	u	107	GLU	2.3
14	T	26	PRO	2.3
4	D	295	SER	2.3
7	h	56	ASP	2.3
3	C	144	SER	2.3
3	C	145	SER	2.3
13	o	32	THR	2.3
2	b	395	GLN	2.3
2	B	474	LEU	2.3
3	c	141	GLU	2.2
7	H	53	LEU	2.2
11	L	6	ASN	2.2
13	O	108	GLN	2.2
16	V	29	LEU	2.2
3	C	149	TYR	2.2
15	U	117	VAL	2.2
19	Z	4	LEU	2.2
16	V	43	LYS	2.2
2	b	294	SER	2.2
17	g	27	MET	2.2
13	O	50	ASP	2.2
13	O	162	ILE	2.2
2	B	491	VAL	2.2
13	o	30	THR	2.2
15	U	39	LEU	2.2
13	O	161	SER	2.2
13	O	220	LYS	2.2
2	b	398	THR	2.1
3	c	44	ASN	2.1
13	o	42	ALA	2.1
16	V	153	GLY	2.1
18	x	17	LYS	2.1
2	b	218	LEU	2.1
18	X	44	ASP	2.1
16	v	133	LEU	2.1
14	T	31	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	475	PHE	2.1
3	c	328	VAL	2.1
4	d	235	PHE	2.1
17	g	29	GLY	2.1
2	b	214	LEU	2.1
7	H	56	ASP	2.1
16	V	44	THR	2.1
2	B	188	ASP	2.1
17	y	45	ASN	2.1
13	o	190	LEU	2.0
18	X	46	VAL	2.0
16	v	103	LYS	2.0
3	c	146	PHE	2.0
10	k	14	ALA	2.0
7	H	6	TRP	2.0
13	o	232	GLY	2.0
8	I	34	ARG	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
33	LMT	i	102	35/35	0.35	1.16	10.65	99,136,146,150	0
31	LMG	c	520	45/55	0.55	1.18	6.72	82,119,140,168	0
27	BCR	B	620	40/40	0.60	0.79	6.17	77,87,92,92	0
31	LMG	C	520	45/55	0.27	1.27	5.74	80,119,142,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	LMT	I	102	35/35	0.39	0.93	5.61	94,136,147,149	0
33	LMT	D	411	31/35	0.59	1.00	4.55	82,132,156,156	0
33	LMT	B	624	35/35	0.64	0.64	4.54	91,142,154,155	0
28	DGD	D	410	63/66	0.56	0.74	4.26	104,127,181,188	0
27	BCR	K	102	40/40	0.73	0.76	4.04	74,85,102,103	0
23	CLA	c	503	65/65	0.88	0.80	4.00	73,89,97,103	0
27	BCR	c	514	40/40	0.77	0.86	3.98	66,80,89,91	0
23	CLA	D	403	65/65	0.82	0.85	3.93	73,85,121,124	0
25	PL9	J	101	35/55	0.30	0.52	3.78	119,157,183,185	0
27	BCR	c	515	40/40	0.77	1.10	3.75	83,95,112,115	0
27	BCR	C	514	40/40	0.78	0.82	3.70	70,80,86,90	0
33	LMT	b	626	35/35	0.55	1.07	3.68	99,143,152,153	0
23	CLA	a	409	65/65	0.74	0.58	3.61	55,69,129,134	0
28	DGD	d	408	63/66	0.56	0.65	3.58	104,127,184,187	0
23	CLA	B	603	65/65	0.88	0.69	3.22	65,80,91,105	0
23	CLA	c	501	65/65	0.86	0.63	3.21	68,81,89,95	0
23	CLA	b	607	65/65	0.84	0.39	3.20	62,67,112,117	0
23	CLA	B	605	65/65	0.85	0.60	3.08	58,77,87,92	0
27	BCR	c	516	40/40	0.69	0.80	3.08	76,86,93,103	0
23	CLA	c	507	65/65	0.83	0.66	3.07	84,94,102,109	0
28	DGD	B	626	52/66	0.71	0.46	3.05	77,104,179,183	0
27	BCR	Z	101	40/40	0.75	0.90	3.01	81,93,117,118	0
27	BCR	J	102	40/40	0.51	0.41	2.96	109,129,176,177	0
23	CLA	A	407	65/65	0.78	0.49	2.92	57,69,128,131	0
23	CLA	b	604	65/65	0.58	0.89	2.83	93,108,130,134	0
23	CLA	C	504	65/65	0.80	0.37	2.80	67,83,133,136	0
31	LMG	a	402	42/55	0.64	0.52	2.75	76,105,121,142	0
27	BCR	H	101	40/40	0.66	1.13	2.71	82,95,131,132	0
27	BCR	b	621	40/40	0.69	0.66	2.64	72,83,92,94	0
33	LMT	b	603	35/35	0.65	0.52	2.56	76,131,155,156	0
33	LMT	B	627	35/35	0.56	0.57	2.53	71,122,138,140	0
30	SQD	d	407	43/54	0.66	0.86	2.51	73,107,144,149	0
23	CLA	c	509	65/65	0.78	0.60	2.48	73,82,91,98	0
23	CLA	C	512	65/65	0.83	0.92	2.43	83,101,147,151	0
23	CLA	B	610	65/65	0.80	0.73	2.36	68,82,87,91	0
27	BCR	a	412	40/40	0.72	0.44	2.32	51,71,82,84	0
30	SQD	f	103	45/54	0.73	0.68	2.28	88,129,148,155	0
23	CLA	C	501	65/65	0.79	0.49	2.27	66,80,90,95	0
23	CLA	B	601	65/65	0.59	0.90	2.26	94,108,129,134	0
27	BCR	k	102	40/40	0.71	0.81	2.23	69,85,106,109	0
23	CLA	B	609	65/65	0.82	0.81	2.23	73,89,105,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	CLA	C	509	65/65	0.81	0.73	2.19	65,81,95,98	0
23	CLA	b	613	65/65	0.75	0.66	2.19	71,81,88,91	0
27	BCR	D	405	40/40	0.58	0.57	2.16	65,80,101,108	0
23	CLA	B	604	65/65	0.84	0.44	2.15	55,66,109,121	0
31	LMG	E	101	44/55	0.49	0.62	2.14	85,123,134,138	0
23	CLA	c	512	65/65	0.81	0.96	2.09	90,102,148,154	0
30	SQD	F	102	45/54	0.69	0.69	2.05	86,129,153,154	0
33	LMT	T	101	35/35	0.60	0.56	2.03	63,115,136,143	0
23	CLA	b	606	65/65	0.84	0.61	1.96	69,79,93,100	0
23	CLA	d	403	65/65	0.81	0.57	1.89	72,88,124,128	0
23	CLA	C	513	65/65	0.76	0.84	1.87	93,108,142,149	0
25	PL9	j	101	35/55	0.34	0.46	1.81	120,159,178,180	0
23	CLA	b	611	65/65	0.79	0.47	1.78	63,76,96,100	0
27	BCR	j	102	40/40	0.50	0.51	1.75	107,125,176,178	0
31	LMG	C	519	48/55	0.68	0.38	1.72	86,99,110,116	0
23	CLA	B	602	65/65	0.88	0.53	1.71	68,87,96,99	0
28	DGD	A	411	56/66	0.72	0.40	1.70	79,100,145,149	0
31	LMG	A	418	42/55	0.64	0.43	1.68	76,107,120,142	0
34	HEM	F	101	43/43	0.87	0.44	1.67	92,104,127,128	0
27	BCR	f	102	40/40	0.73	0.45	1.65	64,83,107,110	0
23	CLA	c	513	65/65	0.68	0.93	1.65	94,107,138,149	0
23	CLA	c	511	65/65	0.78	0.61	1.63	72,91,102,106	0
27	BCR	A	410	40/40	0.65	0.46	1.60	53,68,81,91	0
23	CLA	B	608	65/65	0.85	0.61	1.60	62,74,94,97	0
23	CLA	b	616	65/65	0.93	0.32	1.59	54,68,90,92	0
23	CLA	b	608	65/65	0.84	0.45	1.59	58,76,85,89	0
23	CLA	B	612	65/65	0.88	0.41	1.51	56,69,84,87	0
24	PHO	A	406	64/64	0.79	0.39	1.44	57,69,74,76	0
28	DGD	B	621	58/66	0.77	0.45	1.43	51,69,99,106	0
23	CLA	b	618	65/65	0.80	0.56	1.41	78,97,109,116	0
33	LMT	x	102	31/35	0.54	0.68	1.41	79,130,156,157	0
23	CLA	C	503	65/65	0.76	0.51	1.41	76,88,99,101	0
27	BCR	C	515	40/40	0.71	0.56	1.40	76,87,95,98	0
23	CLA	b	614	65/65	0.87	0.34	1.37	57,71,79,93	0
23	CLA	C	502	65/65	0.73	0.50	1.35	62,72,104,112	0
31	LMG	d	405	46/55	0.84	0.33	1.34	65,71,116,128	0
22	BCT	A	402	4/4	0.93	0.42	1.33	84,88,89,93	0
28	DGD	b	602	52/66	0.61	0.57	1.32	81,104,177,178	0
23	CLA	b	619	65/65	0.72	0.62	1.31	78,99,142,147	0
23	CLA	b	605	65/65	0.84	0.44	1.31	73,87,96,98	0
30	SQD	a	401	54/54	0.73	0.45	1.30	75,116,152,156	0
23	CLA	B	606	65/65	0.80	0.59	1.29	68,84,111,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
27	BCR	B	618	40/40	0.68	0.35	1.28	68,80,90,92	0
23	CLA	C	510	65/65	0.85	0.32	1.26	63,73,85,93	0
31	LMG	M	101	42/55	0.73	0.40	1.25	78,110,135,144	0
23	CLA	C	507	65/65	0.74	0.59	1.24	77,92,101,105	0
24	PHO	a	408	64/64	0.80	0.35	1.22	58,71,81,87	0
23	CLA	b	609	65/65	0.81	0.58	1.21	71,86,111,121	0
23	CLA	b	612	65/65	0.83	0.66	1.20	69,89,104,106	0
23	CLA	B	615	65/65	0.86	0.63	1.17	82,94,108,116	0
31	LMG	e	101	44/55	0.70	0.41	1.15	85,122,133,140	0
25	PL9	a	410	45/55	0.76	0.35	1.08	82,98,119,127	0
23	CLA	c	502	65/65	0.76	0.52	1.07	67,75,101,107	0
34	HEM	V	201	43/43	0.90	0.35	1.04	46,65,74,79	0
33	LMT	B	628	35/35	0.66	0.49	1.03	72,137,162,163	0
28	DGD	a	413	56/66	0.74	0.39	1.03	74,101,145,149	0
26	OEC	A	409	5/9	0.96	0.43	1.00	35,44,46,62	0
28	DGD	c	518	62/66	0.82	0.33	0.98	65,86,138,143	0
23	CLA	c	506	65/65	0.79	0.45	0.98	79,94,122,126	0
28	DGD	C	518	66/66	0.69	0.36	0.96	58,72,106,121	0
28	DGD	C	517	62/66	0.80	0.33	0.91	61,84,132,147	0
23	CLA	C	506	65/65	0.69	0.46	0.91	75,91,123,134	0
27	BCR	b	620	40/40	0.79	0.30	0.90	59,72,79,80	0
30	SQD	D	409	43/54	0.71	0.58	0.88	72,103,147,151	0
31	LMG	M	102	42/55	0.67	0.44	0.85	70,109,133,139	0
30	SQD	b	601	47/54	0.73	0.39	0.84	86,99,139,146	0
29	LHG	a	414	39/49	0.82	0.36	0.79	62,79,91,94	0
29	LHG	A	412	39/49	0.80	0.32	0.77	61,80,92,94	0
23	CLA	B	616	65/65	0.81	0.61	0.77	75,93,144,150	0
26	OEC	a	411	5/9	0.94	0.39	0.74	35,44,62,62	0
30	SQD	a	415	51/54	0.74	0.38	0.74	81,102,128,134	0
23	CLA	b	615	65/65	0.87	0.33	0.74	62,72,83,94	0
23	CLA	a	404	65/65	0.91	0.35	0.73	44,58,65,73	0
32	CL	A	416	1/1	0.74	0.39	0.73	49,49,49,49	0
23	CLA	c	508	65/65	0.89	0.31	0.71	73,84,120,134	0
25	PL9	A	408	45/55	0.72	0.46	0.69	84,103,119,127	0
27	BCR	x	101	40/40	0.70	0.72	0.68	81,97,129,130	0
23	CLA	C	511	65/65	0.81	0.49	0.64	73,90,100,109	0
31	LMG	k	103	48/55	0.73	0.43	0.61	80,100,118,120	0
30	SQD	A	417	54/54	0.77	0.37	0.61	81,116,146,153	0
27	BCR	T	103	40/40	0.77	0.32	0.60	69,79,87,95	0
31	LMG	D	406	46/55	0.86	0.29	0.59	55,74,116,125	0
29	LHG	a	417	37/49	0.63	0.43	0.52	111,134,197,206	0
28	DGD	c	519	66/66	0.76	0.34	0.51	61,72,104,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	SQD	B	625	47/54	0.76	0.38	0.51	73,102,139,146	0
23	CLA	B	613	65/65	0.90	0.27	0.44	44,63,88,92	0
34	HEM	v	201	43/43	0.89	0.46	0.43	61,68,75,78	0
23	CLA	C	505	65/65	0.85	0.34	0.42	69,77,84,88	0
30	SQD	A	413	51/54	0.76	0.34	0.42	81,95,126,130	0
28	DGD	b	622	58/66	0.83	0.34	0.42	57,71,97,102	0
34	HEM	f	101	43/43	0.90	0.38	0.42	77,103,125,130	0
24	PHO	a	407	64/64	0.83	0.32	0.41	52,62,71,76	0
23	CLA	c	505	65/65	0.85	0.30	0.38	66,78,83,86	0
31	LMG	a	416	51/55	0.76	0.33	0.38	61,80,92,99	0
23	CLA	c	510	65/65	0.90	0.33	0.34	66,74,85,87	0
27	BCR	B	617	40/40	0.79	0.28	0.32	64,73,79,80	0
31	LMG	D	407	49/55	0.74	0.35	0.20	59,80,109,117	0
28	DGD	c	517	53/66	0.86	0.28	0.18	58,75,98,102	0
23	CLA	c	504	65/65	0.86	0.28	0.17	69,82,132,136	0
23	CLA	b	617	65/65	0.84	0.31	0.15	67,82,130,135	0
23	CLA	B	614	65/65	0.71	0.42	0.11	64,83,124,132	0
33	LMT	m	101	35/35	0.76	0.51	0.11	71,95,109,109	0
27	BCR	B	619	40/40	0.81	0.27	0.07	62,76,82,84	0
23	CLA	C	508	65/65	0.86	0.30	0.04	70,84,123,140	0
31	LMG	B	622	49/55	0.80	0.30	0.03	50,74,85,91	0
24	PHO	D	402	64/64	0.83	0.30	0.01	48,61,71,77	0
23	CLA	A	404	65/65	0.92	0.33	0.00	39,54,66,70	0
23	CLA	a	405	65/65	0.85	0.33	-0.04	40,54,65,72	0
23	CLA	d	402	65/65	0.86	0.30	-0.04	49,59,79,91	0
25	PL9	d	404	55/55	0.73	0.32	-0.05	48,65,76,86	0
31	LMG	A	414	51/55	0.86	0.27	-0.06	61,74,88,96	0
25	PL9	D	404	55/55	0.81	0.30	-0.07	47,59,70,74	0
31	LMG	D	408	48/55	0.85	0.27	-0.08	52,73,83,120	0
23	CLA	a	406	65/65	0.84	0.29	-0.14	53,70,143,149	0
23	CLA	A	405	65/65	0.86	0.27	-0.15	48,69,139,145	0
23	CLA	A	403	65/65	0.89	0.27	-0.20	47,58,67,68	0
23	CLA	B	611	65/65	0.88	0.32	-0.26	65,73,80,81	0
22	BCT	d	401	4/4	0.88	0.26	-0.27	77,80,82,85	0
23	CLA	b	610	65/65	0.86	0.31	-0.27	52,64,82,88	0
23	CLA	D	401	65/65	0.91	0.26	-0.29	47,58,85,99	0
27	BCR	T	102	40/40	0.85	0.27	-0.34	66,73,83,85	0
29	LHG	A	415	37/49	0.63	0.41	-0.35	108,137,192,202	0
31	LMG	d	406	48/55	0.84	0.26	-0.44	56,71,86,120	0
28	DGD	C	516	53/66	0.92	0.25	-0.47	58,75,97,102	0
33	LMT	M	103	35/35	0.78	0.35	-0.47	68,98,108,115	0
31	LMG	b	624	49/55	0.77	0.29	-0.54	56,76,88,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	LMG	b	623	49/55	0.91	0.25	-0.67	57,80,96,113	0
23	CLA	B	607	65/65	0.90	0.25	-0.83	56,64,84,91	0
32	CL	d	409	1/1	0.88	0.25	-1.14	49,49,49,49	0
21	FE2	A	401	1/1	0.94	0.15	-1.33	60,60,60,60	0
21	FE2	a	403	1/1	0.97	0.13	-3.14	70,70,70,70	0
35	CA	O	301	1/1	0.78	0.31	-	123,123,123,123	0
35	CA	K	101	1/1	0.40	0.51	-	72,72,72,72	0
35	CA	o	301	1/1	0.69	0.43	-	106,106,106,106	0
35	CA	k	101	1/1	0.87	0.21	-	94,94,94,94	0
33	LMT	b	625	35/35	0.75	0.57	-	78,139,172,176	0
33	LMT	B	623	35/35	0.46	0.86	-	76,136,170,172	0
31	LMG	I	101	43/55	0.67	0.70	-	87,115,159,171	0
31	LMG	i	101	43/55	0.67	0.69	-	85,120,158,176	0

6.5 Other polymers

There are no such residues in this entry.