



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 12:13 PM EDT

PDB ID : 4TNI
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 Å resolution
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : unknown
Resolution : 4.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)

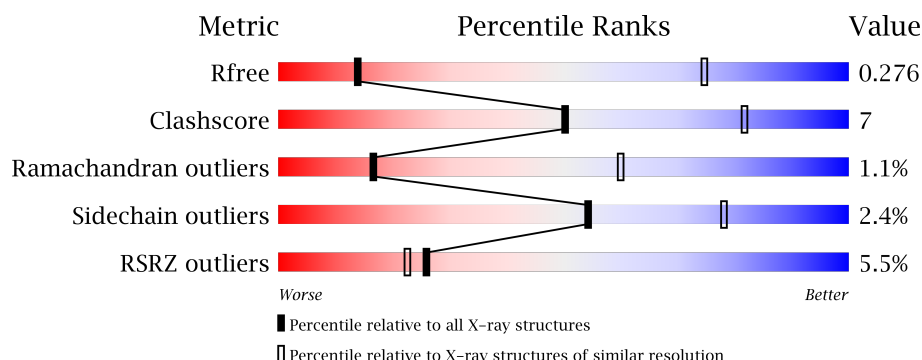
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1005 (5.52-3.66)
Clashscore	112137	1052 (5.50-3.70)
Ramachandran outliers	110173	1041 (5.52-3.66)
Sidechain outliers	110143	1021 (5.50-3.66)
RSRZ outliers	101464	1014 (5.52-3.66)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	615	X	-	-	X
22	CLA	C	501	X	-	-	X
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	X
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	X
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	520	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	D	406	X	-	-	X
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	X	-	-	-
22	CLA	a	407	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	X
22	CLA	b	618	X	-	-	X
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	X
22	CLA	c	506	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	X
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	405	X	-	-	X
22	CLA	d	406	X	-	-	X
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	d	407	-	-	-	X
23	PL9	j	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	513	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	F	102	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	J	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	409	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	513	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	521	-	-	-	X
24	BCR	f	102	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	C	517	-	-	-	X
25	DGD	D	410	-	-	-	X
25	DGD	a	410	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	410	-	-	-	X
27	LMG	A	414	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	m	101	-	-	-	X
28	OEX	A	411	-	-	-	X
28	OEX	a	414	-	-	-	X
29	SQD	B	622	-	-	-	X
29	SQD	B	626	-	-	-	X
29	SQD	F	103	-	-	-	X
29	SQD	a	401	-	-	-	X
29	SQD	b	602	-	-	-	X
29	SQD	d	403	-	-	-	X
29	SQD	f	103	-	-	-	X
30	LMT	B	624	-	-	-	X
30	LMT	B	627	-	-	-	X
30	LMT	B	628	-	-	-	X
30	LMT	D	411	-	-	-	X
30	LMT	I	102	-	-	-	X
30	LMT	M	103	-	-	-	X
30	LMT	b	603	-	-	-	X
30	LMT	b	604	-	-	-	X
30	LMT	b	627	-	-	-	X
30	LMT	d	411	-	-	-	X
30	LMT	i	102	-	-	-	X
31	PHO	d	401	-	-	-	X
32	CL	a	413	-	-	-	X
34	HEM	F	101	-	-	-	X
34	HEM	v	201	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

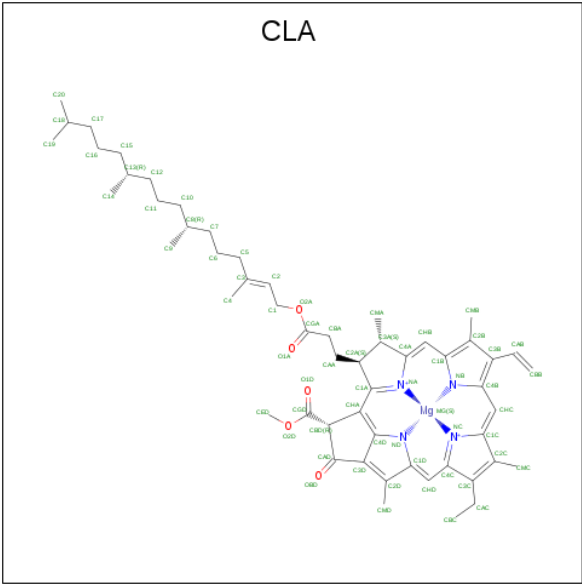
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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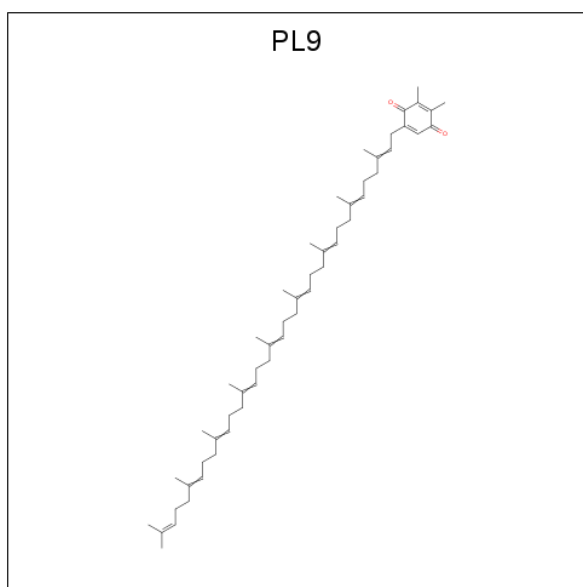
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22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55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

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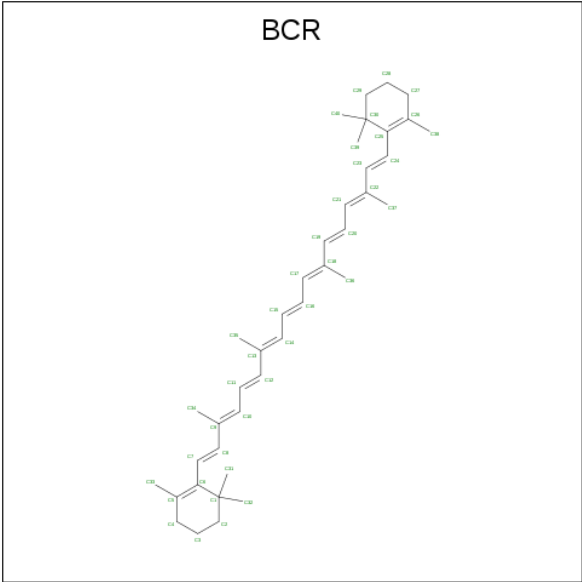
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



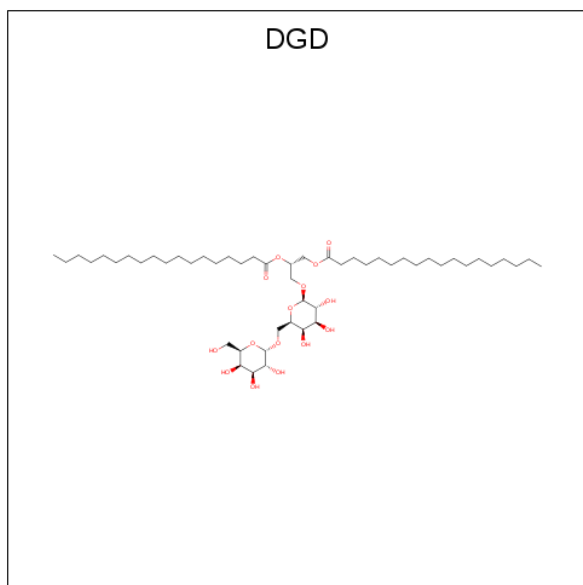
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total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

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

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



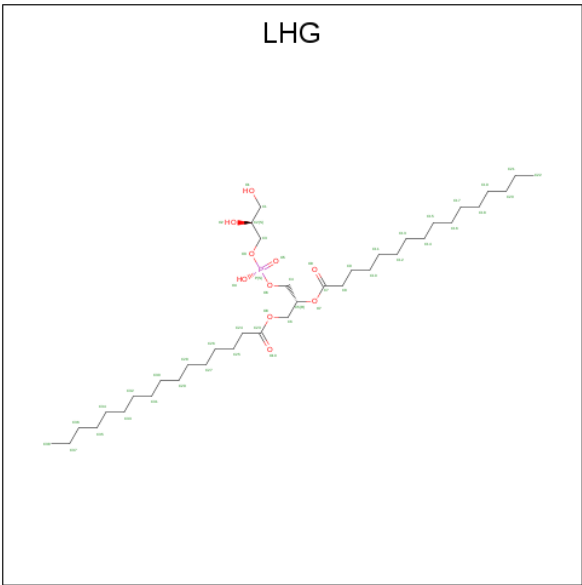
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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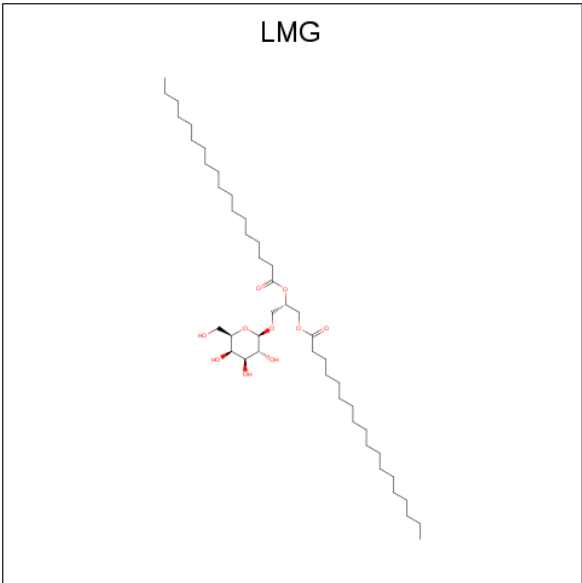
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



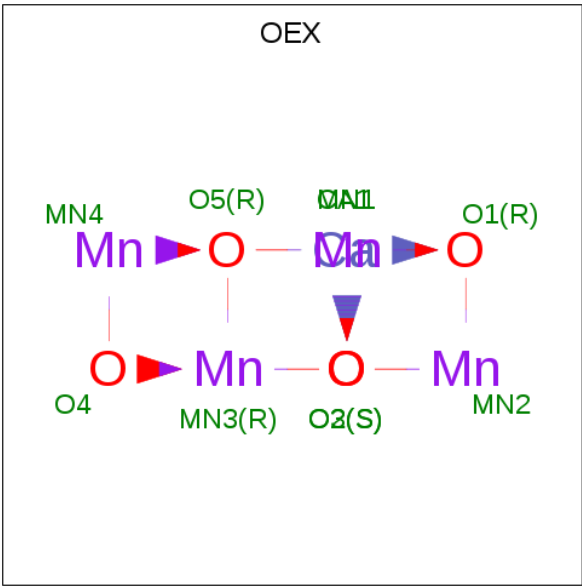
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



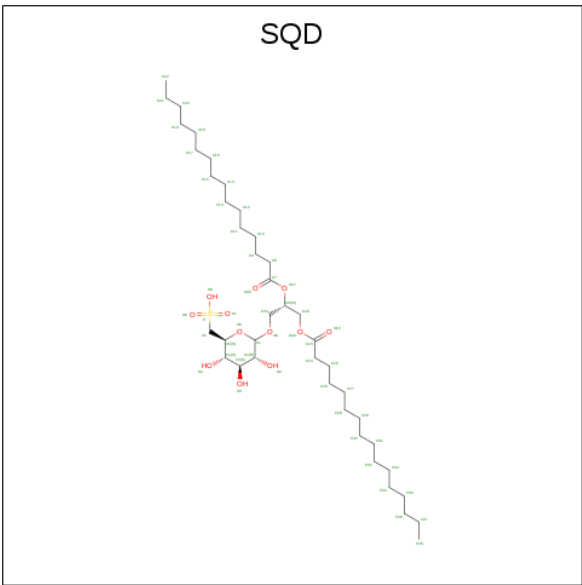
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total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

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



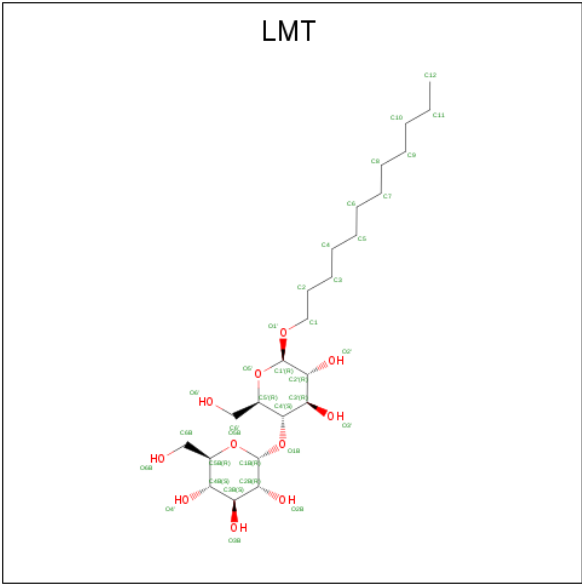
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).



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

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



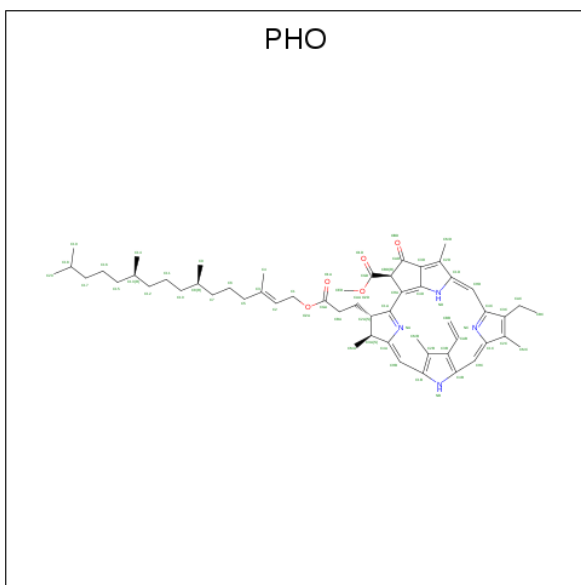
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).

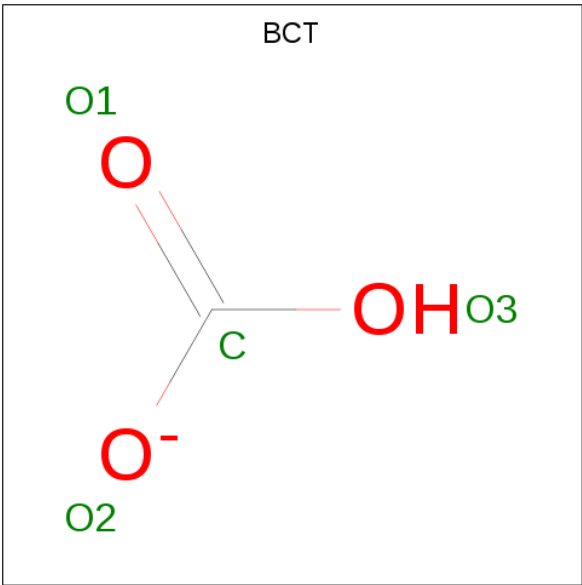


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		

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

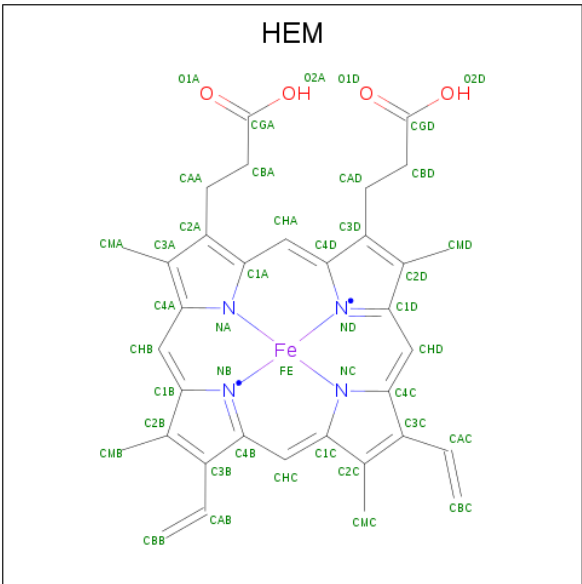
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	a	1	Total	Cl	0	0
			1	1		
32	D	1	Total	Cl	0	0
			1	1		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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

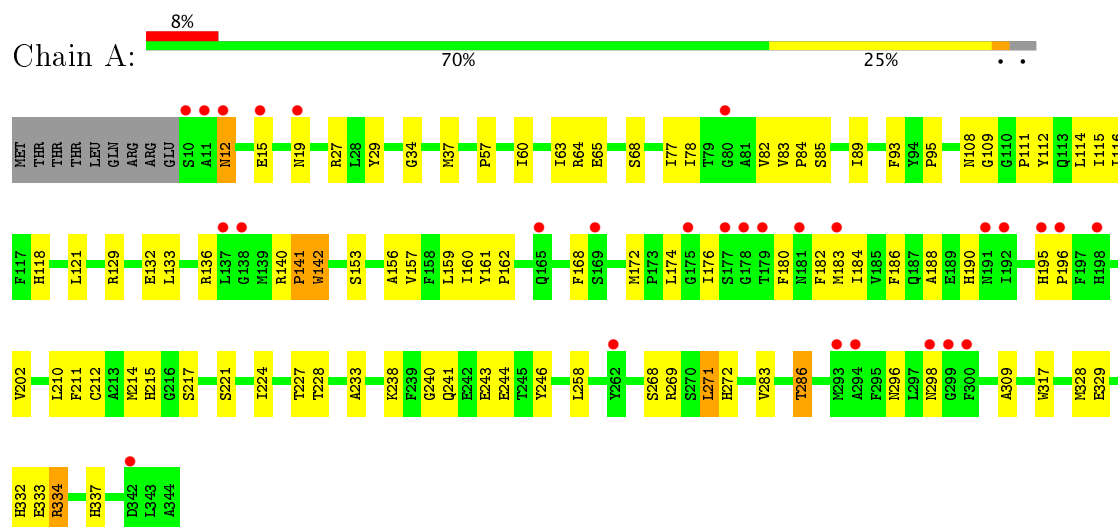
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

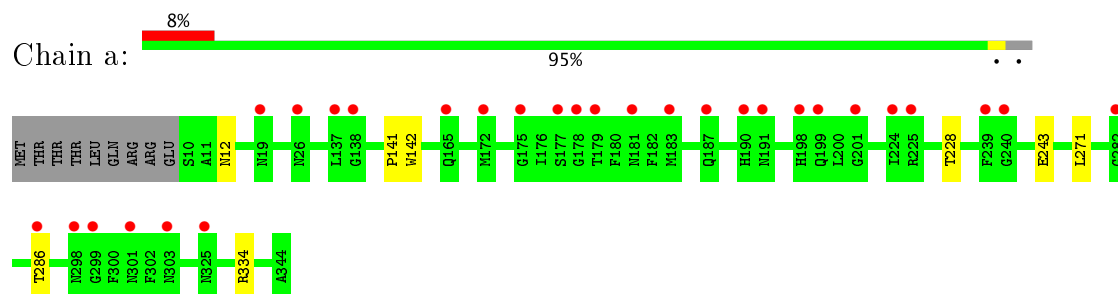
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

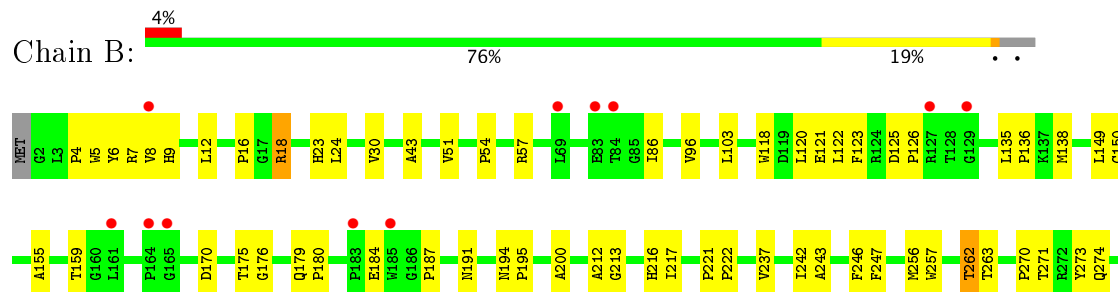
- Molecule 1: Photosystem Q(B) protein 1

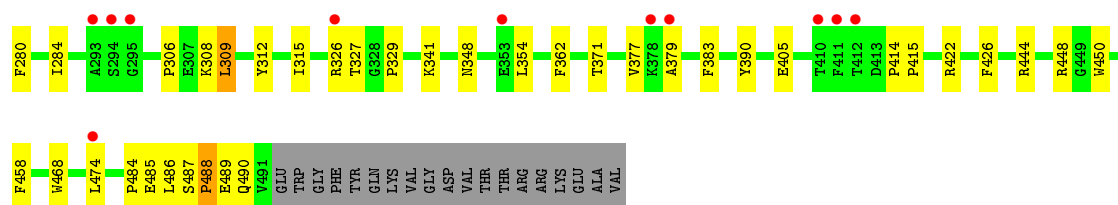


- Molecule 1: Photosystem Q(B) protein 1

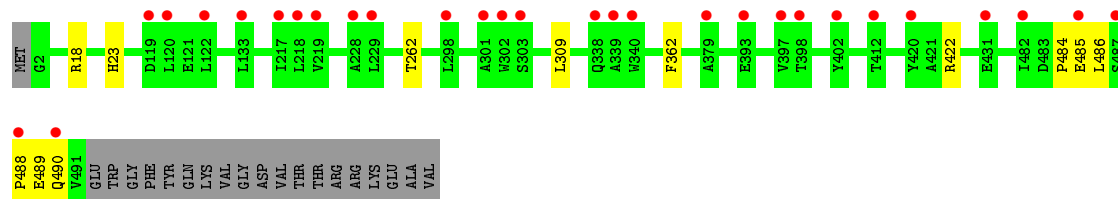


- Molecule 2: Photosystem II core light harvesting protein

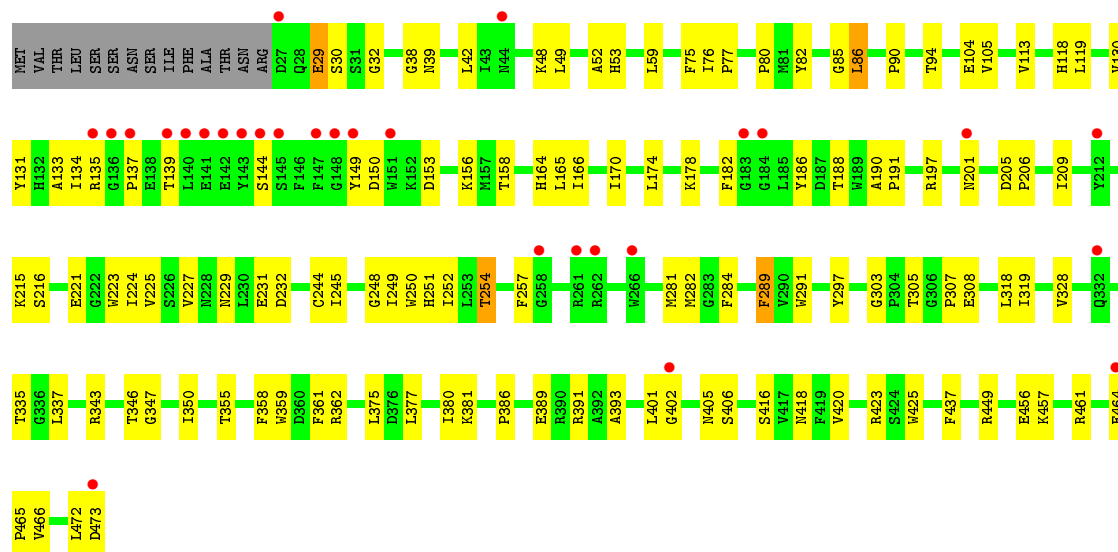




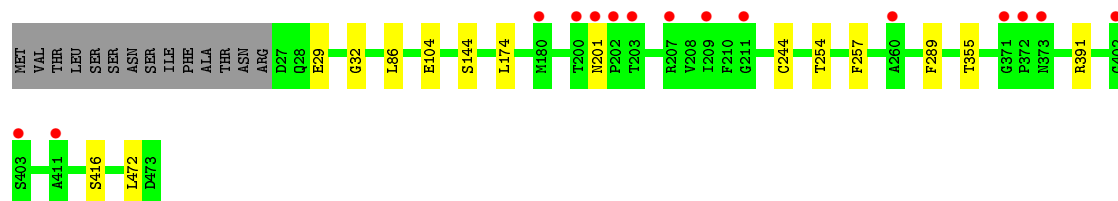
• Molecule 2: Photosystem II core light harvesting protein



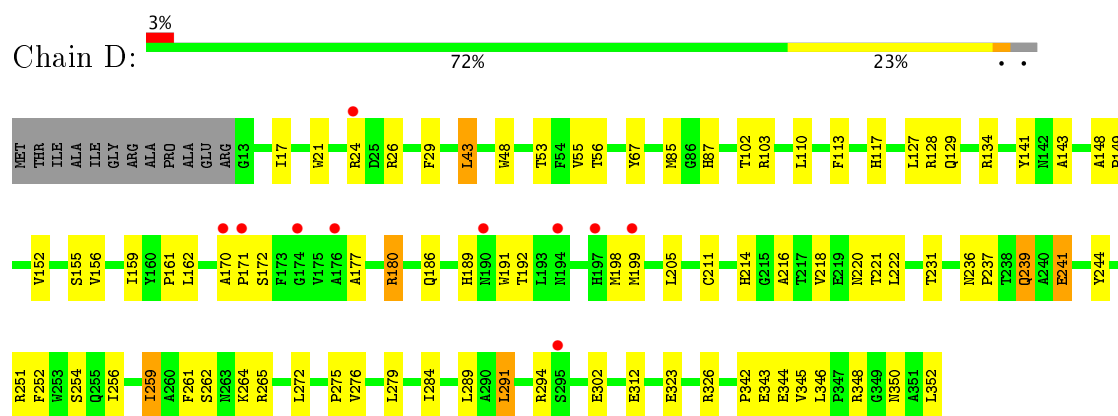
• Molecule 3: Photosystem II CP43 protein



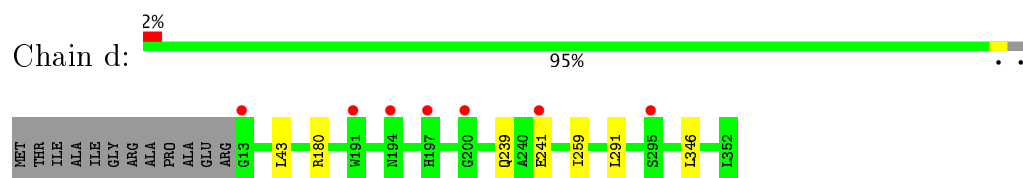
• Molecule 3: Photosystem II CP43 protein



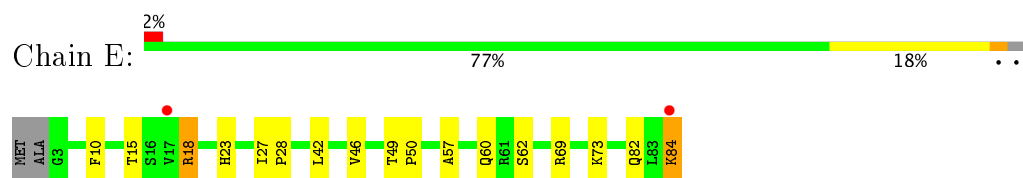
• Molecule 4: Photosystem II D2 protein



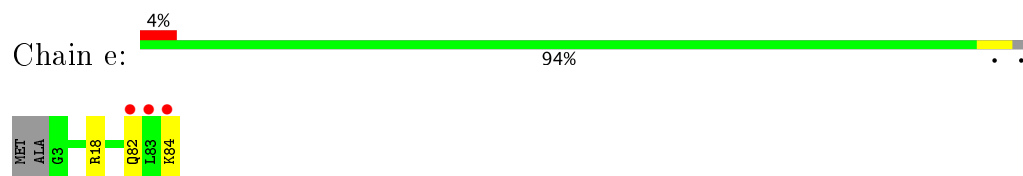
- Molecule 4: Photosystem II D2 protein



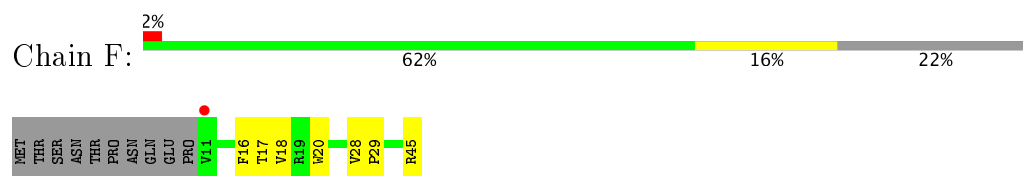
- Molecule 5: Cytochrome b559 subunit alpha



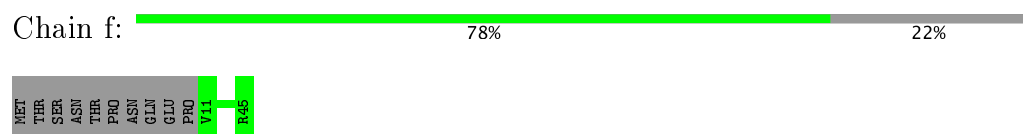
- Molecule 5: Cytochrome b559 subunit alpha



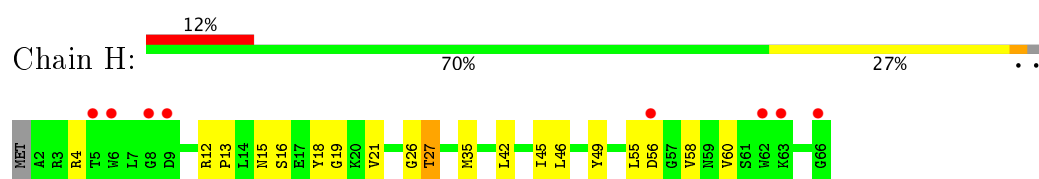
- Molecule 6: Cytochrome b559 subunit beta



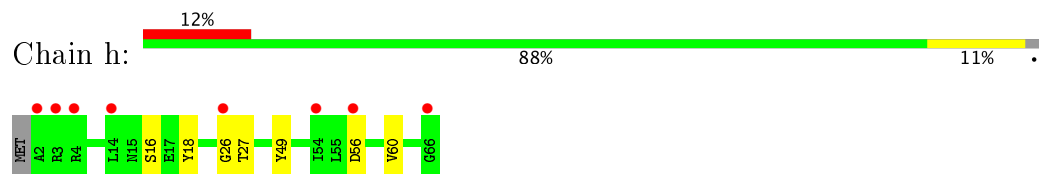
- Molecule 6: Cytochrome b559 subunit beta



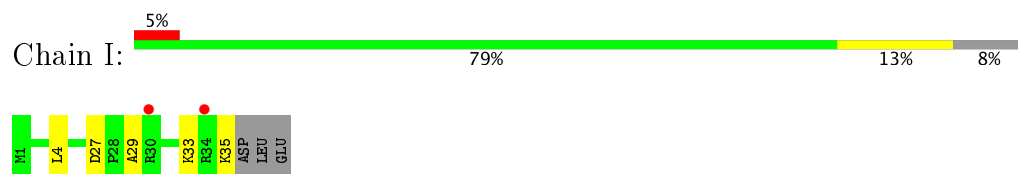
- Molecule 7: Photosystem II reaction center protein H



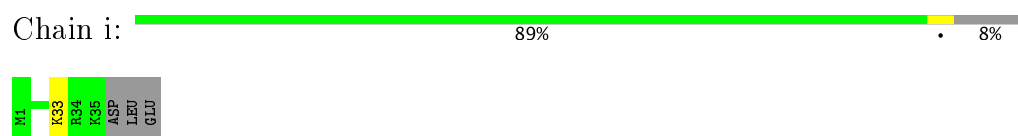
• Molecule 7: Photosystem II reaction center protein H



• Molecule 8: Photosystem II reaction center protein I



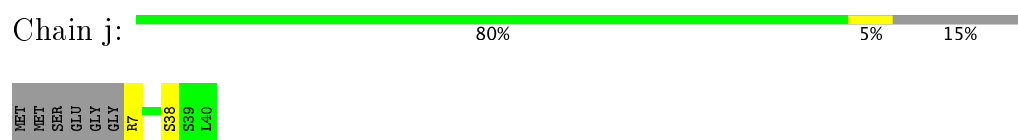
• Molecule 8: Photosystem II reaction center protein I



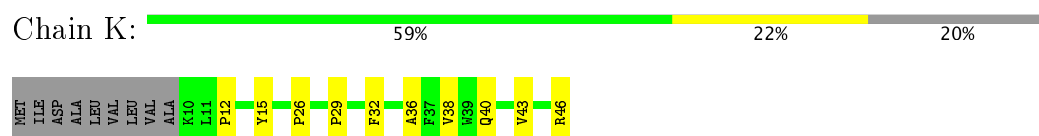
• Molecule 9: Photosystem II reaction center protein J



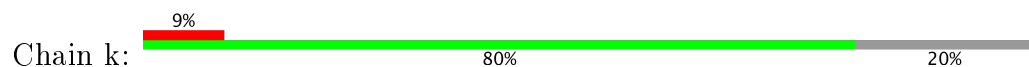
• Molecule 9: Photosystem II reaction center protein J

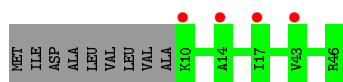


• Molecule 10: Photosystem II reaction center protein K

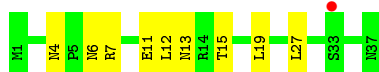
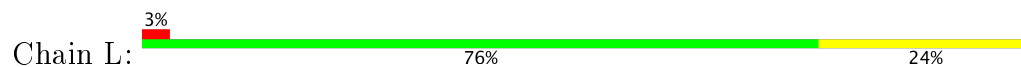


• Molecule 10: Photosystem II reaction center protein K





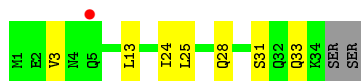
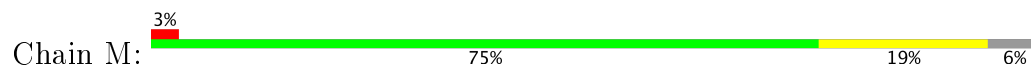
- Molecule 11: Photosystem II reaction center protein L



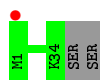
- Molecule 11: Photosystem II reaction center protein L



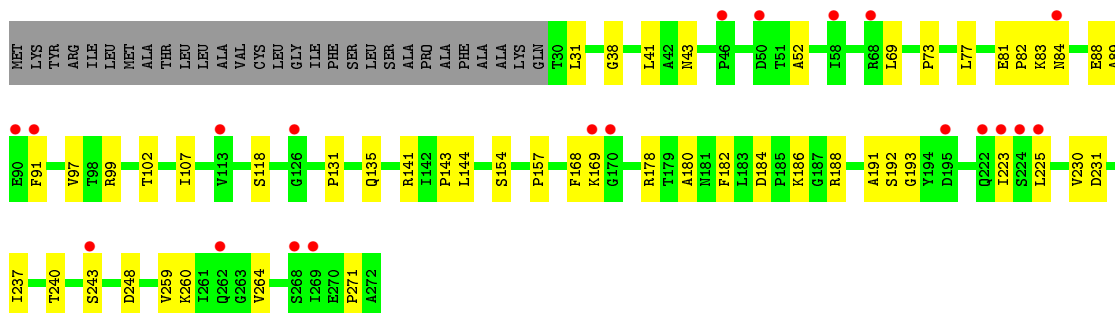
- Molecule 12: Photosystem II reaction center protein M



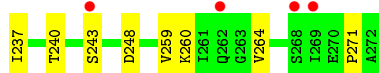
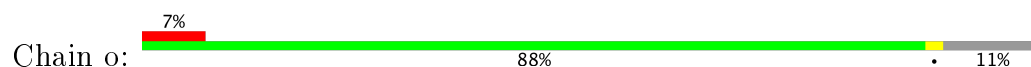
- Molecule 12: Photosystem II reaction center protein M

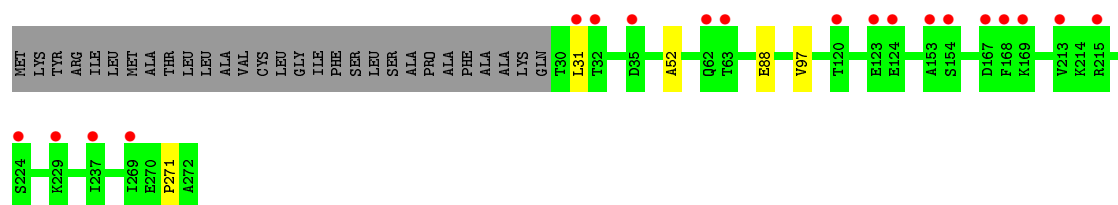


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

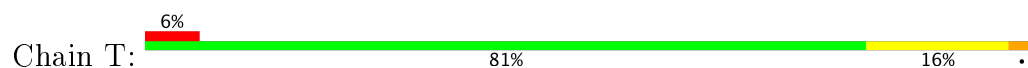


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

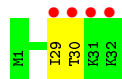




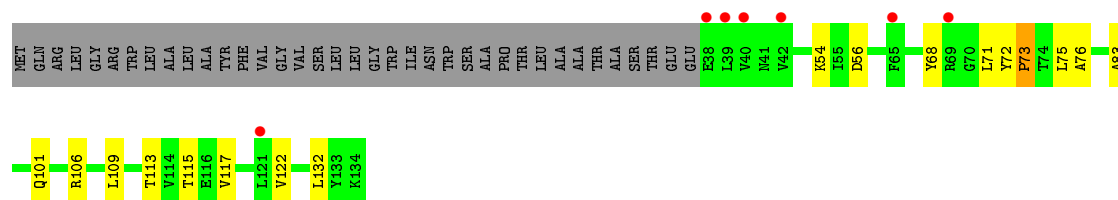
- Molecule 14: Photosystem II reaction center protein T



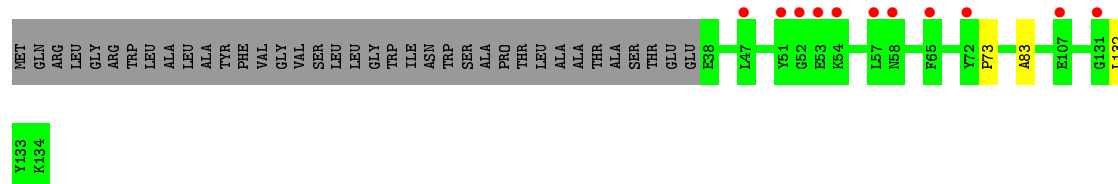
- Molecule 14: Photosystem II reaction center protein T



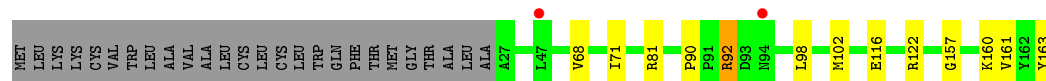
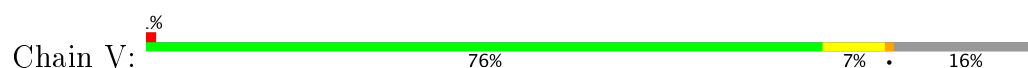
- Molecule 15: Photosystem II 12 kDa extrinsic protein



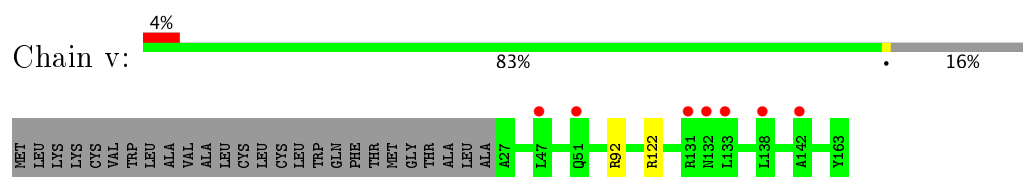
- Molecule 15: Photosystem II 12 kDa extrinsic protein



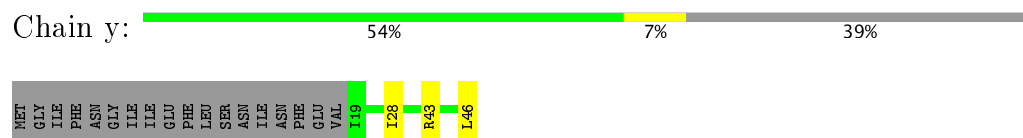
- Molecule 16: Cytochrome c-550



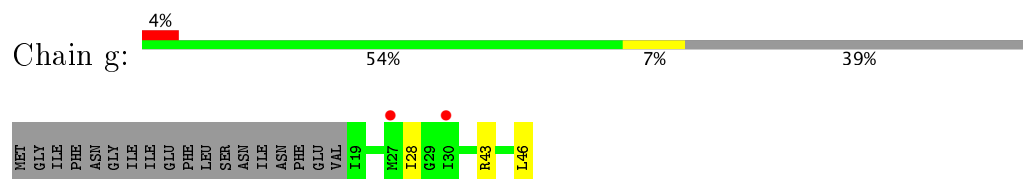
- Molecule 16: Cytochrome c-550



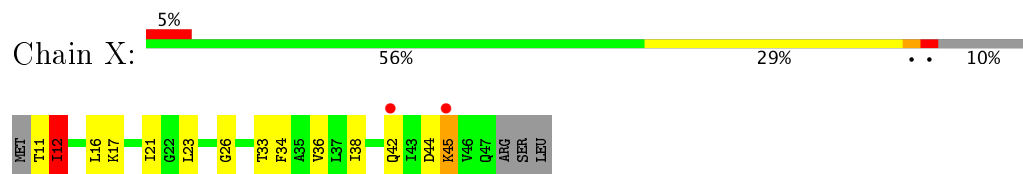
- Molecule 17: Photosystem II reaction center protein Ycf12



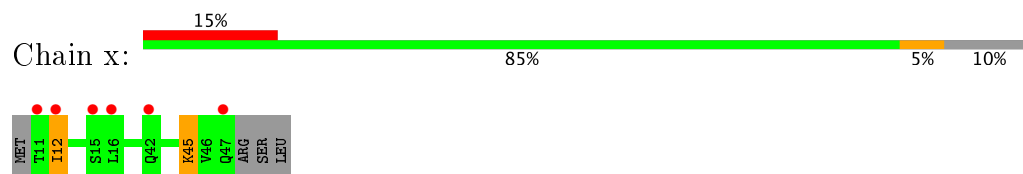
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



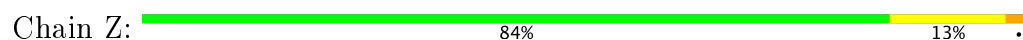
There are no outlier residues recorded for this chain.

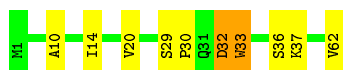
- Molecule 19: Photosystem II reaction center protein Y



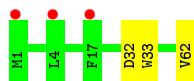
There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z





- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.7 (72.96-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.278 , 0.284 0.273 , 0.276	Depositor DCC
R_{free} test set	2524 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 126.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.22	0/3556	0.41	0/4842
3	c	0.22	0/3556	0.41	0/4842
4	D	0.23	0/2801	0.40	0/3818
4	d	0.24	0/2801	0.40	0/3818
5	E	0.23	0/685	0.42	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.45	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.21	0/255	0.39	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.48	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.43	0/367
12	m	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.42	0/1064
15	u	0.22	0/785	0.43	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.40	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.21	0/202	0.45	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.25	0/273	0.43	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	78	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	83	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	74	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	17	0
7	h	507	0	521	0	0
8	I	286	0	308	3	0
8	i	286	0	308	0	0
9	J	249	0	262	7	0
9	j	249	0	262	0	0
10	K	293	0	305	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	7	0
11	l	304	0	316	0	0
12	M	267	0	289	7	0
12	m	267	0	289	0	0
13	O	1845	0	1801	31	0
13	o	1845	0	1801	0	0
14	T	275	0	288	5	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	44	0
22	B	975	0	1080	90	0
22	C	845	0	936	47	0
22	D	130	0	144	11	0
22	H	65	0	72	9	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	4	0
23	D	55	0	80	12	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	3	0
24	B	160	0	224	10	0
24	C	80	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	40	0	56	4	0
24	H	40	0	56	2	0
24	J	40	0	56	1	0
24	K	40	0	56	3	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	11	0
25	D	63	0	87	2	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	4	0
27	D	143	0	196	11	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	93	0	126	0	0
27	b	49	0	68	0	0
27	c	93	0	126	0	0
27	d	143	0	196	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	m	42	0	54	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	105	0	147	6	0
29	B	90	0	111	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	45	0	54	3	0
29	a	105	0	147	0	0
29	b	47	0	61	0	0
29	d	43	0	50	0	0
29	f	45	0	54	0	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	1	0
30	M	70	0	91	0	0
30	b	140	0	183	0	0
30	d	31	0	35	0	0
30	i	35	0	46	0	0
31	D	128	0	148	15	0
31	d	128	0	148	0	0
32	D	1	0	0	0	0
32	a	1	0	0	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51372	579	0

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

All (579) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.55	0.87
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.51	0.81
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.61	0.80
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.66	0.77
4:D:199:MET:HG2	23:D:407:PL9:H322	1.69	0.74

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.48
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.48
13:O:118:SER:HB3	13:O:157:PRO:HA	1.99	0.48
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.95	0.48
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.70	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
27:C:518:LMG:H292	27:C:518:LMG:H111	1.95	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
22:A:405:CLA:HMA2	23:D:407:PL9:H411	24.71	0.47
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.96	0.47
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.52	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	1.99	0.47
3:C:158:THR:O	3:C:251:HIS:HB3	2.14	0.47
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.47
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.63	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.80	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.97	0.47
22:B:615:CLA:H72	22:B:615:CLA:H12	1.97	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.98	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.47
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.97	0.47
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.97	0.47
22:C:501:CLA:H193	22:C:506:CLA:H111	2.04	0.47
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.47
4:D:262:SER:N	27:D:409:LMG:O3	2.46	0.47
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.47	0.47
22:A:405:CLA:H162	22:A:405:CLA:H141	1.71	0.46
22:B:607:CLA:H18	22:B:608:CLA:H192	1.97	0.46
27:I:101:LMG:H181	30:I:102:LMT:H42	2.04	0.46
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.98	0.46
1:A:202:VAL:HB	22:A:404:CLA:HMB3	12.99	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.01	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
4:D:48:TRP:CE2	31:D:402:PHO:H161	2.50	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.99	0.46
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.05	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:101:CLA:H62	22:H:101:CLA:H41	1.56	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.52	0.46
22:H:101:CLA:H162	22:H:101:CLA:H122	1.50	0.46
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.46
22:A:404:CLA:H161	23:A:406:PL9:H253	1.96	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
4:D:261:PHE:HB2	23:D:407:PL9:H522	1.98	0.46
2:B:170:ASP:OD1	2:B:175:THR:N	2.50	0.46
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.46
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.51	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.18	0.46
31:D:401:PHO:H41	31:D:401:PHO:H62	1.47	0.46
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.51	0.46
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.01	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.98	0.46
24:B:616:BCR:H20C	24:B:616:BCR:H361	1.76	0.46
22:C:510:CLA:H61	22:C:510:CLA:H93	1.81	0.46
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.79	0.46
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.46
27:D:409:LMG:HC1	27:D:409:LMG:O9	2.18	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.52	0.45
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.82	0.45
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.45
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.45
12:M:24:ILE:HG21	27:M:101:LMG:H322	9.39	0.45
22:B:607:CLA:H51	22:B:608:CLA:H101	1.98	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.48	0.45
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.99	0.45
22:B:603:CLA:HMD2	22:B:611:CLA:H193	1.99	0.45
24:B:618:BCR:H361	24:B:618:BCR:H20C	1.82	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.45
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.77	0.45
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.45
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.45
1:A:114:LEU:O	1:A:118:HIS:ND1	2.46	0.45
22:A:402:CLA:HBA1	22:A:402:CLA:H3A	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ALA:O	2:B:216:HIS:ND1	2.52	0.45
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.19	0.45
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.45
22:B:614:CLA:H172	22:B:614:CLA:H111	1.99	0.45
24:C:514:BCR:H361	24:C:514:BCR:H20C	1.83	0.45
13:O:143:PRO:HG2	13:O:248:ASP:HB3	1.98	0.45
22:A:402:CLA:H51	31:D:401:PHO:C3B	2.47	0.45
22:B:611:CLA:H162	22:B:611:CLA:H122	1.76	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.18	0.45
30:B:628:LMT:H122	14:T:7:VAL:HG12	34.40	0.45
16:V:98:LEU:O	16:V:102:MET:HG3	2.22	0.45
1:A:224:ILE:O	4:D:265:ARG:NH2	2.49	0.45
22:A:405:CLA:H162	22:A:405:CLA:H202	3.78	0.45
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.45
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.17	0.45
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.45
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.04	0.45
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.31	0.45
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.03	0.45
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.57	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.27	0.44
22:B:605:CLA:HBA2	22:B:605:CLA:H3A	1.26	0.44
22:C:508:CLA:H11	22:C:508:CLA:H51	1.82	0.44
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.00	0.44
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.42	0.44
22:C:504:CLA:H11	24:C:514:BCR:H312	2.01	0.44
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.44
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.44
22:B:613:CLA:H51	24:B:616:BCR:H372	1.98	0.44
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.44
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.78	0.44
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.99	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.18	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.44
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.99	0.44
22:C:501:CLA:H141	22:C:501:CLA:H162	1.78	0.44
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.71	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.01	0.44
3:C:224:ILE:O	3:C:227:VAL:HG23	2.18	0.44
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.00	0.44
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.44
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.18	0.44
1:A:202:VAL:HB	22:A:402:CLA:HMB3	2.00	0.44
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.53	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.92	0.44
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.00	0.44
22:C:512:CLA:HBA2	22:C:512:CLA:H3A	1.72	0.43
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.43
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.81	0.43
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.06	0.43
3:C:245:ILE:O	3:C:249:ILE:HG12	2.17	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.43
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
22:B:605:CLA:C3D	30:B:623:LMT:H11	2.49	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
1:A:271:LEU:HD21	23:A:406:PL9:HC71	1.99	0.43
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.43
22:C:503:CLA:H201	22:C:503:CLA:HMD2	2.02	0.43
31:D:401:PHO:H13	31:D:401:PHO:H102	1.82	0.43
22:D:405:CLA:H62	22:D:405:CLA:H92	1.79	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.58	0.43
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.18	0.43
22:B:606:CLA:H2	22:B:608:CLA:H93	34.06	0.43
24:C:513:BCR:H24C	24:C:513:BCR:H371	1.78	0.43
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.54	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.43
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.43
22:A:404:CLA:H143	22:A:404:CLA:H161	1.86	0.43
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.06	0.43
30:B:628:LMT:H3'	30:B:628:LMT:H1B	1.53	0.43
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.58	0.43
11:L:4:ASN:OD1	11:L:6:ASN:ND2	2.49	0.43
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:468:TRP:HH2	27:D:408:LMG:HO2	1.63	0.43
22:B:615:CLA:H162	22:B:615:CLA:H122	5.18	0.43
3:C:29:GLU:HB2	3:C:30:SER:H	1.64	0.43
6:F:16:PHE:HB3	29:F:103:SQD:H241	2.07	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.03	0.43
22:B:611:CLA:H171	22:B:612:CLA:HBB2	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.84	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.35	0.43
26:A:409:LHG:H382	22:C:509:CLA:H93	2.01	0.43
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.01	0.43
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.01	0.43
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.76	0.43
22:D:405:CLA:H3A	22:D:405:CLA:HBA1	1.82	0.43
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.67	0.43
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.12	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.42
22:B:606:CLA:H41	22:B:606:CLA:H61	2.89	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.78	0.42
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
7:H:12:ARG:HD3	7:H:12:ARG:O	2.19	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.04	0.42
23:D:407:PL9:H421	23:D:407:PL9:H401	1.86	0.42
24:F:102:BCR:H15C	24:F:102:BCR:H351	1.91	0.42
15:U:72:TYR:O	15:U:76:ALA:HB3	2.19	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.74	0.42
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.88	0.42
25:B:620:DGD:HAW2	22:H:101:CLA:H152	2.02	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.01	0.42
22:C:511:CLA:H61	22:C:511:CLA:H13	2.05	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.53	0.42
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.32	0.42
1:A:140:ARG:HH22	26:A:409:LHG:P	2.41	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.42
22:A:404:CLA:H51	31:D:401:PHO:C3B	21.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.91	0.42
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.86	0.42
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.02	0.42
3:C:377:LEU:O	3:C:381:LYS:HB2	2.20	0.42
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.95	0.42
22:C:511:CLA:H143	22:C:512:CLA:H162	2.02	0.42
22:B:612:CLA:H171	27:D:408:LMG:H401	2.01	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.04	0.42
22:B:613:CLA:H12	22:B:613:CLA:H51	4.48	0.42
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.84	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42
22:A:403:CLA:H42	23:D:407:PL9:H162	2.01	0.42
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.42
3:C:456:GLU:N	3:C:456:GLU:OE1	2.52	0.42
22:C:520:CLA:H112	22:C:520:CLA:H142	1.77	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.02	0.42
22:A:405:CLA:H11	22:A:405:CLA:H51	4.35	0.42
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.42
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.88	0.42
31:D:401:PHO:H202	31:D:401:PHO:H162	1.87	0.42
13:O:192:SER:OG	13:O:193:GLY:N	2.52	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.42
1:A:182:PHE:O	1:A:186:PHE:HB2	2.21	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.02	0.42
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.42
4:D:155:SER:HA	4:D:159:ILE:HB	2.05	0.42
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.63	0.41
22:D:406:CLA:H41	22:D:406:CLA:H61	1.86	0.41
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.83	0.41
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.50	0.41
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.02	0.41
4:D:252:PHE:O	4:D:256:ILE:HG22	2.21	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.48	0.41
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.02	0.41
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.41
22:A:403:CLA:H202	22:A:403:CLA:H162	1.76	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.41
22:B:611:CLA:H18	22:B:612:CLA:H192	22.27	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.41
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
1:A:238:LYS:O	1:A:241:GLN:HG3	2.21	0.41
22:A:403:CLA:H41	22:A:403:CLA:H62	1.76	0.41
22:A:403:CLA:HED2	4:D:198:MET:SD	2.60	0.41
22:B:602:CLA:H92	22:B:602:CLA:HBB2	2.03	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.79	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.84	0.41
24:F:102:BCR:H11C	24:F:102:BCR:H341	1.94	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
3:C:282:MET:HG2	22:C:501:CLA:H61	2.09	0.41
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.54	0.41
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.54	0.41
1:A:269:ARG:NH1	4:D:231:THR:HB	2.38	0.41
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.37	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.41
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.04	0.41
1:A:153:SER:HB2	22:A:404:CLA:H43	19.16	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.97	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.88	0.41
31:D:402:PHO:CHB	22:D:405:CLA:H101	2.51	0.41
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.41
1:A:258:LEU:O	4:D:128:ARG:NH1	2.54	0.41
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.10	0.41
24:A:407:BCR:H341	24:A:407:BCR:H11C	1.94	0.41
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.02	0.41
22:B:611:CLA:H161	22:B:611:CLA:H143	4.42	0.41
3:C:303:GLY:O	3:C:423:ARG:NE	2.41	0.41
3:C:119:LEU:HG	24:C:513:BCR:H10C	2.15	0.41
4:D:342:PRO:O	4:D:345:VAL:HG12	2.22	0.41
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.02	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.21	0.41
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.21	0.41
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:602:CLA:H162	22:B:602:CLA:H192	1.77	0.41
7:H:35:MET:HB2	7:H:35:MET:HE3	1.87	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.07	0.41
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.26	0.41
22:A:404:CLA:H62	22:A:404:CLA:H102	4.12	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.04	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.94	0.41
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.21	0.41
24:H:102:BCR:HC31	24:H:102:BCR:H323	1.89	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.40
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.40
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.40
22:B:605:CLA:H41	22:B:605:CLA:H62	1.86	0.40
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.03	0.40
2:B:179:GLN:HA	2:B:180:PRO:HD3	1.97	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.40
3:C:375:LEU:HB3	3:C:380:ILE:HD11	2.04	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
24:K:102:BCR:H361	24:K:102:BCR:H20C	1.81	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
22:B:602:CLA:H61	22:B:602:CLA:H41	1.67	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.90	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.04	0.40
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.08	0.40
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.61	0.40
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.04	0.40
1:A:180:PHE:O	1:A:184:ILE:HG13	2.26	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.40
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.52	0.40
22:B:606:CLA:H161	22:B:606:CLA:H141	2.05	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.51	0.40
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.86	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.96	0.40
11:L:11:GLU:HG2	11:L:12:LEU:N	2.35	0.40
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.59	0.40
29:A:413:SQD:H332	22:B:609:CLA:H203	66.25	0.40
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.40
2:B:6:TYR:OH	27:D:408:LMG:HC5	2.26	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	15	58
1	a	333/344 (97%)	309 (93%)	20 (6%)	4 (1%)	15	58
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	22	66
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	28	71
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	20	63
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	20	63
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	44	81
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	44	81
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	14	56
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	14	56
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	29
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	29
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	38
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	38
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	15	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	15	58
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	37
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	37
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	8	47
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	8	47
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	34
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4	34
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2	25
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2	25
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	52
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	52
All	All	5138/5618 (92%)	4675 (91%)	408 (8%)	55 (1%)	17	60

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
7	H	26	GLY
9	J	38	SER
13	O	52	ALA
14	T	30	THR
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO

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Mol	Chain	Res	Type
3	c	257	PHE
3	c	416	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
2	B	489	GLU
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
18	X	12	ILE
2	b	489	GLU
3	c	32	GLY
4	d	239	GLN
7	h	26	GLY
9	j	38	SER
13	o	88	GLU
1	A	142	TRP
3	C	32	GLY
5	E	82	GLN
1	a	142	TRP
1	a	334	ARG
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
7	H	16	SER
15	U	73	PRO
3	c	144	SER
7	h	16	SER
15	u	73	PRO
3	C	144	SER
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	267 (98%)	4 (2%)	70	86
1	a	271/280 (97%)	267 (98%)	4 (2%)	70	86
2	B	390/407 (96%)	381 (98%)	9 (2%)	56	79
2	b	390/407 (96%)	381 (98%)	9 (2%)	56	79
3	C	347/362 (96%)	336 (97%)	11 (3%)	44	71
3	c	347/362 (96%)	336 (97%)	11 (3%)	44	71
4	D	275/283 (97%)	269 (98%)	6 (2%)	57	80
4	d	275/283 (97%)	269 (98%)	6 (2%)	57	80
5	E	72/73 (99%)	70 (97%)	2 (3%)	49	74
5	e	72/73 (99%)	70 (97%)	2 (3%)	49	74
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%)	16	49
7	h	53/55 (96%)	49 (92%)	4 (8%)	16	49
8	I	32/35 (91%)	31 (97%)	1 (3%)	45	72
8	i	32/35 (91%)	31 (97%)	1 (3%)	45	72
9	J	24/28 (86%)	23 (96%)	1 (4%)	34	66
9	j	24/28 (86%)	23 (96%)	1 (4%)	34	66
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%)	48	73
11	l	35/35 (100%)	34 (97%)	1 (3%)	48	73
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%)	80	90
13	o	202/228 (89%)	200 (99%)	2 (1%)	80	90
14	T	29/29 (100%)	28 (97%)	1 (3%)	42	71
14	t	29/29 (100%)	28 (97%)	1 (3%)	42	71
15	U	84/112 (75%)	83 (99%)	1 (1%)	75	88
15	u	84/112 (75%)	83 (99%)	1 (1%)	75	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	116/138 (84%)	114 (98%)	2 (2%)	66	85
16	v	116/138 (84%)	114 (98%)	2 (2%)	66	85
17	g	20/37 (54%)	18 (90%)	2 (10%)	9	36
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	36
18	X	30/34 (88%)	28 (93%)	2 (7%)	19	53
18	x	30/34 (88%)	28 (93%)	2 (7%)	19	53
20	Z	52/52 (100%)	50 (96%)	2 (4%)	38	68
20	z	52/52 (100%)	50 (96%)	2 (4%)	38	68
All	All	4244/4594 (92%)	4142 (98%)	102 (2%)	54	78

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG

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Mol	Chain	Res	Type
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	346	LEU
5	E	18	ARG
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU
16	V	92	ARG
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	45	LYS
20	Z	33	TRP
20	Z	62	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU

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Mol	Chain	Res	Type
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	472	LEU
4	d	43	LEU
4	d	180	ARG
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	346	LEU
5	e	18	ARG
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	132	LEU
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	45	LYS
20	z	33	TRP
20	z	62	VAL

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	A	402	-	56,73,73	1.09	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	A	403	-	56,73,73	1.10	4 (7%)	65,113,113	1.26	8 (12%)
22	CLA	A	404	-	56,73,73	1.11	4 (7%)	65,113,113	1.23	7 (10%)
22	CLA	A	405	-	56,73,73	1.10	4 (7%)	65,113,113	1.23	7 (10%)
23	PL9	A	406	-	45,45,55	1.00	4 (8%)	57,57,69	1.51	9 (15%)
24	BCR	A	407	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	7 (12%)
25	DGD	A	408	-	57,57,67	0.93	0	71,71,81	1.45	8 (11%)
26	LHG	A	409	-	38,38,48	0.68	0	39,44,54	1.22	3 (7%)
27	LMG	A	410	-	51,51,55	0.75	1 (1%)	59,59,63	1.37	7 (11%)
28	OEX	A	411	1,3	0,15,15	0.00	-	0,32,32	0.00	-
29	SQD	A	412	-	50,51,54	0.96	4 (8%)	60,62,65	1.93	11 (18%)
29	SQD	A	413	-	53,54,54	0.95	4 (7%)	63,65,65	1.73	10 (15%)
27	LMG	A	414	-	42,42,55	0.83	1 (2%)	50,50,63	1.27	6 (12%)
22	CLA	B	601	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	602	-	56,73,73	1.09	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	B	603	-	56,73,73	1.12	4 (7%)	65,113,113	1.30	10 (15%)
22	CLA	B	604	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	7 (10%)
22	CLA	B	605	-	56,73,73	1.10	4 (7%)	65,113,113	1.23	8 (12%)
22	CLA	B	606	-	56,73,73	1.11	4 (7%)	65,113,113	1.22	9 (13%)
22	CLA	B	607	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	9 (13%)
22	CLA	B	608	-	56,73,73	1.12	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	B	609	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	9 (13%)
22	CLA	B	610	-	56,73,73	1.16	5 (8%)	65,113,113	1.38	9 (13%)
22	CLA	B	611	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	B	612	-	56,73,73	1.08	4 (7%)	65,113,113	1.27	8 (12%)
22	CLA	B	613	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	7 (10%)
22	CLA	B	614	-	56,73,73	1.11	4 (7%)	65,113,113	1.23	9 (13%)
22	CLA	B	615	-	56,73,73	1.11	4 (7%)	65,113,113	1.21	8 (12%)
24	BCR	B	616	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	7 (12%)
24	BCR	B	617	-	41,41,41	1.06	2 (4%)	56,56,56	1.31	8 (14%)
24	BCR	B	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	8 (14%)
24	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	8 (14%)
25	DGD	B	620	-	59,59,67	0.91	1 (1%)	73,73,81	1.37	8 (10%)
27	LMG	B	621	-	49,49,55	0.78	1 (2%)	57,57,63	1.34	6 (10%)
29	SQD	B	622	-	42,43,54	1.05	4 (9%)	52,54,65	1.92	12 (23%)
30	LMT	B	623	-	36,36,36	1.14	5 (13%)	47,47,47	0.99	1 (2%)
30	LMT	B	624	-	36,36,36	1.11	5 (13%)	47,47,47	1.05	2 (4%)
25	DGD	B	625	-	53,53,67	1.07	3 (5%)	67,67,81	1.33	8 (11%)
29	SQD	B	626	-	46,47,54	1.01	5 (10%)	56,58,65	1.91	10 (17%)
30	LMT	B	627	-	36,36,36	1.13	5 (13%)	47,47,47	0.99	1 (2%)
30	LMT	B	628	-	36,36,36	1.15	5 (13%)	47,47,47	1.08	1 (2%)
22	CLA	C	501	-	56,73,73	1.12	4 (7%)	65,113,113	1.20	8 (12%)
22	CLA	C	502	-	56,73,73	1.12	4 (7%)	65,113,113	1.26	7 (10%)
22	CLA	C	503	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	7 (10%)
22	CLA	C	504	-	56,73,73	1.13	4 (7%)	65,113,113	1.26	8 (12%)
22	CLA	C	505	-	56,73,73	1.10	4 (7%)	65,113,113	1.29	7 (10%)
22	CLA	C	506	-	56,73,73	1.09	4 (7%)	65,113,113	1.26	8 (12%)
22	CLA	C	507	-	56,73,73	1.11	4 (7%)	65,113,113	1.30	9 (13%)
22	CLA	C	508	-	56,73,73	1.10	4 (7%)	65,113,113	1.21	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	509	-	56,73,73	1.12	4 (7%)	65,113,113	1.22	9 (13%)
22	CLA	C	510	3	56,73,73	1.10	4 (7%)	65,113,113	1.27	9 (13%)
22	CLA	C	511	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	C	512	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	9 (13%)
24	BCR	C	513	-	41,41,41	1.09	2 (4%)	56,56,56	1.31	9 (16%)
24	BCR	C	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	9 (16%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.29	8 (11%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.47	14 (18%)
25	DGD	C	517	-	67,67,67	0.88	2 (2%)	81,81,81	1.44	12 (14%)
27	LMG	C	518	-	45,45,55	0.78	0	53,53,63	1.29	5 (9%)
26	LHG	C	519	-	36,36,48	0.70	0	37,42,54	1.31	4 (10%)
22	CLA	C	520	-	56,73,73	1.09	4 (7%)	65,113,113	1.23	8 (12%)
27	LMG	C	521	-	48,48,55	0.77	0	56,56,63	1.32	6 (10%)
31	PHO	D	401	-	67,69,69	1.22	8 (11%)	87,99,99	1.02	6 (6%)
31	PHO	D	402	-	67,69,69	1.24	9 (13%)	87,99,99	1.03	6 (6%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	405	-	56,73,73	1.12	4 (7%)	65,113,113	1.20	8 (12%)
22	CLA	D	406	-	56,73,73	1.09	4 (7%)	65,113,113	1.25	7 (10%)
23	PL9	D	407	-	55,55,55	1.04	3 (5%)	69,69,69	1.46	11 (15%)
27	LMG	D	408	-	49,49,55	0.76	0	57,57,63	1.32	5 (8%)
27	LMG	D	409	-	48,48,55	0.78	0	56,56,63	1.41	5 (8%)
25	DGD	D	410	-	64,64,67	0.93	0	78,78,81	1.34	10 (12%)
30	LMT	D	411	-	32,32,36	1.20	5 (15%)	43,43,47	1.06	2 (4%)
27	LMG	D	412	-	46,46,55	0.77	1 (2%)	54,54,63	1.32	5 (9%)
27	LMG	E	101	-	44,44,55	0.77	0	52,52,63	1.31	5 (9%)
34	HEM	F	101	5,6	28,50,50	2.23	6 (21%)	17,82,82	1.44	3 (17%)
24	BCR	F	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
29	SQD	F	103	-	44,45,54	1.03	4 (9%)	54,56,65	1.85	11 (20%)
22	CLA	H	101	-	56,73,73	1.12	4 (7%)	65,113,113	1.23	7 (10%)
24	BCR	H	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	4 (7%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.28	5 (9%)
30	LMT	I	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.04	2 (4%)
23	PL9	J	101	-	35,35,55	1.01	2 (5%)	45,45,69	1.50	7 (15%)
24	BCR	J	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.59	12 (21%)
24	BCR	K	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	M	101	-	42,42,55	0.86	2 (4%)	50,50,63	1.26	4 (8%)
30	LMT	M	102	-	36,36,36	1.16	6 (16%)	47,47,47	1.04	2 (4%)
30	LMT	M	103	-	36,36,36	1.16	5 (13%)	47,47,47	1.03	2 (4%)
34	HEM	V	201	16	28,50,50	2.25	6 (21%)	17,82,82	1.45	2 (11%)
29	SQD	a	401	-	53,54,54	0.95	4 (7%)	63,65,65	1.73	10 (15%)
27	LMG	a	402	-	42,42,55	0.83	0	50,50,63	1.28	5 (10%)
22	CLA	a	404	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	a	405	-	56,73,73	1.09	4 (7%)	65,113,113	1.25	7 (10%)
22	CLA	a	406	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	a	407	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	7 (10%)
23	PL9	a	408	-	45,45,55	1.05	4 (8%)	57,57,69	1.50	9 (15%)
24	BCR	a	409	-	41,41,41	1.07	2 (4%)	56,56,56	1.21	7 (12%)
25	DGD	a	410	-	57,57,67	0.93	1 (1%)	71,71,81	1.43	7 (9%)
26	LHG	a	411	-	38,38,48	0.67	1 (2%)	39,44,54	1.23	3 (7%)
27	LMG	a	412	-	51,51,55	0.76	1 (1%)	59,59,63	1.35	7 (11%)
28	OEX	a	414	1,3	0,15,15	0.00	-	0,32,32	0.00	-
29	SQD	a	415	-	50,51,54	0.97	4 (8%)	60,62,65	1.95	11 (18%)
25	DGD	b	601	-	53,53,67	1.06	4 (7%)	67,67,81	1.33	8 (11%)
29	SQD	b	602	-	46,47,54	1.02	5 (10%)	56,58,65	1.93	10 (17%)
30	LMT	b	603	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	1 (2%)
30	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.08	1 (2%)
22	CLA	b	605	-	56,73,73	1.11	4 (7%)	65,113,113	1.26	8 (12%)
22	CLA	b	606	-	56,73,73	1.09	4 (7%)	65,113,113	1.24	9 (13%)
22	CLA	b	607	-	56,73,73	1.12	4 (7%)	65,113,113	1.29	10 (15%)
22	CLA	b	608	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	7 (10%)
22	CLA	b	609	-	56,73,73	1.10	4 (7%)	65,113,113	1.23	8 (12%)
22	CLA	b	610	-	56,73,73	1.10	4 (7%)	65,113,113	1.23	9 (13%)
22	CLA	b	611	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	7 (10%)
22	CLA	b	612	-	56,73,73	1.12	4 (7%)	65,113,113	1.21	7 (10%)
22	CLA	b	613	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	b	614	-	56,73,73	1.17	5 (8%)	65,113,113	1.38	9 (13%)
22	CLA	b	615	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	b	616	-	56,73,73	1.10	4 (7%)	65,113,113	1.28	8 (12%)
22	CLA	b	617	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	7 (10%)
22	CLA	b	618	-	56,73,73	1.11	4 (7%)	65,113,113	1.23	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	619	-	56,73,73	1.11	4 (7%)	65,113,113	1.19	7 (10%)
24	BCR	b	620	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
24	BCR	b	621	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	9 (16%)
24	BCR	b	622	-	41,41,41	1.09	2 (4%)	56,56,56	1.35	10 (17%)
24	BCR	b	623	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	8 (14%)
25	DGD	b	624	-	59,59,67	0.91	0	73,73,81	1.35	7 (9%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.34	6 (10%)
30	LMT	b	626	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	1 (2%)
30	LMT	b	627	-	36,36,36	1.11	5 (13%)	47,47,47	1.03	2 (4%)
22	CLA	c	501	-	56,73,73	1.12	4 (7%)	65,113,113	1.21	9 (13%)
22	CLA	c	502	-	56,73,73	1.12	4 (7%)	65,113,113	1.25	7 (10%)
22	CLA	c	503	-	56,73,73	1.11	4 (7%)	65,113,113	1.23	8 (12%)
22	CLA	c	504	-	56,73,73	1.14	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	c	505	-	56,73,73	1.10	4 (7%)	65,113,113	1.28	7 (10%)
22	CLA	c	506	-	56,73,73	1.09	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	c	507	-	56,73,73	1.10	4 (7%)	65,113,113	1.32	8 (12%)
22	CLA	c	508	-	56,73,73	1.11	4 (7%)	65,113,113	1.21	9 (13%)
22	CLA	c	509	-	56,73,73	1.11	4 (7%)	65,113,113	1.22	8 (12%)
22	CLA	c	510	3	56,73,73	1.10	4 (7%)	65,113,113	1.26	7 (10%)
22	CLA	c	511	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	9 (13%)
22	CLA	c	512	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	10 (15%)
24	BCR	c	513	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	9 (16%)
24	BCR	c	514	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	8 (14%)
25	DGD	c	515	-	54,54,67	0.96	1 (1%)	68,68,81	1.29	8 (11%)
25	DGD	c	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.47	14 (18%)
25	DGD	c	517	-	67,67,67	0.88	2 (2%)	81,81,81	1.43	10 (12%)
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.29	6 (11%)
26	LHG	c	519	-	36,36,48	0.71	0	37,42,54	1.30	4 (10%)
22	CLA	c	520	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	9 (13%)
24	BCR	c	521	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	7 (12%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.31	6 (10%)
31	PHO	d	401	-	67,69,69	1.22	8 (11%)	87,99,99	1.03	6 (6%)
31	PHO	d	402	-	67,69,69	1.23	8 (11%)	87,99,99	1.00	5 (5%)
29	SQD	d	403	-	42,43,54	1.05	4 (9%)	52,54,65	1.93	11 (21%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	d	405	-	56,73,73	1.14	4 (7%)	65,113,113	1.21	9 (13%)
22	CLA	d	406	-	56,73,73	1.10	4 (7%)	65,113,113	1.26	8 (12%)
23	PL9	d	407	-	55,55,55	1.05	2 (3%)	69,69,69	1.47	14 (20%)
27	LMG	d	408	-	49,49,55	0.76	0	57,57,63	1.32	4 (7%)
27	LMG	d	409	-	48,48,55	0.78	0	56,56,63	1.40	4 (7%)
25	DGD	d	410	-	64,64,67	0.93	2 (3%)	78,78,81	1.35	9 (11%)
30	LMT	d	411	-	32,32,36	1.19	5 (15%)	43,43,47	1.04	2 (4%)
27	LMG	d	412	-	46,46,55	0.78	0	54,54,63	1.32	5 (9%)
27	LMG	e	101	-	44,44,55	0.76	0	52,52,63	1.31	5 (9%)
34	HEM	f	101	5,6	28,50,50	2.23	6 (21%)	17,82,82	1.48	3 (17%)
24	BCR	f	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
29	SQD	f	103	-	44,45,54	1.03	4 (9%)	54,56,65	1.85	11 (20%)
24	BCR	g	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	7 (12%)
22	CLA	h	101	-	56,73,73	1.11	4 (7%)	65,113,113	1.22	7 (10%)
27	LMG	i	101	-	43,43,55	0.81	0	51,51,63	1.29	5 (9%)
30	LMT	i	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.01	2 (4%)
23	PL9	j	101	-	35,35,55	0.99	2 (5%)	45,45,69	1.51	7 (15%)
24	BCR	j	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.58	12 (21%)
27	LMG	m	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.26	4 (8%)
34	HEM	v	201	16	28,50,50	2.26	6 (21%)	17,82,82	1.41	2 (11%)
24	BCR	x	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.16	2 (3%)
24	BCR	y	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.24	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	BCR	A	407	-	-	0/29/63/63	0/2/2/2
25	DGD	A	408	-	-	0/45/85/95	0/2/2/2
26	LHG	A	409	-	-	0/43/43/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	A	410	-	-	0/46/66/70	0/1/1/1
28	OEX	A	411	1,3	-	0/0/68/68	0/0/6/6
29	SQD	A	412	-	-	0/46/66/69	0/1/1/1
29	SQD	A	413	-	-	0/49/69/69	0/1/1/1
27	LMG	A	414	-	-	0/37/57/70	0/1/1/1
22	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	B	616	-	-	0/29/63/63	0/2/2/2
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	DGD	B	620	-	-	0/47/87/95	0/2/2/2
27	LMG	B	621	-	-	0/44/64/70	0/1/1/1
29	SQD	B	622	-	-	1/38/58/69	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
30	LMT	B	624	-	-	0/21/61/61	0/2/2/2
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
29	SQD	B	626	-	-	0/42/62/69	0/1/1/1
30	LMT	B	627	-	-	0/21/61/61	0/2/2/2
30	LMT	B	628	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	C	513	-	-	0/29/63/63	0/2/2/2
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	DGD	C	515	-	-	0/42/82/95	0/2/2/2
25	DGD	C	516	-	-	1/51/91/95	0/2/2/2
25	DGD	C	517	-	-	0/55/95/95	0/2/2/2
27	LMG	C	518	-	-	0/40/60/70	0/1/1/1
26	LHG	C	519	-	-	0/41/41/53	0/0/0/0
22	CLA	C	520	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LMG	C	521	-	-	0/43/63/70	0/1/1/1
31	PHO	D	401	-	-	0/53/103/103	0/1/6/6
31	PHO	D	402	-	-	0/53/103/103	0/1/6/6
33	BCT	D	404	21	-	0/0/0/0	0/0/0/0
22	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	D	406	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PL9	D	407	-	-	0/53/73/73	0/1/1/1
27	LMG	D	408	-	-	0/44/64/70	0/1/1/1
27	LMG	D	409	-	-	0/43/63/70	0/1/1/1
25	DGD	D	410	-	-	0/52/92/95	0/2/2/2
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
27	LMG	D	412	-	-	0/41/61/70	0/1/1/1
27	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/6/54/54	0/0/8/8
24	BCR	F	102	-	-	0/29/63/63	0/2/2/2
29	SQD	F	103	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	H	102	-	-	0/29/63/63	0/2/2/2
27	LMG	I	101	-	-	0/38/58/70	0/1/1/1
30	LMT	I	102	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
24	BCR	J	102	-	-	0/29/63/63	0/2/2/2
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	-	0/37/57/70	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
29	SQD	a	401	-	-	0/49/69/69	0/1/1/1
27	LMG	a	402	-	-	0/37/57/70	0/1/1/1
22	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	a	408	-	-	0/41/61/73	0/1/1/1
24	BCR	a	409	-	-	0/29/63/63	0/2/2/2
25	DGD	a	410	-	-	0/45/85/95	0/2/2/2
26	LHG	a	411	-	-	0/43/43/53	0/0/0/0
27	LMG	a	412	-	-	0/46/66/70	0/1/1/1
28	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
29	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2
29	SQD	b	602	-	-	0/42/62/69	0/1/1/1
30	LMT	b	603	-	-	0/21/61/61	0/2/2/2
30	LMT	b	604	-	-	0/21/61/61	0/2/2/2
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	b	624	-	-	0/47/87/95	0/2/2/2
27	LMG	b	625	-	-	0/44/64/70	0/1/1/1
30	LMT	b	626	-	-	0/21/61/61	0/2/2/2
30	LMT	b	627	-	-	0/21/61/61	0/2/2/2
22	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	513	-	-	0/29/63/63	0/2/2/2
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	DGD	c	515	-	-	0/42/82/95	0/2/2/2
25	DGD	c	516	-	-	1/51/91/95	0/2/2/2
25	DGD	c	517	-	-	0/55/95/95	0/2/2/2
27	LMG	c	518	-	-	0/40/60/70	0/1/1/1
26	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	LMG	c	522	-	-	0/43/63/70	0/1/1/1
31	PHO	d	401	-	-	0/53/103/103	0/1/6/6
31	PHO	d	402	-	-	0/53/103/103	0/1/6/6
29	SQD	d	403	-	-	1/38/58/69	0/1/1/1
33	BCT	d	404	21	-	0/0/0/0	0/0/0/0
22	CLA	d	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	406	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	d	407	-	-	0/53/73/73	0/1/1/1
27	LMG	d	408	-	-	0/44/64/70	0/1/1/1
27	LMG	d	409	-	-	0/43/63/70	0/1/1/1
25	DGD	d	410	-	-	0/52/92/95	0/2/2/2
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
27	LMG	d	412	-	-	0/41/61/70	0/1/1/1
27	LMG	e	101	-	-	0/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HEM	f	101	5,6	-	0/6/54/54	0/0/8/8
24	BCR	f	102	-	-	0/29/63/63	0/2/2/2
29	SQD	f	103	-	-	0/40/60/69	0/1/1/1
24	BCR	g	101	-	-	0/29/63/63	0/2/2/2
22	CLA	h	101	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LMG	i	101	-	-	0/38/58/70	0/1/1/1
30	LMT	i	102	-	-	0/21/61/61	0/2/2/2
23	PL9	j	101	-	-	0/29/49/73	0/1/1/1
24	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/6/54/54	0/0/8/8
24	BCR	x	101	-	-	0/29/63/63	0/2/2/2
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

All (549) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	C3B-C2B	-5.08	1.33	1.40
34	F	101	HEM	C3B-C2B	-5.07	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.80	1.34	1.40
34	V	201	HEM	C3C-C2C	-4.77	1.34	1.40
34	v	201	HEM	C3B-C2B	-3.92	1.35	1.40
34	V	201	HEM	C3B-C2B	-3.91	1.35	1.40
34	F	101	HEM	C3C-C2C	-3.89	1.35	1.40
34	f	101	HEM	C3C-C2C	-3.84	1.35	1.40
23	d	407	PL9	C7-C3	-3.82	1.47	1.51
24	y	101	BCR	C1-C6	-3.76	1.48	1.53
22	b	614	CLA	CMB-C2B	-3.76	1.44	1.51
24	H	102	BCR	C1-C6	-3.70	1.48	1.53
24	g	101	BCR	C1-C6	-3.68	1.48	1.53
22	B	610	CLA	CMB-C2B	-3.66	1.44	1.51
24	F	102	BCR	C1-C6	-3.65	1.48	1.53
24	f	102	BCR	C1-C6	-3.60	1.48	1.53
24	x	101	BCR	C1-C6	-3.59	1.48	1.53
23	D	407	PL9	C7-C3	-3.52	1.47	1.51
23	a	408	PL9	C7-C3	-3.46	1.47	1.51
24	B	616	BCR	C1-C6	-3.38	1.49	1.53
24	C	514	BCR	C1-C6	-3.37	1.49	1.53
24	c	514	BCR	C1-C6	-3.36	1.49	1.53
24	b	620	BCR	C1-C6	-3.33	1.49	1.53
24	b	621	BCR	C1-C6	-3.30	1.49	1.53
24	y	101	BCR	C30-C25	-3.29	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	622	BCR	C30-C25	-3.28	1.49	1.53
24	B	617	BCR	C1-C6	-3.23	1.49	1.53
24	J	102	BCR	C30-C25	-3.23	1.49	1.53
24	g	101	BCR	C30-C25	-3.23	1.49	1.53
24	C	513	BCR	C1-C6	-3.23	1.49	1.53
24	j	102	BCR	C30-C25	-3.21	1.49	1.53
24	c	513	BCR	C1-C6	-3.19	1.49	1.53
24	B	618	BCR	C30-C25	-3.17	1.49	1.53
24	K	102	BCR	C30-C25	-3.17	1.49	1.53
24	F	102	BCR	C30-C25	-3.14	1.49	1.53
24	c	521	BCR	C30-C25	-3.12	1.49	1.53
24	A	407	BCR	C30-C25	-3.11	1.49	1.53
23	J	101	PL9	C7-C3	-3.11	1.48	1.51
24	B	618	BCR	C1-C6	-3.10	1.49	1.53
23	A	406	PL9	C7-C3	-3.09	1.48	1.51
24	a	409	BCR	C30-C25	-3.09	1.49	1.53
24	f	102	BCR	C30-C25	-3.08	1.49	1.53
24	B	619	BCR	C30-C25	-3.08	1.49	1.53
24	b	623	BCR	C1-C6	-3.08	1.49	1.53
24	B	616	BCR	C30-C25	-3.08	1.49	1.53
24	b	620	BCR	C30-C25	-3.07	1.49	1.53
24	b	623	BCR	C30-C25	-3.06	1.49	1.53
24	B	619	BCR	C1-C6	-3.05	1.49	1.53
24	b	622	BCR	C1-C6	-3.05	1.49	1.53
24	A	407	BCR	C1-C6	-3.05	1.49	1.53
24	a	409	BCR	C1-C6	-3.04	1.49	1.53
24	C	514	BCR	C30-C25	-3.00	1.49	1.53
24	K	102	BCR	C1-C6	-3.00	1.49	1.53
23	j	101	PL9	C7-C3	-2.99	1.48	1.51
24	C	513	BCR	C30-C25	-2.97	1.49	1.53
24	c	514	BCR	C30-C25	-2.97	1.49	1.53
24	x	101	BCR	C30-C25	-2.92	1.49	1.53
24	c	521	BCR	C1-C6	-2.90	1.49	1.53
24	H	102	BCR	C30-C25	-2.87	1.49	1.53
24	J	102	BCR	C1-C6	-2.80	1.50	1.53
24	j	102	BCR	C1-C6	-2.79	1.50	1.53
24	c	513	BCR	C30-C25	-2.79	1.50	1.53
24	b	621	BCR	C30-C25	-2.74	1.50	1.53
24	B	617	BCR	C30-C25	-2.72	1.50	1.53
30	d	411	LMT	O3'-C3'	-2.68	1.36	1.43
30	b	627	LMT	O3'-C3'	-2.68	1.36	1.43
22	C	507	CLA	CMB-C2B	-2.66	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	411	LMT	O3'-C3'	-2.66	1.36	1.43
30	M	102	LMT	O3'-C3'	-2.65	1.36	1.43
22	c	507	CLA	CMB-C2B	-2.65	1.46	1.51
30	I	102	LMT	O3'-C3'	-2.65	1.36	1.43
30	M	103	LMT	O3'-C3'	-2.65	1.36	1.43
23	a	408	PL9	C3-C4	-2.64	1.45	1.49
30	b	626	LMT	O3'-C3'	-2.63	1.36	1.43
22	B	611	CLA	CMD-C2D	-2.63	1.46	1.51
30	b	603	LMT	O3'-C3'	-2.62	1.36	1.43
30	b	604	LMT	O3'-C3'	-2.61	1.36	1.43
30	B	627	LMT	O3'-C3'	-2.61	1.37	1.43
30	B	624	LMT	O3'-C3'	-2.60	1.37	1.43
23	D	407	PL9	C3-C4	-2.60	1.45	1.49
30	i	102	LMT	O3'-C3'	-2.59	1.37	1.43
30	B	623	LMT	O3'-C3'	-2.58	1.37	1.43
22	b	615	CLA	CMD-C2D	-2.57	1.46	1.51
23	d	407	PL9	C3-C4	-2.55	1.45	1.49
22	a	404	CLA	CMB-C2B	-2.55	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.55	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.54	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.54	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.53	1.46	1.51
22	A	403	CLA	CMB-C2B	-2.53	1.46	1.51
30	B	628	LMT	O3'-C3'	-2.53	1.37	1.43
22	B	609	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	603	CLA	CMB-C2B	-2.52	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.52	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.52	1.46	1.51
22	c	504	CLA	CMD-C2D	-2.51	1.46	1.51
22	A	404	CLA	CMB-C2B	-2.51	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.51	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.51	1.46	1.51
22	a	407	CLA	CMB-C2B	-2.51	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.50	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.50	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.50	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	504	CLA	CMD-C2D	-2.49	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.49	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	509	CLA	CMD-C2D	-2.48	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.48	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.47	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.47	1.46	1.51
22	D	405	CLA	CMD-C2D	-2.47	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	406	PL9	C3-C4	-2.47	1.45	1.49
22	h	101	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.46	1.46	1.51
22	D	406	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.45	1.46	1.51
22	d	406	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.44	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	611	CLA	CMD-C2D	-2.43	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	CMD-C2D	-2.42	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.42	1.46	1.51
22	A	402	CLA	CMD-C2D	-2.41	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.41	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	515	DGD	O2G-C2G	-2.40	1.40	1.46
30	I	102	LMT	O2'-C2'	-2.40	1.37	1.43
22	b	606	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.40	1.46	1.51
22	A	404	CLA	CMD-C2D	-2.39	1.46	1.51
22	a	406	CLA	CMD-C2D	-2.39	1.46	1.51
22	a	404	CLA	CMD-C2D	-2.39	1.46	1.51
30	I	102	LMT	O2B-C2B	-2.39	1.37	1.43
22	b	614	CLA	C3B-C2B	-2.38	1.37	1.40
22	B	613	CLA	CMB-C2B	-2.38	1.46	1.51
22	b	607	CLA	CMD-C2D	-2.38	1.46	1.51
22	b	619	CLA	CMD-C2D	-2.37	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.37	1.46	1.51
30	i	102	LMT	O2'-C2'	-2.37	1.37	1.43
22	B	615	CLA	CMD-C2D	-2.37	1.46	1.51
30	i	102	LMT	O2B-C2B	-2.37	1.37	1.43
30	b	626	LMT	O2'-C2'	-2.37	1.37	1.43
22	d	405	CLA	CMD-C2D	-2.36	1.46	1.51
22	a	405	CLA	CMD-C2D	-2.36	1.46	1.51
22	A	403	CLA	CMD-C2D	-2.36	1.46	1.51
22	B	602	CLA	CMD-C2D	-2.35	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.35	1.46	1.51
22	B	604	CLA	CMD-C2D	-2.34	1.46	1.51
22	H	101	CLA	CMD-C2D	-2.34	1.46	1.51
22	b	608	CLA	CMD-C2D	-2.34	1.46	1.51
22	C	502	CLA	CMD-C2D	-2.33	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.33	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.33	1.46	1.51
22	h	101	CLA	CMD-C2D	-2.33	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.32	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.32	1.46	1.51
22	B	610	CLA	C3B-C2B	-2.32	1.37	1.40
22	C	507	CLA	CMD-C2D	-2.32	1.46	1.51
22	B	614	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.32	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	520	CLA	CMD-C2D	-2.32	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.32	1.46	1.51
30	M	103	LMT	O2'-C2'	-2.32	1.37	1.43
30	B	623	LMT	O2'-C2'	-2.32	1.37	1.43
22	b	606	CLA	CMD-C2D	-2.31	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.31	1.46	1.51
22	C	503	CLA	CMD-C2D	-2.31	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.31	1.46	1.51
22	C	511	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	609	CLA	CMD-C2D	-2.31	1.46	1.51
22	c	507	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.31	1.46	1.51
22	b	616	CLA	CMD-C2D	-2.31	1.46	1.51
30	M	103	LMT	O3B-C3B	-2.31	1.37	1.43
22	c	503	CLA	CMD-C2D	-2.31	1.46	1.51
30	b	627	LMT	O2'-C2'	-2.31	1.37	1.43
22	B	613	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.31	1.46	1.51
22	c	505	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	601	CLA	CMD-C2D	-2.31	1.46	1.51
22	b	618	CLA	CMD-C2D	-2.30	1.46	1.51
30	B	627	LMT	O2'-C2'	-2.30	1.37	1.43
22	c	511	CLA	CMD-C2D	-2.30	1.46	1.51
22	C	520	CLA	CMD-C2D	-2.30	1.46	1.51
30	B	628	LMT	O3B-C3B	-2.30	1.37	1.43
30	M	102	LMT	O3B-C3B	-2.30	1.37	1.43
30	b	627	LMT	O3B-C3B	-2.30	1.37	1.43
30	M	103	LMT	O2B-C2B	-2.29	1.37	1.43
22	B	605	CLA	CMD-C2D	-2.29	1.46	1.51
30	M	102	LMT	O2'-C2'	-2.29	1.37	1.43
30	b	603	LMT	O2B-C2B	-2.29	1.37	1.43
30	D	411	LMT	O3B-C3B	-2.29	1.37	1.43
30	b	603	LMT	O3B-C3B	-2.29	1.37	1.43
22	a	407	CLA	CMD-C2D	-2.29	1.46	1.51
22	c	510	CLA	CMD-C2D	-2.28	1.46	1.51
22	d	406	CLA	CMD-C2D	-2.28	1.46	1.51
22	c	506	CLA	CMD-C2D	-2.28	1.46	1.51
30	B	623	LMT	O3B-C3B	-2.28	1.37	1.43
22	B	612	CLA	CMD-C2D	-2.28	1.46	1.51
22	c	501	CLA	CMD-C2D	-2.28	1.46	1.51
30	M	102	LMT	O2B-C2B	-2.28	1.37	1.43
30	b	626	LMT	O2B-C2B	-2.28	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	CMD-C2D	-2.28	1.46	1.51
22	b	613	CLA	CMD-C2D	-2.27	1.46	1.51
30	b	604	LMT	O3B-C3B	-2.27	1.37	1.43
22	C	510	CLA	CMD-C2D	-2.27	1.46	1.51
22	D	406	CLA	CMD-C2D	-2.27	1.46	1.51
30	B	624	LMT	O3B-C3B	-2.27	1.37	1.43
30	I	102	LMT	O3B-C3B	-2.27	1.37	1.43
30	D	411	LMT	O2'-C2'	-2.26	1.37	1.43
30	B	627	LMT	O2B-C2B	-2.26	1.37	1.43
30	d	411	LMT	O3B-C3B	-2.26	1.37	1.43
29	b	602	SQD	O2-C2	-2.26	1.37	1.43
22	B	610	CLA	CMD-C2D	-2.25	1.46	1.51
30	b	603	LMT	O2'-C2'	-2.25	1.37	1.43
22	c	512	CLA	CMD-C2D	-2.25	1.46	1.51
31	D	401	PHO	C1C-NC	-2.25	1.33	1.38
22	C	501	CLA	CMD-C2D	-2.25	1.46	1.51
30	b	604	LMT	O2B-C2B	-2.24	1.37	1.43
30	d	411	LMT	O2'-C2'	-2.24	1.37	1.43
30	D	411	LMT	O2B-C2B	-2.24	1.37	1.43
30	b	626	LMT	O3B-C3B	-2.24	1.37	1.43
30	B	624	LMT	O2'-C2'	-2.24	1.37	1.43
30	i	102	LMT	O3B-C3B	-2.24	1.37	1.43
31	d	402	PHO	C1C-NC	-2.24	1.33	1.38
30	B	627	LMT	O3B-C3B	-2.23	1.37	1.43
30	B	628	LMT	O2'-C2'	-2.23	1.37	1.43
30	B	628	LMT	O2B-C2B	-2.23	1.37	1.43
22	b	614	CLA	CMD-C2D	-2.23	1.46	1.51
29	B	626	SQD	O2-C2	-2.23	1.37	1.43
31	D	402	PHO	C1C-NC	-2.23	1.33	1.38
31	d	401	PHO	C1C-NC	-2.23	1.33	1.38
25	C	515	DGD	O1G-C1G	-2.22	1.40	1.45
30	B	623	LMT	O2B-C2B	-2.22	1.37	1.43
30	d	411	LMT	O2B-C2B	-2.22	1.37	1.43
22	C	512	CLA	CMD-C2D	-2.22	1.46	1.51
23	D	407	PL9	C6-C1	-2.21	1.44	1.48
30	b	604	LMT	O2'-C2'	-2.20	1.37	1.43
23	a	408	PL9	C53-C6	-2.19	1.46	1.50
29	A	413	SQD	O3-C3	-2.16	1.38	1.43
30	b	627	LMT	O2B-C2B	-2.15	1.38	1.43
30	B	624	LMT	O2B-C2B	-2.15	1.38	1.43
23	A	406	PL9	C53-C6	-2.14	1.46	1.50
29	a	401	SQD	O3-C3	-2.13	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	M	103	LMT	O4'-C4B	-2.13	1.38	1.43
24	g	101	BCR	C33-C5	-2.13	1.47	1.51
29	f	103	SQD	O3-C3	-2.12	1.38	1.43
29	A	412	SQD	O2-C2	-2.12	1.38	1.43
25	c	515	DGD	O2G-C2G	-2.12	1.41	1.46
29	a	415	SQD	O2-C2	-2.11	1.38	1.43
25	a	410	DGD	O1G-C1G	-2.10	1.40	1.45
29	b	602	SQD	O3-C3	-2.10	1.38	1.43
29	f	103	SQD	O2-C2	-2.10	1.38	1.43
30	B	628	LMT	O4'-C4B	-2.10	1.38	1.43
23	A	406	PL9	C6-C1	-2.10	1.44	1.48
29	F	103	SQD	O3-C3	-2.10	1.38	1.43
30	M	102	LMT	O4'-C4B	-2.09	1.38	1.43
29	B	626	SQD	O3-C3	-2.08	1.38	1.43
29	d	403	SQD	O2-C2	-2.08	1.38	1.43
29	F	103	SQD	O2-C2	-2.08	1.38	1.43
30	d	411	LMT	O4'-C4B	-2.08	1.38	1.43
29	d	403	SQD	O3-C3	-2.07	1.38	1.43
30	b	603	LMT	O4'-C4B	-2.07	1.38	1.43
29	B	622	SQD	O3-C3	-2.07	1.38	1.43
30	B	623	LMT	O4'-C4B	-2.07	1.38	1.43
29	B	622	SQD	O2-C2	-2.07	1.38	1.43
25	c	516	DGD	O2G-C2G	-2.07	1.41	1.46
30	B	627	LMT	O4'-C4B	-2.06	1.38	1.43
30	D	411	LMT	O4'-C4B	-2.06	1.38	1.43
29	a	415	SQD	O3-C3	-2.06	1.38	1.43
30	I	102	LMT	O4'-C4B	-2.06	1.38	1.43
30	b	627	LMT	O4'-C4B	-2.05	1.38	1.43
26	a	411	LHG	O7-C5	-2.05	1.41	1.46
30	b	604	LMT	O4'-C4B	-2.05	1.38	1.43
24	y	101	BCR	C33-C5	-2.05	1.47	1.51
29	A	413	SQD	O2-C2	-2.05	1.38	1.43
29	A	412	SQD	O3-C3	-2.04	1.38	1.43
23	a	408	PL9	C6-C1	-2.04	1.45	1.48
23	J	101	PL9	C3-C4	-2.04	1.46	1.49
25	C	516	DGD	O2G-C2G	-2.04	1.41	1.46
29	B	626	SQD	O4-C4	-2.04	1.38	1.43
30	b	626	LMT	O4'-C4B	-2.03	1.38	1.43
30	B	624	LMT	O4'-C4B	-2.03	1.38	1.43
29	b	602	SQD	O4-C4	-2.02	1.38	1.43
30	i	102	LMT	O4'-C4B	-2.02	1.38	1.43
25	d	410	DGD	O1G-C1G	-2.02	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	412	LMG	O7-C8	-2.02	1.41	1.46
29	a	401	SQD	O2-C2	-2.02	1.38	1.43
30	M	102	LMT	O1'-C1'	-2.02	1.36	1.40
25	B	620	DGD	O2G-C2G	-2.02	1.41	1.46
23	j	101	PL9	C3-C4	-2.00	1.46	1.49
27	A	414	LMG	C4-C5	2.00	1.57	1.53
27	M	101	LMG	C4-C5	2.00	1.57	1.53
31	D	402	PHO	C1B-C2B	2.02	1.50	1.45
31	d	401	PHO	C4B-NB	2.05	1.41	1.36
25	c	517	DGD	C3G-C2G	2.07	1.56	1.50
31	d	402	PHO	C4B-NB	2.07	1.41	1.36
31	D	402	PHO	C4B-NB	2.07	1.41	1.36
31	D	401	PHO	C4B-NB	2.07	1.41	1.36
25	b	601	DGD	C4D-C5D	2.09	1.57	1.53
25	d	410	DGD	C1D-C2D	2.11	1.58	1.52
25	C	517	DGD	C3G-C2G	2.11	1.56	1.50
27	A	410	LMG	C7-C8	2.13	1.56	1.50
27	b	625	LMG	C4-C5	2.14	1.57	1.53
27	m	101	LMG	C7-C8	2.16	1.56	1.50
27	M	101	LMG	C7-C8	2.18	1.56	1.50
27	a	412	LMG	C7-C8	2.18	1.56	1.50
25	c	517	DGD	C1G-C2G	2.19	1.56	1.50
25	C	517	DGD	C1G-C2G	2.20	1.57	1.50
27	B	621	LMG	C4-C5	2.22	1.57	1.53
31	d	401	PHO	CHD-C1D	2.22	1.43	1.38
31	D	401	PHO	CHD-C1D	2.24	1.43	1.38
25	b	601	DGD	C1G-C2G	2.25	1.57	1.50
31	d	401	PHO	C4C-C3C	2.28	1.49	1.45
31	D	402	PHO	C4C-C3C	2.29	1.49	1.45
25	b	601	DGD	C3G-C2G	2.29	1.57	1.50
31	D	401	PHO	C4C-C3C	2.31	1.49	1.45
25	B	625	DGD	C3G-C2G	2.33	1.57	1.50
31	d	402	PHO	C4C-C3C	2.34	1.49	1.45
31	D	402	PHO	CHD-C1D	2.38	1.43	1.38
34	f	101	HEM	C4D-ND	2.39	1.39	1.36
22	b	614	CLA	CHC-C1C	2.40	1.42	1.35
31	d	402	PHO	CHD-C1D	2.40	1.43	1.38
22	B	610	CLA	CHC-C1C	2.41	1.42	1.35
34	F	101	HEM	C4D-ND	2.41	1.39	1.36
25	B	625	DGD	C4D-C5D	2.41	1.58	1.53
31	d	402	PHO	C1A-NA	2.47	1.42	1.37
31	D	401	PHO	C1A-NA	2.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	401	PHO	C1A-NA	2.53	1.42	1.37
31	D	402	PHO	C1A-NA	2.53	1.42	1.37
22	a	405	CLA	CHC-C1C	2.57	1.42	1.35
22	c	501	CLA	CHC-C1C	2.57	1.42	1.35
22	B	615	CLA	CHC-C1C	2.58	1.42	1.35
22	A	405	CLA	CHC-C1C	2.59	1.42	1.35
22	B	611	CLA	CHC-C1C	2.59	1.42	1.35
22	b	619	CLA	CHC-C1C	2.59	1.42	1.35
22	D	406	CLA	CHC-C1C	2.59	1.42	1.35
22	C	503	CLA	CHC-C1C	2.60	1.42	1.35
22	C	501	CLA	CHC-C1C	2.60	1.42	1.35
22	b	615	CLA	CHC-C1C	2.61	1.42	1.35
22	c	506	CLA	CHC-C1C	2.61	1.42	1.35
34	V	201	HEM	C4D-ND	2.61	1.39	1.36
22	C	507	CLA	CHC-C1C	2.61	1.42	1.35
34	v	201	HEM	C4D-ND	2.61	1.39	1.36
22	b	605	CLA	CHC-C1C	2.61	1.42	1.35
22	B	601	CLA	CHC-C1C	2.62	1.42	1.35
22	b	609	CLA	CHC-C1C	2.62	1.42	1.35
31	d	401	PHO	C4C-NC	2.62	1.42	1.36
31	D	401	PHO	C4C-NC	2.62	1.42	1.36
22	C	506	CLA	CHC-C1C	2.62	1.42	1.35
22	c	520	CLA	CHC-C1C	2.62	1.42	1.35
22	b	610	CLA	CHC-C1C	2.63	1.42	1.35
22	A	402	CLA	CHC-C1C	2.63	1.42	1.35
22	B	612	CLA	CHC-C1C	2.63	1.42	1.35
22	c	503	CLA	CHC-C1C	2.63	1.42	1.35
22	C	510	CLA	CHC-C1C	2.63	1.42	1.35
22	b	608	CLA	CHC-C1C	2.63	1.42	1.35
22	B	606	CLA	CHC-C1C	2.63	1.42	1.35
22	B	605	CLA	CHC-C1C	2.64	1.43	1.35
22	A	403	CLA	CHC-C1C	2.64	1.43	1.35
22	b	613	CLA	CHC-C1C	2.64	1.43	1.35
22	C	520	CLA	CHC-C1C	2.64	1.43	1.35
22	A	404	CLA	CHC-C1C	2.65	1.43	1.35
31	D	402	PHO	C4C-NC	2.65	1.42	1.36
22	c	510	CLA	CHC-C1C	2.65	1.43	1.35
22	C	508	CLA	CHC-C1C	2.65	1.43	1.35
22	c	508	CLA	CHC-C1C	2.66	1.43	1.35
22	B	604	CLA	CHC-C1C	2.66	1.43	1.35
22	B	614	CLA	CHC-C1C	2.66	1.43	1.35
22	C	504	CLA	CHC-C1C	2.66	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	618	CLA	CHC-C1C	2.66	1.43	1.35
22	B	602	CLA	CHC-C1C	2.66	1.43	1.35
22	b	607	CLA	CHC-C1C	2.66	1.43	1.35
22	b	616	CLA	CHC-C1C	2.66	1.43	1.35
22	B	603	CLA	CHC-C1C	2.67	1.43	1.35
22	B	609	CLA	CHC-C1C	2.67	1.43	1.35
22	a	407	CLA	CHC-C1C	2.67	1.43	1.35
22	D	405	CLA	CHC-C1C	2.67	1.43	1.35
22	c	505	CLA	CHC-C1C	2.67	1.43	1.35
22	C	509	CLA	CHC-C1C	2.67	1.43	1.35
22	c	504	CLA	CHC-C1C	2.67	1.43	1.35
22	a	406	CLA	CHC-C1C	2.67	1.43	1.35
22	C	502	CLA	CHC-C1C	2.68	1.43	1.35
22	d	405	CLA	CHC-C1C	2.68	1.43	1.35
22	c	509	CLA	CHC-C1C	2.68	1.43	1.35
22	C	511	CLA	CHC-C1C	2.68	1.43	1.35
31	d	402	PHO	C4C-NC	2.68	1.42	1.36
22	c	512	CLA	CHC-C1C	2.68	1.43	1.35
22	c	511	CLA	CHC-C1C	2.68	1.43	1.35
22	C	512	CLA	CHC-C1C	2.68	1.43	1.35
22	c	507	CLA	CHC-C1C	2.69	1.43	1.35
22	C	505	CLA	CHC-C1C	2.69	1.43	1.35
22	d	406	CLA	CHC-C1C	2.70	1.43	1.35
22	c	502	CLA	CHC-C1C	2.70	1.43	1.35
22	a	404	CLA	CHC-C1C	2.70	1.43	1.35
22	B	607	CLA	CHC-C1C	2.70	1.43	1.35
22	b	617	CLA	CHC-C1C	2.71	1.43	1.35
22	b	606	CLA	CHC-C1C	2.72	1.43	1.35
22	b	611	CLA	CHC-C1C	2.73	1.43	1.35
22	b	612	CLA	CHC-C1C	2.74	1.43	1.35
22	H	101	CLA	CHC-C1C	2.74	1.43	1.35
29	f	103	SQD	O47-C7	2.74	1.42	1.34
29	B	626	SQD	O47-C7	2.75	1.42	1.34
22	h	101	CLA	CHC-C1C	2.75	1.43	1.35
29	b	602	SQD	O47-C7	2.76	1.42	1.34
22	B	613	CLA	CHC-C1C	2.77	1.43	1.35
22	B	608	CLA	CHC-C1C	2.78	1.43	1.35
29	F	103	SQD	O47-C7	2.79	1.42	1.34
29	A	412	SQD	O47-C7	2.81	1.42	1.34
29	A	413	SQD	O47-C7	2.81	1.42	1.34
31	d	401	PHO	CHC-C1C	2.82	1.44	1.38
29	a	401	SQD	O47-C7	2.82	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	415	SQD	O47-C7	2.83	1.42	1.34
29	B	622	SQD	O47-C7	2.84	1.42	1.34
31	D	401	PHO	CHC-C1C	2.86	1.44	1.38
29	d	403	SQD	O47-C7	2.86	1.42	1.34
25	B	625	DGD	C1E-C2E	2.87	1.60	1.52
25	b	601	DGD	C1E-C2E	2.94	1.61	1.52
31	d	402	PHO	CHC-C1C	2.94	1.44	1.38
31	D	402	PHO	CHC-C1C	2.96	1.44	1.38
29	A	412	SQD	O48-C23	3.03	1.42	1.33
31	d	401	PHO	C3B-C4B	3.06	1.49	1.43
29	a	415	SQD	O48-C23	3.08	1.42	1.33
29	B	626	SQD	O48-C23	3.09	1.42	1.33
29	B	622	SQD	O48-C23	3.10	1.42	1.33
29	A	413	SQD	O48-C23	3.10	1.42	1.33
29	F	103	SQD	O48-C23	3.12	1.42	1.33
29	f	103	SQD	O48-C23	3.13	1.42	1.33
29	d	403	SQD	O48-C23	3.13	1.42	1.33
29	b	602	SQD	O48-C23	3.15	1.42	1.33
31	D	401	PHO	C3B-C4B	3.15	1.50	1.43
29	a	401	SQD	O48-C23	3.16	1.42	1.33
31	d	402	PHO	C3B-C4B	3.24	1.50	1.43
31	D	402	PHO	C3B-C4B	3.25	1.50	1.43
34	f	101	HEM	C3B-CAB	3.65	1.55	1.47
34	F	101	HEM	C3B-CAB	3.69	1.55	1.47
34	V	201	HEM	C3C-CAC	3.87	1.55	1.47
34	v	201	HEM	C3C-CAC	3.89	1.55	1.47
22	B	610	CLA	CHB-C4A	3.90	1.38	1.33
22	b	614	CLA	CHB-C4A	3.93	1.38	1.33
34	v	201	HEM	C3B-CAB	3.93	1.55	1.47
22	a	404	CLA	CHB-C4A	3.94	1.38	1.33
34	F	101	HEM	C3C-CAC	3.95	1.55	1.47
34	V	201	HEM	C3B-CAB	3.95	1.55	1.47
22	c	505	CLA	CHB-C4A	3.96	1.38	1.33
22	c	507	CLA	CHB-C4A	3.96	1.38	1.33
22	A	402	CLA	CHB-C4A	3.96	1.38	1.33
22	C	505	CLA	CHB-C4A	3.97	1.38	1.33
22	A	403	CLA	CHB-C4A	3.98	1.38	1.33
22	a	405	CLA	CHB-C4A	3.98	1.38	1.33
22	b	606	CLA	CHB-C4A	3.99	1.38	1.33
22	C	520	CLA	CHB-C4A	3.99	1.38	1.33
34	f	101	HEM	C3C-CAC	4.00	1.55	1.47
22	a	407	CLA	CHB-C4A	4.01	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	406	CLA	CHB-C4A	4.01	1.38	1.33
22	C	506	CLA	CHB-C4A	4.01	1.38	1.33
22	C	508	CLA	CHB-C4A	4.02	1.38	1.33
22	b	611	CLA	CHB-C4A	4.02	1.38	1.33
22	c	509	CLA	CHB-C4A	4.03	1.38	1.33
22	B	602	CLA	CHB-C4A	4.04	1.38	1.33
22	A	405	CLA	CHB-C4A	4.05	1.38	1.33
22	b	610	CLA	CHB-C4A	4.06	1.38	1.33
22	c	506	CLA	CHB-C4A	4.06	1.38	1.33
22	A	404	CLA	CHB-C4A	4.06	1.38	1.33
22	B	609	CLA	CHB-C4A	4.07	1.38	1.33
22	d	406	CLA	CHB-C4A	4.07	1.38	1.33
22	b	613	CLA	CHB-C4A	4.09	1.38	1.33
22	B	612	CLA	CHB-C4A	4.09	1.38	1.33
22	B	607	CLA	CHB-C4A	4.09	1.38	1.33
22	b	608	CLA	CHB-C4A	4.09	1.38	1.33
22	c	508	CLA	CHB-C4A	4.09	1.38	1.33
22	c	520	CLA	CHB-C4A	4.09	1.38	1.33
22	C	509	CLA	CHB-C4A	4.12	1.38	1.33
22	B	608	CLA	CHB-C4A	4.12	1.38	1.33
22	a	406	CLA	CHB-C4A	4.12	1.38	1.33
22	B	605	CLA	CHB-C4A	4.12	1.38	1.33
22	B	606	CLA	CHB-C4A	4.12	1.38	1.33
22	h	101	CLA	CHB-C4A	4.13	1.38	1.33
22	b	612	CLA	CHB-C4A	4.14	1.38	1.33
22	c	512	CLA	CHB-C4A	4.14	1.38	1.33
22	B	601	CLA	CHB-C4A	4.17	1.38	1.33
22	b	615	CLA	CHB-C4A	4.17	1.38	1.33
22	B	615	CLA	CHB-C4A	4.17	1.38	1.33
22	b	605	CLA	CHB-C4A	4.17	1.38	1.33
22	C	507	CLA	CHB-C4A	4.17	1.38	1.33
22	C	512	CLA	CHB-C4A	4.17	1.38	1.33
22	B	604	CLA	CHB-C4A	4.17	1.38	1.33
22	C	503	CLA	CHB-C4A	4.18	1.38	1.33
22	c	501	CLA	CHB-C4A	4.18	1.38	1.33
22	b	616	CLA	CHB-C4A	4.19	1.38	1.33
22	c	511	CLA	CHB-C4A	4.19	1.38	1.33
22	b	618	CLA	CHB-C4A	4.19	1.38	1.33
22	C	511	CLA	CHB-C4A	4.20	1.38	1.33
22	C	510	CLA	CHB-C4A	4.21	1.38	1.33
22	c	502	CLA	CHB-C4A	4.21	1.38	1.33
22	c	510	CLA	CHB-C4A	4.21	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	CHB-C4A	4.21	1.38	1.33
22	H	101	CLA	CHB-C4A	4.21	1.38	1.33
22	C	502	CLA	CHB-C4A	4.23	1.38	1.33
22	b	617	CLA	CHB-C4A	4.23	1.38	1.33
22	b	619	CLA	CHB-C4A	4.23	1.38	1.33
22	B	613	CLA	CHB-C4A	4.25	1.38	1.33
22	C	501	CLA	CHB-C4A	4.25	1.38	1.33
22	b	609	CLA	CHB-C4A	4.26	1.39	1.33
22	B	603	CLA	CHB-C4A	4.28	1.39	1.33
22	C	504	CLA	CHB-C4A	4.28	1.39	1.33
22	B	611	CLA	CHB-C4A	4.29	1.39	1.33
22	b	607	CLA	CHB-C4A	4.29	1.39	1.33
22	c	503	CLA	CHB-C4A	4.32	1.39	1.33
22	D	405	CLA	CHB-C4A	4.34	1.39	1.33
22	c	504	CLA	CHB-C4A	4.41	1.39	1.33
22	d	405	CLA	CHB-C4A	4.48	1.39	1.33
34	f	101	HEM	C3D-C2D	5.43	1.53	1.37
34	F	101	HEM	C3D-C2D	5.45	1.53	1.37
34	v	201	HEM	C3D-C2D	5.64	1.54	1.37
34	V	201	HEM	C3D-C2D	5.65	1.54	1.37

All (1226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	CMB-C2B-C1B	-5.16	120.54	128.46
22	b	614	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
25	A	408	DGD	O3G-C3G-C2G	-4.95	99.22	110.99
25	a	410	DGD	O3G-C3G-C2G	-4.85	99.46	110.99
25	C	517	DGD	O3G-C3G-C2G	-4.56	100.13	110.99
25	c	517	DGD	O3G-C3G-C2G	-4.36	100.61	110.99
27	D	409	LMG	C1-C2-C3	-4.32	101.95	109.98
27	d	409	LMG	C1-C2-C3	-4.29	102.01	109.98
22	c	507	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
22	C	507	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
22	b	616	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
22	B	612	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
25	c	516	DGD	O5D-C6D-C5D	-4.08	102.11	108.94
24	J	102	BCR	C11-C10-C9	-3.93	121.71	127.31
22	b	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	C	516	DGD	O5D-C6D-C5D	-3.91	102.40	108.94
22	B	607	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
29	F	103	SQD	O9-S-O7	-3.79	100.74	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	103	SQD	O9-S-O7	-3.77	100.78	113.86
24	j	102	BCR	C11-C10-C9	-3.74	121.97	127.31
22	c	510	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
29	A	412	SQD	O9-S-O7	-3.74	100.90	113.86
29	a	415	SQD	O9-S-O7	-3.73	100.93	113.86
29	d	403	SQD	O9-S-O7	-3.72	100.97	113.86
22	b	615	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
29	B	622	SQD	O9-S-O7	-3.69	101.06	113.86
29	a	401	SQD	O9-S-O7	-3.69	101.07	113.86
29	B	626	SQD	O9-S-O7	-3.69	101.08	113.86
22	b	617	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	B	602	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
29	b	602	SQD	O9-S-O7	-3.67	101.12	113.86
29	A	413	SQD	O9-S-O7	-3.67	101.13	113.86
22	c	512	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	C	505	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	B	613	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
22	B	611	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
22	b	613	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	C	506	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
22	c	503	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
22	A	405	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	C	510	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	c	506	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	B	609	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	C	516	DGD	O3G-C3G-C2G	-3.62	102.37	110.99
25	c	516	DGD	O3G-C3G-C2G	-3.62	102.39	110.99
25	d	410	DGD	O6D-C1D-O3G	-3.61	101.46	110.02
22	a	404	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
22	C	512	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
25	D	410	DGD	O6D-C1D-O3G	-3.58	101.51	110.02
22	c	511	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	a	407	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	C	502	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
22	A	402	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	c	502	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
22	D	405	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	D	406	CLA	CMB-C2B-C1B	-3.50	123.08	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	C	509	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
22	b	605	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
22	d	405	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
22	c	520	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	a	405	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	c	509	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
22	B	601	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
25	B	620	DGD	O3G-C3G-C2G	-3.45	102.78	110.99
22	B	605	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
22	C	520	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
22	b	618	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	d	406	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	j	101	PL9	C7-C3-C2	-3.43	118.36	123.23
22	A	403	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	b	607	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	C	515	DGD	O3G-C3G-C2G	-3.40	102.89	110.99
22	C	508	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
25	c	515	DGD	O3G-C3G-C2G	-3.39	102.93	110.99
22	A	404	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
23	J	101	PL9	C7-C3-C2	-3.38	118.42	123.23
22	b	608	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
25	b	624	DGD	O3G-C3G-C2G	-3.37	102.98	110.99
22	H	101	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
22	h	101	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	b	609	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	b	610	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	B	603	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
22	b	619	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
22	a	406	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
23	d	407	PL9	C7-C3-C2	-3.29	118.55	123.23
30	B	628	LMT	C1'-O5'-C5'	-3.25	107.59	113.72
25	d	410	DGD	O3G-C3G-C2G	-3.24	103.28	110.99
24	b	622	BCR	C24-C23-C22	-3.22	121.38	126.21
24	j	102	BCR	C24-C23-C22	-3.21	121.38	126.21
23	D	407	PL9	C7-C3-C2	-3.21	118.66	123.23
23	A	406	PL9	C7-C3-C2	-3.21	118.66	123.23
25	c	517	DGD	C1D-C2D-C3D	-3.21	104.01	109.98
22	B	606	CLA	CMB-C2B-C1B	-3.20	123.54	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
30	b	604	LMT	C1'-O5'-C5'	-3.18	107.73	113.72
22	B	608	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
24	J	102	BCR	C24-C23-C22	-3.17	121.44	126.21
25	D	410	DGD	O3G-C3G-C2G	-3.17	103.44	110.99
25	B	625	DGD	C1D-C2D-C3D	-3.15	104.12	109.98
25	b	624	DGD	O6D-C1D-O3G	-3.15	102.54	110.02
25	C	517	DGD	C1D-C2D-C3D	-3.14	104.14	109.98
25	B	620	DGD	O6D-C1D-O3G	-3.13	102.58	110.02
23	a	408	PL9	C7-C3-C2	-3.13	118.78	123.23
22	B	605	CLA	O2D-CGD-O1D	-3.12	117.54	123.82
25	c	516	DGD	O6D-C1D-O3G	-3.12	102.62	110.02
30	B	624	LMT	C3'-C4'-C5'	-3.09	104.31	110.88
22	B	603	CLA	O2D-CGD-O1D	-3.09	117.60	123.82
22	b	609	CLA	O2D-CGD-O1D	-3.09	117.60	123.82
25	b	601	DGD	C1D-C2D-C3D	-3.08	104.26	109.98
22	B	613	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
25	A	408	DGD	O6D-C1D-O3G	-3.06	102.75	110.02
25	C	517	DGD	O5D-C6D-C5D	-3.06	103.82	108.94
25	c	517	DGD	O5D-C6D-C5D	-3.05	103.83	108.94
22	C	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
24	J	102	BCR	C3-C4-C5	-3.05	108.53	113.78
24	j	102	BCR	C7-C8-C9	-3.05	121.63	126.21
25	C	516	DGD	O6D-C1D-O3G	-3.05	102.79	110.02
22	c	504	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
22	c	503	CLA	O2D-CGD-O1D	-3.04	117.70	123.82
24	J	102	BCR	C7-C8-C9	-3.02	121.67	126.21
22	b	617	CLA	O2D-CGD-O1D	-3.02	117.74	123.82
22	b	606	CLA	O2D-CGD-O1D	-3.02	117.75	123.82
24	B	617	BCR	C33-C5-C6	-3.01	121.14	124.51
30	b	627	LMT	C3'-C4'-C5'	-3.00	104.50	110.88
24	b	621	BCR	C33-C5-C6	-3.00	121.15	124.51
24	B	617	BCR	C15-C16-C17	-2.99	117.07	123.46
24	j	102	BCR	C3-C4-C5	-2.99	108.63	113.78
22	c	507	CLA	O2D-CGD-O1D	-2.99	117.81	123.82
22	b	607	CLA	O2D-CGD-O1D	-2.98	117.83	123.82
22	C	505	CLA	O2D-CGD-O1D	-2.97	117.84	123.82
22	C	503	CLA	O2D-CGD-O1D	-2.97	117.85	123.82
22	c	504	CLA	O2D-CGD-O1D	-2.96	117.87	123.82
22	B	608	CLA	O2D-CGD-O1D	-2.96	117.87	123.82
22	b	610	CLA	O2D-CGD-O1D	-2.96	117.87	123.82
27	d	408	LMG	O6-C1-O1	-2.96	103.00	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
25	c	515	DGD	O6D-C1D-O3G	-2.94	103.04	110.02
22	B	606	CLA	O2D-CGD-O1D	-2.94	117.90	123.82
22	C	504	CLA	O2D-CGD-O1D	-2.94	117.91	123.82
22	b	605	CLA	O2D-CGD-O1D	-2.93	117.92	123.82
24	F	102	BCR	C33-C5-C6	-2.93	121.22	124.51
24	H	102	BCR	C33-C5-C6	-2.93	121.23	124.51
25	a	410	DGD	O6D-C1D-O3G	-2.93	103.06	110.02
24	b	621	BCR	C15-C16-C17	-2.93	117.21	123.46
25	b	601	DGD	C3G-C2G-C1G	-2.92	105.27	111.86
22	c	501	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
24	x	101	BCR	C33-C5-C6	-2.90	121.27	124.51
24	f	102	BCR	C33-C5-C6	-2.90	121.27	124.51
24	J	102	BCR	C35-C13-C14	-2.89	118.87	122.92
22	b	611	CLA	O2D-CGD-O1D	-2.89	118.00	123.82
25	C	515	DGD	O6D-C1D-O3G	-2.89	103.16	110.02
22	b	608	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
25	A	408	DGD	O5D-C6D-C5D	-2.88	104.12	108.94
22	B	602	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
25	B	625	DGD	C3G-C2G-C1G	-2.87	105.39	111.86
25	c	517	DGD	CDB-CCB-CBB	-2.86	99.70	114.45
25	C	517	DGD	CDB-CCB-CBB	-2.86	99.70	114.45
22	B	604	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
27	M	101	LMG	C1-C2-C3	-2.86	104.67	109.98
22	b	612	CLA	O2D-CGD-O1D	-2.86	118.08	123.82
25	b	601	DGD	O3G-C3G-C2G	-2.85	104.20	110.99
22	a	406	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
22	c	505	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
22	C	507	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
22	C	506	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
22	a	404	CLA	O2D-CGD-O1D	-2.84	118.10	123.82
22	B	607	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
22	c	520	CLA	O2D-CGD-O1D	-2.83	118.14	123.82
22	C	501	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
22	c	511	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
27	D	408	LMG	O6-C1-O1	-2.82	103.33	110.02
22	C	510	CLA	O2D-CGD-O1D	-2.82	118.15	123.82
22	c	501	CLA	O2D-CGD-O1D	-2.82	118.15	123.82
22	d	406	CLA	O2D-CGD-O1D	-2.82	118.15	123.82
22	b	616	CLA	O2D-CGD-O1D	-2.82	118.16	123.82
22	c	506	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
22	C	501	CLA	CMB-C2B-C1B	-2.81	124.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	402	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
22	c	512	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
25	c	516	DGD	CDB-CCB-CBB	-2.81	99.97	114.45
22	A	403	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
22	c	510	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
22	b	613	CLA	O2D-CGD-O1D	-2.80	118.18	123.82
22	B	601	CLA	O2D-CGD-O1D	-2.79	118.20	123.82
22	H	101	CLA	O2D-CGD-O1D	-2.79	118.20	123.82
29	A	413	SQD	C5-C6-S	-2.79	110.45	114.34
27	B	621	LMG	C1-C2-C3	-2.79	104.79	109.98
24	j	102	BCR	C35-C13-C14	-2.79	119.02	122.92
25	C	516	DGD	CDB-CCB-CBB	-2.79	100.10	114.45
25	B	625	DGD	O3G-C3G-C2G	-2.78	104.37	110.99
22	B	609	CLA	O2D-CGD-O1D	-2.78	118.23	123.82
22	B	612	CLA	O2D-CGD-O1D	-2.77	118.24	123.82
24	b	621	BCR	C15-C14-C13	-2.77	123.36	127.31
22	b	618	CLA	O2D-CGD-O1D	-2.77	118.25	123.82
22	c	502	CLA	O2D-CGD-O1D	-2.77	118.26	123.82
22	B	614	CLA	O2D-CGD-O1D	-2.76	118.27	123.82
22	C	520	CLA	O2D-CGD-O1D	-2.75	118.28	123.82
25	D	410	DGD	CDB-CCB-CBB	-2.75	100.31	114.45
22	D	406	CLA	O2D-CGD-O1D	-2.74	118.30	123.82
24	j	102	BCR	C15-C14-C13	-2.74	123.40	127.31
22	d	405	CLA	O2D-CGD-O1D	-2.73	118.32	123.82
25	d	410	DGD	CDB-CCB-CBB	-2.73	100.39	114.45
22	C	509	CLA	O2D-CGD-O1D	-2.73	118.34	123.82
22	A	404	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
31	D	402	PHO	O2D-CGD-O1D	-2.72	118.34	123.82
30	M	102	LMT	C1'-O5'-C5'	-2.72	108.59	113.72
24	c	513	BCR	C11-C10-C9	-2.71	123.44	127.31
25	C	517	DGD	C1D-O6D-C5D	-2.71	108.61	113.72
24	B	618	BCR	C24-C23-C22	-2.71	122.14	126.21
25	c	517	DGD	C1D-O6D-C5D	-2.71	108.62	113.72
25	a	410	DGD	O5D-C6D-C5D	-2.70	104.42	108.94
27	C	518	LMG	O6-C1-O1	-2.70	103.61	110.02
22	b	614	CLA	O2D-CGD-O1D	-2.70	118.39	123.82
22	h	101	CLA	O2D-CGD-O1D	-2.70	118.39	123.82
24	J	102	BCR	C15-C14-C13	-2.69	123.47	127.31
30	B	623	LMT	C1'-O5'-C5'	-2.69	108.65	113.72
27	i	101	LMG	O6-C1-O1	-2.68	103.65	110.02
23	d	407	PL9	C7-C8-C9	-2.68	122.22	126.71
22	C	512	CLA	O2D-CGD-O1D	-2.68	118.42	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	101	BCR	C7-C8-C9	-2.68	122.19	126.21
24	B	619	BCR	C3-C4-C5	-2.67	109.18	113.78
24	K	102	BCR	C15-C16-C17	-2.67	117.75	123.46
24	c	521	BCR	C15-C16-C17	-2.67	117.76	123.46
24	y	101	BCR	C38-C26-C25	-2.67	121.52	124.51
23	J	101	PL9	C7-C8-C9	-2.67	122.25	126.71
22	B	610	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
27	E	101	LMG	C1-C2-C3	-2.67	105.02	109.98
22	C	511	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
22	c	509	CLA	O2D-CGD-O1D	-2.66	118.46	123.82
27	b	625	LMG	C1-C2-C3	-2.66	105.03	109.98
27	I	101	LMG	O6-C1-O1	-2.66	103.71	110.02
24	c	514	BCR	C11-C10-C9	-2.66	123.51	127.31
24	b	623	BCR	C3-C4-C5	-2.66	109.21	113.78
22	a	405	CLA	O2D-CGD-O1D	-2.66	118.47	123.82
24	g	101	BCR	C38-C26-C25	-2.65	121.54	124.51
31	D	401	PHO	O2D-CGD-O1D	-2.65	118.49	123.82
24	C	514	BCR	C15-C16-C17	-2.65	117.81	123.46
23	j	101	PL9	C7-C8-C9	-2.65	122.28	126.71
24	B	617	BCR	C28-C27-C26	-2.65	109.23	113.78
24	B	618	BCR	C11-C10-C9	-2.63	123.55	127.31
30	M	102	LMT	C3'-C4'-C5'	-2.63	105.28	110.88
31	d	401	PHO	O2D-CGD-O1D	-2.63	118.53	123.82
23	A	406	PL9	C22-C23-C24	-2.63	121.07	127.68
27	c	518	LMG	O6-C1-O1	-2.62	103.79	110.02
24	b	621	BCR	C28-C27-C26	-2.62	109.27	113.78
22	a	407	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
23	D	407	PL9	C7-C8-C9	-2.61	122.34	126.71
24	b	620	BCR	C33-C5-C6	-2.61	121.58	124.51
24	g	101	BCR	C7-C8-C9	-2.61	122.29	126.21
23	a	408	PL9	C22-C23-C24	-2.61	121.13	127.68
24	B	616	BCR	C33-C5-C6	-2.60	121.59	124.51
25	d	410	DGD	C3G-C2G-C1G	-2.60	105.99	111.86
30	M	103	LMT	C3'-C4'-C5'	-2.60	105.35	110.88
30	b	626	LMT	C1'-O5'-C5'	-2.60	108.82	113.72
22	b	619	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
22	A	405	CLA	O2D-CGD-O1D	-2.60	118.60	123.82
30	M	103	LMT	C1'-O5'-C5'	-2.59	108.83	113.72
24	B	618	BCR	C15-C14-C13	-2.59	123.62	127.31
27	a	402	LMG	O6-C1-O1	-2.59	103.88	110.02
24	C	513	BCR	C24-C23-C22	-2.58	122.34	126.21
27	e	101	LMG	C1-C2-C3	-2.58	105.19	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	402	PHO	CBD-CHA-C4D	-2.58	105.64	108.54
23	a	408	PL9	C7-C8-C9	-2.57	122.41	126.71
31	D	401	PHO	CBD-CHA-C4D	-2.57	105.64	108.54
22	c	508	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
22	D	405	CLA	O2D-CGD-O1D	-2.57	118.66	123.82
31	d	401	PHO	CBD-CHA-C4D	-2.56	105.65	108.54
24	g	101	BCR	C33-C5-C6	-2.56	121.64	124.51
24	C	514	BCR	C11-C10-C9	-2.56	123.66	127.31
31	d	402	PHO	O2D-CGD-O1D	-2.55	118.68	123.82
34	f	101	HEM	CBD-CAD-C3D	-2.55	107.60	112.47
23	D	407	PL9	C22-C23-C24	-2.55	121.27	127.68
29	a	415	SQD	C5-C6-S	-2.55	110.78	114.34
27	m	101	LMG	O2-C2-C1	-2.55	104.70	110.03
30	D	411	LMT	C1'-O5'-C5'	-2.55	108.92	113.72
31	d	402	PHO	CBD-CHA-C4D	-2.54	105.67	108.54
24	c	514	BCR	C28-C27-C26	-2.54	109.41	113.78
24	J	102	BCR	C38-C26-C25	-2.54	121.66	124.51
34	F	101	HEM	C1D-C2D-C3D	-2.54	105.23	107.00
24	c	521	BCR	C15-C14-C13	-2.53	123.69	127.31
24	B	617	BCR	C15-C14-C13	-2.53	123.70	127.31
24	C	514	BCR	C15-C14-C13	-2.53	123.70	127.31
24	b	622	BCR	C11-C10-C9	-2.53	123.70	127.31
27	A	410	LMG	C1-C2-C3	-2.53	105.28	109.98
22	B	615	CLA	O2D-CGD-O1D	-2.52	118.74	123.82
24	C	513	BCR	C15-C16-C17	-2.52	118.08	123.46
24	C	513	BCR	C15-C14-C13	-2.52	123.71	127.31
24	B	619	BCR	C7-C8-C9	-2.52	122.42	126.21
25	B	620	DGD	C1D-C2D-C3D	-2.52	105.30	109.98
27	A	414	LMG	O6-C1-O1	-2.51	104.05	110.02
24	C	514	BCR	C28-C27-C26	-2.51	109.46	113.78
30	d	411	LMT	C3'-C4'-C5'	-2.51	105.54	110.88
25	D	410	DGD	CFB-CEB-CDB	-2.51	101.50	114.45
34	f	101	HEM	C1D-C2D-C3D	-2.51	105.25	107.00
27	D	408	LMG	O2-C2-C1	-2.50	104.79	110.03
27	A	410	LMG	O3-C3-C2	-2.50	104.91	110.36
22	a	407	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
27	m	101	LMG	C1-C2-C3	-2.50	105.33	109.98
25	c	515	DGD	C3G-C2G-C1G	-2.50	106.22	111.86
24	j	102	BCR	C38-C26-C25	-2.50	121.72	124.51
24	y	101	BCR	C33-C5-C6	-2.50	121.72	124.51
25	c	516	DGD	C3G-C2G-C1G	-2.49	106.23	111.86
27	C	521	LMG	O2-C2-C1	-2.49	104.81	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
24	b	623	BCR	C7-C8-C9	-2.49	122.47	126.21
22	b	615	CLA	O2D-CGD-O1D	-2.49	118.81	123.82
27	D	412	LMG	C1-C2-C3	-2.49	105.36	109.98
25	C	515	DGD	C3G-C2G-C1G	-2.49	106.25	111.86
27	i	101	LMG	O2-C2-C1	-2.48	104.83	110.03
22	B	606	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
30	b	603	LMT	C1'-O5'-C5'	-2.48	109.04	113.72
27	D	409	LMG	O6-C1-C2	-2.48	105.50	110.30
25	b	624	DGD	C1D-C2D-C3D	-2.48	105.36	109.98
24	c	514	BCR	C15-C16-C17	-2.48	118.17	123.46
23	J	101	PL9	C22-C23-C24	-2.48	121.45	127.68
24	B	618	BCR	C15-C16-C17	-2.48	118.17	123.46
25	C	516	DGD	C3G-C2G-C1G	-2.48	106.27	111.86
24	C	514	BCR	C33-C5-C6	-2.47	121.74	124.51
25	d	410	DGD	CFB-CEB-CDB	-2.47	101.72	114.45
27	I	101	LMG	O2-C2-C1	-2.47	104.87	110.03
23	A	406	PL9	C7-C8-C9	-2.47	122.59	126.71
23	d	407	PL9	C22-C23-C24	-2.46	121.49	127.68
27	d	412	LMG	C38-C37-C36	-2.46	101.77	114.45
25	D	410	DGD	C3G-C2G-C1G	-2.46	106.31	111.86
22	C	504	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
24	K	102	BCR	C24-C23-C22	-2.46	122.52	126.21
27	d	408	LMG	O2-C2-C1	-2.46	104.89	110.03
27	d	409	LMG	C38-C37-C36	-2.45	101.81	114.45
22	b	610	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
27	D	412	LMG	C38-C37-C36	-2.45	101.83	114.45
30	B	627	LMT	C1'-O5'-C5'	-2.45	109.10	113.72
25	a	410	DGD	CBB-CAB-C9B	-2.45	101.83	114.45
27	d	412	LMG	C1-C2-C3	-2.45	105.42	109.98
24	c	514	BCR	C33-C5-C6	-2.45	121.77	124.51
24	c	513	BCR	C15-C14-C13	-2.45	123.82	127.31
25	c	515	DGD	O5D-C6D-C5D	-2.45	104.85	108.94
23	j	101	PL9	C22-C23-C24	-2.44	121.54	127.68
27	A	410	LMG	C40-C39-C38	-2.44	101.86	114.45
30	D	411	LMT	C3'-C4'-C5'	-2.44	105.69	110.88
24	y	101	BCR	C1-C6-C5	-2.44	119.16	122.59
27	a	412	LMG	O3-C3-C2	-2.44	105.05	110.36
27	a	412	LMG	C1-C2-C3	-2.44	105.44	109.98
25	A	408	DGD	CBB-CAB-C9B	-2.44	101.89	114.45
22	C	508	CLA	O2D-CGD-O1D	-2.44	118.92	123.82
25	a	410	DGD	C1D-C2D-C3D	-2.43	105.45	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	DGD	C1D-C2D-C3D	-2.43	105.45	109.98
24	b	623	BCR	C11-C10-C9	-2.43	123.84	127.31
24	b	622	BCR	C15-C14-C13	-2.43	123.84	127.31
22	c	505	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
24	K	102	BCR	C15-C14-C13	-2.43	123.84	127.31
30	i	102	LMT	C1'-O5'-C5'	-2.43	109.14	113.72
22	A	403	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
25	c	516	DGD	O6E-C1E-O5D	-2.42	104.27	110.02
22	a	405	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	b	606	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
26	c	519	LHG	C11-C10-C9	-2.42	101.99	114.45
22	C	511	CLA	O2A-CGA-O1A	-2.42	117.55	123.55
24	b	622	BCR	C15-C16-C17	-2.42	118.31	123.46
25	C	516	DGD	O6E-C1E-O5D	-2.41	104.29	110.02
27	c	522	LMG	O2-C2-C1	-2.41	104.98	110.03
24	b	621	BCR	C35-C13-C14	-2.41	119.54	122.92
24	b	620	BCR	C11-C10-C9	-2.41	123.86	127.31
27	D	412	LMG	O3-C3-C2	-2.41	105.11	110.36
22	B	611	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
24	j	102	BCR	C15-C16-C17	-2.41	118.31	123.46
22	B	608	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	E	101	LMG	O6-C1-O1	-2.41	104.31	110.02
22	b	608	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	b	612	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
24	c	513	BCR	C15-C16-C17	-2.40	118.34	123.46
27	D	409	LMG	C38-C37-C36	-2.40	102.10	114.45
27	d	408	LMG	C38-C37-C36	-2.40	102.10	114.45
25	B	620	DGD	CBB-CAB-C9B	-2.40	102.10	114.45
27	c	522	LMG	O6-C1-O1	-2.40	104.33	110.02
29	a	401	SQD	C5-C6-S	-2.40	111.00	114.34
22	A	404	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	B	602	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
25	b	624	DGD	CBB-CAB-C9B	-2.39	102.13	114.45
24	B	616	BCR	C11-C10-C9	-2.39	123.90	127.31
27	b	625	LMG	O2-C2-C1	-2.39	105.03	110.03
24	c	513	BCR	C7-C8-C9	-2.39	122.62	126.21
26	C	519	LHG	C11-C10-C9	-2.39	102.14	114.45
27	a	412	LMG	C40-C39-C38	-2.39	102.15	114.45
30	d	411	LMT	C1'-O5'-C5'	-2.39	109.22	113.72
22	A	405	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	B	603	CLA	C1-C2-C3	-2.39	121.56	125.96
22	b	607	CLA	C1-C2-C3	-2.39	121.56	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	404	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	a	406	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
27	C	521	LMG	C40-C39-C38	-2.38	102.19	114.45
25	C	517	DGD	CFB-CEB-CDB	-2.38	102.19	114.45
27	B	621	LMG	O6-C1-O1	-2.38	104.37	110.02
27	M	101	LMG	O2-C2-C1	-2.38	105.05	110.03
25	c	517	DGD	CFB-CEB-CDB	-2.38	102.21	114.45
24	c	514	BCR	C15-C14-C13	-2.37	123.92	127.31
22	A	402	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	C	506	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	c	515	DGD	C1D-C2D-C3D	-2.37	105.57	109.98
22	c	507	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	B	601	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	b	611	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	C	516	DGD	O3D-C3D-C4D	-2.36	105.21	110.36
22	C	520	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
25	c	516	DGD	O3D-C3D-C4D	-2.36	105.21	110.36
24	g	101	BCR	C1-C6-C5	-2.36	119.27	122.59
27	c	522	LMG	C40-C39-C38	-2.36	102.28	114.45
22	H	101	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	h	101	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
34	v	201	HEM	C1D-C2D-C3D	-2.36	105.36	107.00
34	V	201	HEM	C1D-C2D-C3D	-2.36	105.36	107.00
25	c	516	DGD	CFB-CEB-CDB	-2.36	102.32	114.45
25	A	408	DGD	C3G-C2G-C1G	-2.35	106.55	111.86
27	D	408	LMG	C38-C37-C36	-2.35	102.34	114.45
27	C	521	LMG	O6-C1-O1	-2.35	104.44	110.02
27	d	408	LMG	O3-C3-C2	-2.35	105.25	110.36
27	e	101	LMG	O6-C1-O1	-2.35	104.45	110.02
22	d	406	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
27	C	518	LMG	O2-C2-C1	-2.34	105.13	110.03
27	c	518	LMG	O2-C2-C1	-2.34	105.13	110.03
22	B	613	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	604	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	c	506	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
27	A	410	LMG	C38-C37-C36	-2.34	102.42	114.45
25	d	410	DGD	C3D-C4D-C5D	-2.33	106.10	110.22
25	a	410	DGD	C3G-C2G-C1G	-2.33	106.59	111.86
24	B	619	BCR	C11-C10-C9	-2.33	123.98	127.31
22	b	605	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
24	F	102	BCR	C11-C10-C9	-2.33	123.99	127.31
34	f	101	HEM	CAA-CBA-CGA	-2.33	108.68	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	I	102	LMT	C1'-O5'-C5'	-2.33	109.33	113.72
22	c	504	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	c	511	CLA	O2A-CGA-O1A	-2.33	117.78	123.55
27	C	518	LMG	C38-C37-C36	-2.32	102.49	114.45
25	C	515	DGD	O5D-C6D-C5D	-2.32	105.06	108.94
27	D	408	LMG	O3-C3-C2	-2.32	105.31	110.36
25	A	408	DGD	C1D-C2D-C3D	-2.32	105.67	109.98
27	b	625	LMG	O3-C3-C2	-2.32	105.31	110.36
27	a	402	LMG	O3-C3-C2	-2.32	105.31	110.36
27	a	412	LMG	O2-C2-C1	-2.32	105.18	110.03
27	B	621	LMG	O3-C3-C2	-2.32	105.32	110.36
27	A	410	LMG	O2-C2-C1	-2.31	105.19	110.03
25	B	620	DGD	C3G-C2G-C1G	-2.31	106.64	111.86
27	d	412	LMG	O2-C2-C1	-2.31	105.19	110.03
27	I	101	LMG	O3-C3-C2	-2.31	105.33	110.36
22	D	405	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	B	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
24	C	513	BCR	C11-C10-C9	-2.31	124.01	127.31
24	c	513	BCR	C24-C23-C22	-2.31	122.74	126.21
24	K	102	BCR	C11-C10-C9	-2.31	124.02	127.31
27	B	621	LMG	O2-C2-C1	-2.31	105.20	110.03
27	d	412	LMG	O3-C3-C2	-2.31	105.34	110.36
22	B	605	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
24	J	102	BCR	C20-C21-C22	-2.31	124.02	127.31
27	d	412	LMG	O6-C1-O1	-2.31	104.55	110.02
27	a	402	LMG	O2-C2-C1	-2.31	105.21	110.03
27	B	621	LMG	C40-C39-C38	-2.31	102.58	114.45
27	c	518	LMG	C38-C37-C36	-2.31	102.58	114.45
25	C	516	DGD	CFB-CEB-CDB	-2.30	102.58	114.45
27	b	625	LMG	O6-C1-O1	-2.30	104.56	110.02
22	D	406	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
24	j	102	BCR	C20-C21-C22	-2.30	124.03	127.31
22	B	603	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
25	b	601	DGD	O6D-C1D-O3G	-2.29	104.58	110.02
22	B	607	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
27	i	101	LMG	O1-C7-C8	-2.29	105.55	110.99
24	f	102	BCR	C11-C10-C9	-2.29	124.05	127.31
27	a	412	LMG	C38-C37-C36	-2.29	102.68	114.45
27	b	625	LMG	C40-C39-C38	-2.28	102.70	114.45
23	D	407	PL9	C27-C28-C29	-2.28	121.95	127.68
22	c	502	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
25	b	624	DGD	C3G-C2G-C1G	-2.27	106.73	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	412	LMG	O2-C2-C1	-2.27	105.28	110.03
27	c	522	LMG	O3-C3-C2	-2.27	105.42	110.36
24	B	616	BCR	C15-C14-C13	-2.27	124.07	127.31
27	m	101	LMG	C1-O6-C5	-2.27	109.44	113.72
30	B	624	LMT	C1'-O5'-C5'	-2.27	109.44	113.72
22	b	617	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
24	c	521	BCR	C11-C10-C9	-2.27	124.07	127.31
27	C	521	LMG	O3-C3-C2	-2.27	105.42	110.36
22	b	613	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
27	i	101	LMG	O3-C3-C2	-2.27	105.42	110.36
24	b	620	BCR	C15-C14-C13	-2.27	124.08	127.31
29	F	103	SQD	C5-C6-S	-2.27	111.18	114.34
22	c	520	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	C	502	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
27	d	409	LMG	O6-C1-C2	-2.26	105.94	110.30
27	e	101	LMG	O3-C3-C2	-2.26	105.44	110.36
22	c	512	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
24	B	617	BCR	C35-C13-C14	-2.26	119.76	122.92
27	C	521	LMG	C38-C37-C36	-2.26	102.82	114.45
27	D	412	LMG	O6-C1-O1	-2.26	104.66	110.02
22	b	616	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
27	A	414	LMG	O3-C3-C2	-2.26	105.45	110.36
22	c	509	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
27	c	518	LMG	O3-C3-C2	-2.25	105.46	110.36
24	a	409	BCR	C15-C16-C17	-2.25	118.67	123.46
22	B	609	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	C	512	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	a	408	PL9	C27-C28-C29	-2.24	122.05	127.68
22	C	509	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
22	b	609	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
27	b	625	LMG	C38-C37-C36	-2.24	102.91	114.45
22	b	607	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
24	B	617	BCR	C11-C10-C9	-2.24	124.12	127.31
23	A	406	PL9	C27-C28-C29	-2.24	122.06	127.68
34	F	101	HEM	CAA-CBA-CGA	-2.24	108.84	112.66
22	C	508	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
24	a	409	BCR	C33-C5-C6	-2.23	122.01	124.51
23	d	407	PL9	C27-C28-C29	-2.23	122.07	127.68
24	A	407	BCR	C15-C14-C13	-2.23	124.12	127.31
27	a	402	LMG	O1-C7-C8	-2.23	105.69	110.99
22	c	510	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
27	C	518	LMG	O3-C3-C2	-2.22	105.53	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	BCR	C15-C14-C13	-2.22	124.14	127.31
22	C	510	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
22	b	614	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
30	b	627	LMT	C1'-O5'-C5'	-2.22	109.54	113.72
27	c	522	LMG	C38-C37-C36	-2.22	103.04	114.45
24	C	513	BCR	C3-C4-C5	-2.22	109.97	113.78
29	B	622	SQD	C5-C6-S	-2.21	111.25	114.34
24	K	102	BCR	C33-C5-C6	-2.21	122.03	124.51
22	c	506	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
25	C	516	DGD	C3D-C4D-C5D	-2.21	106.32	110.22
24	J	102	BCR	C15-C16-C17	-2.21	118.74	123.46
22	B	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
34	F	101	HEM	CBD-CAD-C3D	-2.21	108.25	112.47
22	d	406	CLA	C1-C2-C3	-2.21	121.89	125.96
22	b	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
27	B	621	LMG	C38-C37-C36	-2.21	103.08	114.45
22	C	511	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
27	E	101	LMG	O3-C3-C2	-2.21	105.56	110.36
25	D	410	DGD	C3D-C4D-C5D	-2.20	106.33	110.22
22	b	618	CLA	O2A-CGA-O1A	-2.20	118.09	123.55
22	C	501	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
27	M	101	LMG	O3-C3-C2	-2.20	105.57	110.36
22	C	507	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
27	A	414	LMG	O2-C2-C1	-2.20	105.43	110.03
22	c	501	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
24	A	407	BCR	C33-C5-C6	-2.20	122.05	124.51
23	D	407	PL9	C37-C38-C39	-2.20	122.17	127.68
25	c	516	DGD	O2D-C2D-C1D	-2.19	105.44	110.03
25	B	625	DGD	O6D-C1D-O3G	-2.19	104.81	110.02
27	d	409	LMG	O6-C1-O1	-2.19	104.82	110.02
27	e	101	LMG	O1-C7-C8	-2.19	105.77	110.99
24	A	407	BCR	C15-C16-C17	-2.19	118.79	123.46
27	D	409	LMG	O6-C1-O1	-2.19	104.83	110.02
22	C	503	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
24	B	616	BCR	C15-C16-C17	-2.19	118.80	123.46
22	c	511	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
25	a	410	DGD	CAB-C9B-C8B	-2.18	103.22	114.45
24	c	521	BCR	C24-C23-C22	-2.18	122.94	126.21
27	m	101	LMG	O3-C3-C2	-2.18	105.62	110.36
24	b	622	BCR	C7-C8-C9	-2.18	122.94	126.21
23	d	407	PL9	C37-C38-C39	-2.17	122.22	127.68
24	c	513	BCR	C3-C4-C5	-2.17	110.04	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	516	DGD	O2D-C2D-C1D	-2.17	105.48	110.03
22	B	601	CLA	O2A-CGA-O1A	-2.17	118.16	123.55
22	B	611	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
22	b	618	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
22	B	603	CLA	O2A-CGA-O1A	-2.17	118.17	123.55
27	E	101	LMG	O1-C7-C8	-2.17	105.83	110.99
25	c	516	DGD	CBB-CAB-C9B	-2.17	103.29	114.45
24	b	621	BCR	C11-C10-C9	-2.17	124.22	127.31
26	a	411	LHG	C27-C26-C25	-2.17	103.29	114.45
22	c	508	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	b	614	CLA	C1-C2-C3	-2.16	121.97	125.96
27	e	101	LMG	O2-C2-C1	-2.16	105.50	110.03
22	d	405	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
24	F	102	BCR	C15-C16-C17	-2.16	118.85	123.46
24	g	101	BCR	C3-C2-C1	-2.16	106.82	114.59
22	b	619	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
25	A	408	DGD	CAB-C9B-C8B	-2.16	103.33	114.45
25	C	516	DGD	CBB-CAB-C9B	-2.16	103.33	114.45
27	E	101	LMG	O2-C2-C1	-2.16	105.51	110.03
27	A	414	LMG	O1-C7-C8	-2.16	105.86	110.99
24	b	621	BCR	C7-C8-C9	-2.15	122.97	126.21
25	C	517	DGD	CBB-CAB-C9B	-2.15	103.35	114.45
22	B	610	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
24	b	623	BCR	C24-C23-C22	-2.15	122.98	126.21
22	B	614	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
25	b	601	DGD	CBB-CAB-C9B	-2.15	103.38	114.45
25	c	515	DGD	O2D-C2D-C1D	-2.15	105.54	110.03
29	A	412	SQD	C5-C6-S	-2.15	111.35	114.34
24	C	513	BCR	C7-C8-C9	-2.15	122.99	126.21
25	C	516	DGD	C1D-C2D-C3D	-2.15	105.99	109.98
24	c	521	BCR	C33-C5-C6	-2.14	122.11	124.51
23	D	407	PL9	C32-C33-C34	-2.14	122.30	127.68
25	C	517	DGD	O2D-C2D-C1D	-2.14	105.55	110.03
22	B	610	CLA	C1-C2-C3	-2.14	122.01	125.96
24	F	102	BCR	C7-C8-C9	-2.14	123.00	126.21
24	b	623	BCR	C38-C26-C25	-2.14	122.11	124.51
22	c	509	CLA	O2A-CGA-O1A	-2.14	118.24	123.55
24	C	514	BCR	C38-C26-C25	-2.14	122.11	124.51
25	C	516	DGD	CAB-C9B-C8B	-2.14	103.45	114.45
22	B	602	CLA	O2A-CGA-O1A	-2.13	118.25	123.55
22	D	405	CLA	O2A-CGA-O1A	-2.13	118.25	123.55
27	M	101	LMG	C1-O6-C5	-2.13	109.70	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	607	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
22	c	503	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
25	B	620	DGD	C4E-C3E-C2E	-2.13	107.08	110.84
29	f	103	SQD	C5-C6-S	-2.13	111.37	114.34
22	B	608	CLA	C1-C2-C3	-2.13	122.04	125.96
24	B	619	BCR	C38-C26-C25	-2.13	122.13	124.51
24	B	617	BCR	C7-C8-C9	-2.13	123.02	126.21
25	B	625	DGD	CBB-CAB-C9B	-2.12	103.51	114.45
24	b	623	BCR	C33-C5-C6	-2.12	122.13	124.51
24	f	102	BCR	C15-C16-C17	-2.12	118.93	123.46
22	b	615	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
25	c	517	DGD	CBB-CAB-C9B	-2.12	103.52	114.45
24	B	618	BCR	C7-C8-C9	-2.12	123.02	126.21
22	C	506	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
26	A	409	LHG	C27-C26-C25	-2.12	103.54	114.45
24	C	514	BCR	C24-C23-C22	-2.12	123.03	126.21
25	C	515	DGD	O3E-C3E-C2E	-2.11	105.76	110.36
22	B	611	CLA	O2A-CGA-O1A	-2.11	118.30	123.55
25	b	601	DGD	CAB-C9B-C8B	-2.11	103.58	114.45
22	B	612	CLA	O2A-CGA-O1A	-2.11	118.31	123.55
24	y	101	BCR	C3-C2-C1	-2.11	107.01	114.59
25	C	515	DGD	O2D-C2D-C1D	-2.11	105.62	110.03
24	B	619	BCR	C24-C23-C22	-2.11	123.05	126.21
27	D	409	LMG	O3-C3-C2	-2.11	105.77	110.36
31	d	401	PHO	C2B-C1B-NB	-2.11	106.70	109.82
27	C	521	LMG	C1-C2-C3	-2.11	106.06	109.98
25	c	516	DGD	C3D-C4D-C5D	-2.11	106.51	110.22
22	C	501	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
25	d	410	DGD	C5B-C4B-C3B	-2.10	103.64	114.45
24	c	514	BCR	C24-C23-C22	-2.10	123.06	126.21
24	H	102	BCR	C16-C15-C14	-2.10	118.98	123.46
23	d	407	PL9	O1-C4-C3	-2.10	118.33	120.71
24	g	101	BCR	C15-C16-C17	-2.10	118.99	123.46
25	c	517	DGD	CAB-C9B-C8B	-2.10	103.66	114.45
27	A	414	LMG	C1-C2-C3	-2.09	106.09	109.98
27	c	518	LMG	O7-C10-O9	-2.09	118.45	123.68
23	d	407	PL9	O2-C1-C2	-2.09	116.88	121.77
22	b	616	CLA	O2A-CGA-O1A	-2.09	118.36	123.55
25	B	625	DGD	CAB-C9B-C8B	-2.09	103.68	114.45
22	B	606	CLA	O2A-CGA-O1A	-2.09	118.36	123.55
22	B	614	CLA	O2A-CGA-O1A	-2.09	118.36	123.55
22	b	610	CLA	O2A-CGA-O1A	-2.09	118.36	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	101	PL9	O2-C1-C2	-2.09	116.89	121.77
24	b	622	BCR	C33-C5-C6	-2.08	122.17	124.51
22	C	520	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
22	c	508	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
27	I	101	LMG	O7-C10-O9	-2.08	118.48	123.68
26	C	519	LHG	C27-C26-C25	-2.08	103.73	114.45
22	c	520	CLA	O2A-CGA-O1A	-2.08	118.39	123.55
22	C	508	CLA	O2A-CGA-O1A	-2.08	118.39	123.55
25	D	410	DGD	C5B-C4B-C3B	-2.08	103.75	114.45
24	B	619	BCR	C33-C5-C6	-2.08	122.18	124.51
24	c	514	BCR	C38-C26-C25	-2.08	122.19	124.51
22	C	512	CLA	O2A-CGA-O1A	-2.07	118.40	123.55
25	b	601	DGD	O3E-C3E-C2E	-2.07	105.85	110.36
22	a	405	CLA	O2A-CGA-O1A	-2.07	118.41	123.55
23	D	407	PL9	O1-C4-C3	-2.07	118.36	120.71
22	c	501	CLA	O2A-CGA-O1A	-2.07	118.41	123.55
25	C	517	DGD	CAB-C9B-C8B	-2.07	103.79	114.45
23	d	407	PL9	C32-C33-C34	-2.07	122.48	127.68
27	D	408	LMG	O1-C7-C8	-2.07	106.07	110.99
25	c	516	DGD	CAB-C9B-C8B	-2.07	103.81	114.45
23	J	101	PL9	O2-C1-C2	-2.06	116.94	121.77
22	b	606	CLA	O2A-CGA-O1A	-2.06	118.43	123.55
24	a	409	BCR	C24-C23-C22	-2.06	123.11	126.21
25	B	620	DGD	O2D-C2D-C1D	-2.06	105.72	110.03
26	c	519	LHG	C27-C26-C25	-2.06	103.84	114.45
31	D	402	PHO	C2B-C1B-NB	-2.06	106.77	109.82
25	C	515	DGD	C5B-C4B-C3B	-2.06	103.85	114.45
27	C	518	LMG	O7-C10-O9	-2.06	118.54	123.68
25	D	410	DGD	O3E-C3E-C2E	-2.06	105.88	110.36
27	a	412	LMG	C1-O6-C5	-2.06	109.84	113.72
25	c	515	DGD	C5B-C4B-C3B	-2.05	103.87	114.45
24	y	101	BCR	C15-C16-C17	-2.05	119.08	123.46
27	c	522	LMG	C1-C2-C3	-2.05	106.16	109.98
31	D	402	PHO	CMB-C2B-C1B	-2.05	121.85	125.04
24	c	513	BCR	C8-C7-C6	-2.05	121.51	127.25
25	b	624	DGD	O2D-C2D-C1D	-2.05	105.74	110.03
22	c	512	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
25	c	515	DGD	O3E-C3E-C2E	-2.05	105.90	110.36
27	a	412	LMG	O7-C10-O9	-2.05	118.57	123.68
31	D	401	PHO	C2B-C1B-NB	-2.05	106.79	109.82
22	B	609	CLA	O2A-CGA-O1A	-2.05	118.47	123.55
24	A	407	BCR	C38-C26-C25	-2.05	122.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	410	LMG	O7-C10-O9	-2.05	118.57	123.68
23	D	407	PL9	O2-C1-C2	-2.04	116.99	121.77
24	C	514	BCR	C7-C8-C9	-2.04	123.14	126.21
22	d	405	CLA	O2A-CGA-O1A	-2.04	118.48	123.55
23	A	406	PL9	O2-C1-C2	-2.04	117.00	121.77
24	K	102	BCR	C7-C8-C9	-2.04	123.15	126.21
23	a	408	PL9	O2-C1-C2	-2.04	117.00	121.77
24	C	513	BCR	C8-C7-C6	-2.04	121.55	127.25
25	D	410	DGD	CAB-C9B-C8B	-2.04	103.96	114.45
23	d	407	PL9	C36-C34-C33	-2.04	116.94	121.10
22	B	607	CLA	O2A-CGA-O1A	-2.03	118.50	123.55
22	C	507	CLA	C1-C2-C3	-2.03	122.21	125.96
24	b	622	BCR	C20-C21-C22	-2.03	124.41	127.31
27	a	402	LMG	C1-C2-C3	-2.03	106.20	109.98
25	D	410	DGD	CBB-CAB-C9B	-2.03	103.98	114.45
27	A	410	LMG	C1-O6-C5	-2.03	109.89	113.72
24	a	409	BCR	C38-C26-C25	-2.03	122.24	124.51
25	d	410	DGD	CAB-C9B-C8B	-2.03	104.00	114.45
31	d	402	PHO	CMB-C2B-C1B	-2.03	121.88	125.04
31	d	401	PHO	O2A-CGA-O1A	-2.03	118.52	123.55
27	A	414	LMG	O7-C10-O9	-2.03	118.62	123.68
25	b	624	DGD	CAB-C9B-C8B	-2.02	104.02	114.45
31	D	401	PHO	O2A-CGA-O1A	-2.02	118.53	123.55
25	d	410	DGD	CBB-CAB-C9B	-2.02	104.03	114.45
24	b	621	BCR	C24-C23-C22	-2.02	123.17	126.21
22	A	403	CLA	O2A-CGA-O1A	-2.02	118.53	123.55
25	B	625	DGD	O3E-C3E-C2E	-2.02	105.95	110.36
24	B	618	BCR	C33-C5-C6	-2.02	122.25	124.51
25	c	516	DGD	C1D-C2D-C3D	-2.02	106.23	109.98
27	c	518	LMG	O1-C7-C8	-2.02	106.19	110.99
23	d	407	PL9	C31-C32-C33	-2.02	105.05	111.97
22	b	613	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
25	c	517	DGD	C5B-C4B-C3B	-2.01	104.08	114.45
25	c	516	DGD	C1D-O6D-C5D	-2.01	109.92	113.72
25	C	517	DGD	C5B-C4B-C3B	-2.01	104.08	114.45
24	A	407	BCR	C11-C10-C9	-2.01	124.44	127.31
24	H	102	BCR	C7-C8-C9	-2.01	123.19	126.21
25	B	620	DGD	C5B-C4B-C3B	-2.01	104.09	114.45
27	I	101	LMG	O1-C7-C8	-2.01	106.21	110.99
25	C	516	DGD	C5B-C4B-C3B	-2.01	104.12	114.45
22	b	605	CLA	O2A-CGA-O1A	-2.01	118.57	123.55
22	C	510	CLA	O2A-CGA-O1A	-2.00	118.57	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	615	CLA	O2A-CGA-O1A	-2.00	118.58	123.55
25	A	408	DGD	C5B-C4B-C3B	-2.00	104.14	114.45
25	c	517	DGD	O2D-C2D-C1D	-2.00	105.84	110.03
22	C	509	CLA	O2A-CGA-O1A	-2.00	118.58	123.55
25	C	517	DGD	O3E-C3E-C2E	-2.00	106.00	110.36
27	i	101	LMG	O7-C10-O9	-2.00	118.68	123.68
24	B	616	BCR	C7-C8-C9	-2.00	123.21	126.21
22	B	606	CLA	C1D-CHD-C4C	2.00	125.22	122.48
22	c	511	CLA	C1D-CHD-C4C	2.01	125.23	122.48
22	c	508	CLA	C1D-CHD-C4C	2.01	125.23	122.48
22	c	512	CLA	O1D-CGD-CBD	2.01	128.21	124.60
22	B	610	CLA	O1D-CGD-CBD	2.01	128.22	124.60
22	b	606	CLA	C1D-CHD-C4C	2.01	125.24	122.48
31	d	402	PHO	C1B-NB-C4B	2.02	110.53	106.52
22	b	618	CLA	C1D-CHD-C4C	2.02	125.25	122.48
22	c	501	CLA	O1D-CGD-CBD	2.02	128.24	124.60
22	c	503	CLA	O2D-CGD-CBD	2.03	114.93	111.30
22	a	406	CLA	C1D-CHD-C4C	2.04	125.27	122.48
25	C	517	DGD	C3G-O3G-C1D	2.04	117.94	113.76
22	C	510	CLA	O1D-CGD-CBD	2.04	128.27	124.60
23	A	406	PL9	O2-C1-C6	2.04	124.25	120.57
31	D	401	PHO	C1B-NB-C4B	2.04	110.57	106.52
23	d	407	PL9	O2-C1-C6	2.05	124.26	120.57
24	b	622	BCR	C27-C26-C25	2.05	125.75	122.74
31	d	401	PHO	C1B-NB-C4B	2.05	110.58	106.52
22	b	614	CLA	C1D-CHD-C4C	2.06	125.30	122.48
23	J	101	PL9	O2-C1-C6	2.06	124.28	120.57
24	H	102	BCR	C29-C30-C25	2.07	113.71	110.48
22	A	403	CLA	CMD-C2D-C3D	2.07	128.74	124.89
23	a	408	PL9	O2-C1-C6	2.07	124.31	120.57
22	c	512	CLA	C1D-CHD-C4C	2.08	125.32	122.48
23	j	101	PL9	O2-C1-C6	2.08	124.32	120.57
22	B	607	CLA	O1D-CGD-CBD	2.09	128.35	124.60
34	V	201	HEM	CMB-C2B-C3B	2.09	128.77	124.89
22	C	509	CLA	C1D-CHD-C4C	2.10	125.35	122.48
31	D	402	PHO	C1B-NB-C4B	2.10	110.67	106.52
22	a	406	CLA	CMD-C2D-C3D	2.10	128.78	124.89
22	D	405	CLA	CHB-C4A-NA	2.10	127.41	124.51
22	c	507	CLA	O2D-CGD-CBD	2.10	115.05	111.30
22	c	508	CLA	CMD-C2D-C3D	2.10	128.79	124.89
22	c	520	CLA	C1D-CHD-C4C	2.10	125.36	122.48
22	B	614	CLA	C1D-CHD-C4C	2.10	125.36	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	O1D-CGD-CBD	2.11	128.38	124.60
22	b	610	CLA	C1D-CHD-C4C	2.11	125.37	122.48
34	v	201	HEM	CMB-C2B-C3B	2.11	128.81	124.89
22	d	405	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	A	402	CLA	CMD-C2D-C3D	2.12	128.83	124.89
29	A	413	SQD	C1-O5-C5	2.13	117.72	113.72
29	d	403	SQD	C4-C3-C2	2.13	114.59	110.84
22	b	610	CLA	CMD-C2D-C3D	2.13	128.84	124.89
22	b	609	CLA	CMD-C2D-C3D	2.13	128.84	124.89
22	A	402	CLA	O1D-CGD-CBD	2.13	128.43	124.60
22	A	404	CLA	CMD-C2D-C3D	2.13	128.85	124.89
24	F	102	BCR	C27-C26-C25	2.14	125.88	122.74
22	b	614	CLA	O1D-CGD-CBD	2.14	128.45	124.60
24	x	101	BCR	C29-C30-C25	2.14	113.83	110.48
29	B	622	SQD	C4-C3-C2	2.15	114.62	110.84
22	B	604	CLA	CMD-C2D-C3D	2.15	128.88	124.89
24	f	102	BCR	C27-C26-C25	2.15	125.90	122.74
22	C	509	CLA	CMD-C2D-C3D	2.15	128.89	124.89
22	C	507	CLA	C1D-CHD-C4C	2.15	125.43	122.48
22	a	404	CLA	CMD-C2D-C3D	2.16	128.90	124.89
22	a	404	CLA	O1D-CGD-CBD	2.16	128.49	124.60
22	C	508	CLA	CMD-C2D-C3D	2.17	128.91	124.89
22	B	610	CLA	C4A-NA-C1A	2.17	109.14	106.45
23	A	406	PL9	C20-C19-C21	2.17	119.05	115.29
24	C	513	BCR	C27-C26-C25	2.18	125.94	122.74
22	c	509	CLA	CMD-C2D-C3D	2.19	128.95	124.89
24	c	513	BCR	C27-C26-C25	2.19	125.95	122.74
24	b	620	BCR	C27-C26-C25	2.20	125.96	122.74
22	b	619	CLA	CMD-C2D-C3D	2.20	128.97	124.89
22	B	606	CLA	CMD-C2D-C3D	2.20	128.97	124.89
22	B	609	CLA	C1D-CHD-C4C	2.20	125.49	122.48
22	B	615	CLA	CMD-C2D-C3D	2.20	128.98	124.89
22	b	608	CLA	CMD-C2D-C3D	2.20	128.98	124.89
22	B	610	CLA	C1D-CHD-C4C	2.20	125.50	122.48
22	b	614	CLA	C4A-NA-C1A	2.20	109.19	106.45
24	B	616	BCR	C27-C26-C25	2.21	125.99	122.74
22	c	520	CLA	CMD-C2D-C3D	2.22	129.00	124.89
29	f	103	SQD	O48-C23-C24	2.22	118.37	111.90
22	c	503	CLA	CMD-C2D-C3D	2.22	129.02	124.89
22	c	512	CLA	CMD-C2D-C3D	2.23	129.03	124.89
22	c	510	CLA	CMD-C2D-C3D	2.23	129.03	124.89
24	J	102	BCR	C29-C30-C25	2.23	113.97	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	f	103	SQD	C3-C4-C5	2.23	114.15	110.22
22	B	609	CLA	CMD-C2D-C3D	2.23	129.04	124.89
29	F	103	SQD	C3-C4-C5	2.23	114.15	110.22
29	A	412	SQD	C4-C3-C2	2.24	114.78	110.84
22	C	505	CLA	CMD-C2D-C3D	2.24	129.04	124.89
23	j	101	PL9	C20-C19-C21	2.24	119.17	115.29
22	B	605	CLA	CMD-C2D-C3D	2.24	129.05	124.89
22	C	504	CLA	O1D-CGD-CBD	2.24	128.63	124.60
22	b	616	CLA	CMD-C2D-C3D	2.25	129.06	124.89
22	C	512	CLA	CMD-C2D-C3D	2.27	129.10	124.89
22	B	614	CLA	CMD-C2D-C3D	2.27	129.11	124.89
22	C	520	CLA	CMD-C2D-C3D	2.27	129.11	124.89
24	j	102	BCR	C29-C30-C25	2.27	114.03	110.48
22	b	609	CLA	O1D-CGD-CBD	2.28	128.69	124.60
22	B	601	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	B	616	BCR	C2-C1-C6	2.29	114.05	110.48
22	H	101	CLA	CMD-C2D-C3D	2.29	129.15	124.89
22	C	501	CLA	CMB-C2B-C3B	2.30	129.16	124.89
22	b	605	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	C	510	CLA	CMD-C2D-C3D	2.31	129.17	124.89
22	c	504	CLA	O1D-CGD-CBD	2.31	128.75	124.60
22	b	618	CLA	CMD-C2D-C3D	2.31	129.17	124.89
22	c	505	CLA	CMD-C2D-C3D	2.31	129.18	124.89
22	C	503	CLA	CMD-C2D-C3D	2.31	129.18	124.89
22	C	507	CLA	CMD-C2D-C3D	2.31	129.18	124.89
22	b	607	CLA	CMD-C2D-C3D	2.31	129.18	124.89
22	b	619	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	d	407	PL9	C20-C19-C21	2.32	119.32	115.29
22	B	612	CLA	CMD-C2D-C3D	2.33	129.22	124.89
22	c	501	CLA	CMD-C2D-C3D	2.33	129.22	124.89
24	B	619	BCR	C27-C26-C25	2.33	126.17	122.74
23	J	101	PL9	C20-C19-C21	2.34	119.34	115.29
29	F	103	SQD	O48-C23-C24	2.34	118.71	111.90
24	a	409	BCR	C27-C26-C25	2.34	126.18	122.74
23	D	407	PL9	C20-C19-C21	2.34	119.35	115.29
22	c	506	CLA	CMD-C2D-C3D	2.34	129.24	124.89
24	b	623	BCR	C27-C26-C25	2.34	126.18	122.74
29	a	415	SQD	C4-C3-C2	2.34	114.97	110.84
24	B	617	BCR	C29-C30-C25	2.35	114.15	110.48
24	b	621	BCR	C29-C30-C25	2.35	114.16	110.48
22	B	615	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	d	405	CLA	O1D-CGD-CBD	2.36	128.84	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	CMD-C2D-C3D	2.36	129.27	124.89
24	A	407	BCR	C27-C26-C25	2.36	126.21	122.74
22	b	606	CLA	CMD-C2D-C3D	2.37	129.28	124.89
22	A	405	CLA	CMD-C2D-C3D	2.37	129.29	124.89
22	C	501	CLA	CMD-C2D-C3D	2.37	129.29	124.89
29	b	602	SQD	O48-C23-C24	2.37	118.80	111.90
22	B	605	CLA	O1D-CGD-CBD	2.37	128.86	124.60
22	d	406	CLA	CMD-C2D-C3D	2.37	129.30	124.89
23	A	406	PL9	C41-C39-C40	2.37	120.14	114.60
24	b	620	BCR	C2-C1-C6	2.38	114.19	110.48
22	B	613	CLA	CMD-C2D-C3D	2.38	129.31	124.89
29	F	103	SQD	C44-O6-C1	2.38	118.64	113.76
22	b	613	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	C	507	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	a	408	PL9	C20-C19-C21	2.38	119.42	115.29
22	C	509	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	b	606	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	b	606	CLA	C4A-NA-C1A	2.39	109.42	106.45
22	a	404	CLA	C4A-NA-C1A	2.39	109.42	106.45
22	c	509	CLA	CHB-C4A-NA	2.40	127.82	124.51
22	b	605	CLA	CMD-C2D-C3D	2.40	129.34	124.89
22	c	501	CLA	CMB-C2B-C3B	2.40	129.35	124.89
22	C	502	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	b	612	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	D	406	CLA	CMD-C2D-C3D	2.40	129.35	124.89
29	a	401	SQD	C1-O5-C5	2.41	118.25	113.72
22	H	101	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	K	102	BCR	C27-C26-C25	2.41	126.28	122.74
22	B	603	CLA	CMD-C2D-C3D	2.41	129.36	124.89
22	b	612	CLA	C4A-NA-C1A	2.41	109.45	106.45
22	B	602	CLA	CMD-C2D-C3D	2.41	129.37	124.89
22	B	601	CLA	CMD-C2D-C3D	2.42	129.37	124.89
22	c	507	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	h	101	CLA	CMD-C2D-C3D	2.42	129.38	124.89
22	b	605	CLA	C4A-NA-C1A	2.42	109.46	106.45
22	C	506	CLA	CMD-C2D-C3D	2.42	129.39	124.89
24	c	521	BCR	C27-C26-C25	2.42	126.30	122.74
22	B	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	b	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
29	A	413	SQD	O48-C23-C24	2.43	118.96	111.90
22	B	607	CLA	CMD-C2D-C3D	2.43	129.40	124.89
22	b	611	CLA	CMD-C2D-C3D	2.43	129.41	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	405	CLA	C4A-NA-C1A	2.43	109.47	106.45
22	h	101	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	B	601	CLA	C4A-NA-C1A	2.43	109.47	106.45
22	b	613	CLA	C4A-NA-C1A	2.44	109.48	106.45
22	D	406	CLA	C4A-NA-C1A	2.44	109.48	106.45
29	B	626	SQD	O48-C23-C24	2.44	119.00	111.90
22	A	405	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	c	502	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	c	509	CLA	C4A-NA-C1A	2.45	109.49	106.45
22	C	503	CLA	CHB-C4A-NA	2.45	127.89	124.51
24	c	514	BCR	C29-C30-C25	2.45	114.30	110.48
22	B	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	b	617	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	D	406	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	C	509	CLA	C4A-NA-C1A	2.45	109.49	106.45
22	A	402	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	A	402	CLA	C4A-NA-C1A	2.45	109.50	106.45
23	a	408	PL9	C41-C39-C40	2.45	120.33	114.60
29	d	403	SQD	O48-C23-C24	2.46	119.05	111.90
22	b	612	CLA	CMD-C2D-C3D	2.46	129.46	124.89
22	C	502	CLA	CMD-C2D-C3D	2.46	129.46	124.89
22	C	502	CLA	C4A-NA-C1A	2.46	109.51	106.45
24	C	514	BCR	C29-C30-C25	2.47	114.34	110.48
22	a	404	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	C	508	CLA	C4A-NA-C1A	2.47	109.52	106.45
22	d	406	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	b	617	CLA	CMD-C2D-C3D	2.48	129.49	124.89
22	B	607	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	b	611	CLA	C4A-NA-C1A	2.48	109.53	106.45
22	b	607	CLA	O1D-CGD-CBD	2.48	129.06	124.60
22	b	616	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	b	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	608	CLA	CMD-C2D-C3D	2.49	129.51	124.89
22	C	508	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	606	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	D	405	CLA	CMD-C2D-C3D	2.50	129.52	124.89
29	a	415	SQD	O48-C23-C24	2.50	119.16	111.90
22	c	503	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	609	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	512	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	d	406	CLA	C4A-NA-C1A	2.50	109.56	106.45
22	c	507	CLA	CMD-C2D-C3D	2.50	129.54	124.89
22	D	405	CLA	C4A-NA-C1A	2.51	109.56	106.45
22	c	501	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	c	504	CLA	CMD-C2D-C3D	2.51	129.55	124.89
22	B	602	CLA	C4A-NA-C1A	2.51	109.57	106.45
22	a	407	CLA	CMD-C2D-C3D	2.51	129.55	124.89
22	c	510	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	B	604	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	c	504	CLA	CMB-C2B-C3B	2.52	129.57	124.89
22	c	512	CLA	C4A-NA-C1A	2.52	109.58	106.45
22	d	405	CLA	CMD-C2D-C3D	2.52	129.57	124.89
22	c	502	CLA	C4A-NA-C1A	2.52	109.58	106.45
22	c	508	CLA	C4A-NA-C1A	2.52	109.58	106.45
22	a	407	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	c	507	CLA	C4A-NA-C1A	2.52	109.59	106.45
29	B	626	SQD	C4-C3-C2	2.53	115.30	110.84
22	c	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	A	404	CLA	C4A-NA-C1A	2.53	109.59	106.45
22	b	618	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	b	615	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	B	611	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	b	610	CLA	C4A-NA-C1A	2.54	109.60	106.45
22	B	609	CLA	C4A-NA-C1A	2.54	109.60	106.45
29	a	401	SQD	O48-C23-C24	2.54	119.30	111.90
29	B	622	SQD	C44-O6-C1	2.54	118.97	113.76
22	B	608	CLA	C4A-NA-C1A	2.54	109.61	106.45
22	C	511	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	H	101	CLA	C4A-NA-C1A	2.55	109.61	106.45
22	B	608	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	C	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	607	CLA	C4A-NA-C1A	2.55	109.62	106.45
22	c	505	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	c	508	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	613	CLA	C4A-NA-C1A	2.55	109.62	106.45
29	B	622	SQD	O48-C23-C24	2.55	119.33	111.90
22	h	101	CLA	C4A-NA-C1A	2.55	109.62	106.45
22	C	512	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	b	619	CLA	C4A-NA-C1A	2.56	109.63	106.45
22	c	502	CLA	CMD-C2D-C3D	2.56	129.64	124.89
22	B	610	CLA	CMD-C2D-C3D	2.56	129.65	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	CHB-C4A-NA	2.56	128.06	124.51
24	b	622	BCR	C29-C30-C25	2.57	114.49	110.48
22	c	520	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	a	406	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	c	505	CLA	C4A-NA-C1A	2.57	109.65	106.45
22	a	407	CLA	C4A-NA-C1A	2.57	109.65	106.45
22	C	503	CLA	C4A-NA-C1A	2.57	109.65	106.45
22	c	511	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	b	615	CLA	CMD-C2D-C3D	2.58	129.67	124.89
22	C	507	CLA	C4A-NA-C1A	2.58	109.65	106.45
22	B	604	CLA	C4A-NA-C1A	2.58	109.65	106.45
22	B	611	CLA	CMD-C2D-C3D	2.58	129.68	124.89
22	C	504	CLA	CMB-C2B-C3B	2.59	129.69	124.89
22	c	510	CLA	C4A-NA-C1A	2.59	109.66	106.45
22	C	505	CLA	C4A-NA-C1A	2.59	109.67	106.45
22	a	406	CLA	C4A-NA-C1A	2.59	109.67	106.45
22	b	619	CLA	CMB-C2B-C3B	2.59	129.70	124.89
29	f	103	SQD	C44-O6-C1	2.59	119.07	113.76
22	b	617	CLA	C4A-NA-C1A	2.59	109.67	106.45
29	A	412	SQD	O48-C23-C24	2.59	119.44	111.90
22	B	615	CLA	CMB-C2B-C3B	2.59	129.71	124.89
22	c	506	CLA	C4A-NA-C1A	2.60	109.67	106.45
22	B	603	CLA	O1D-CGD-CBD	2.60	129.28	124.60
22	C	506	CLA	C4A-NA-C1A	2.60	109.69	106.45
22	C	504	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	b	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	B	612	CLA	C4A-NA-C1A	2.61	109.69	106.45
22	c	506	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	c	508	CLA	CMB-C2B-C3B	2.61	129.73	124.89
22	C	520	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	B	614	CLA	C4A-NA-C1A	2.61	109.70	106.45
22	B	615	CLA	C4A-NA-C1A	2.62	109.70	106.45
22	C	505	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	C	510	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	C	512	CLA	C4A-NA-C1A	2.62	109.70	106.45
22	C	506	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	A	402	CLA	CMB-C2B-C3B	2.63	129.76	124.89
29	b	602	SQD	C4-C3-C2	2.63	115.47	110.84
29	d	403	SQD	C44-O6-C1	2.63	119.15	113.76
22	A	405	CLA	C4A-NA-C1A	2.63	109.72	106.45
22	c	511	CLA	C4A-NA-C1A	2.63	109.72	106.45
22	b	608	CLA	CHB-C4A-NA	2.63	128.15	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	CMB-C2B-C3B	2.63	129.78	124.89
22	B	606	CLA	CMB-C2B-C3B	2.63	129.78	124.89
22	c	520	CLA	C4A-NA-C1A	2.64	109.72	106.45
22	a	406	CLA	CMB-C2B-C3B	2.64	129.78	124.89
22	B	601	CLA	CMB-C2B-C3B	2.64	129.78	124.89
22	B	606	CLA	C4A-NA-C1A	2.64	109.73	106.45
22	b	608	CLA	C4A-NA-C1A	2.64	109.73	106.45
31	D	401	PHO	O1D-CGD-CBD	2.64	129.35	124.60
22	C	504	CLA	CMD-C2D-C3D	2.65	129.81	124.89
22	C	511	CLA	CMD-C2D-C3D	2.65	129.81	124.89
22	B	608	CLA	CMB-C2B-C3B	2.65	129.81	124.89
22	C	511	CLA	C4A-NA-C1A	2.65	109.75	106.45
22	b	607	CLA	CHB-C4A-NA	2.66	128.18	124.51
22	b	618	CLA	C4A-NA-C1A	2.66	109.75	106.45
22	a	404	CLA	CMB-C2B-C3B	2.66	129.83	124.89
22	a	405	CLA	CHB-C4A-NA	2.66	128.19	124.51
24	F	102	BCR	C29-C30-C25	2.66	114.64	110.48
22	b	614	CLA	CMD-C2D-C3D	2.66	129.83	124.89
22	b	612	CLA	CMB-C2B-C3B	2.66	129.83	124.89
24	B	618	BCR	C29-C30-C25	2.66	114.64	110.48
22	c	511	CLA	CMD-C2D-C3D	2.67	129.84	124.89
22	B	605	CLA	C4A-NA-C1A	2.67	109.77	106.45
22	c	501	CLA	C4A-NA-C1A	2.67	109.77	106.45
31	d	401	PHO	O1D-CGD-CBD	2.67	129.41	124.60
22	C	520	CLA	C4A-NA-C1A	2.67	109.77	106.45
22	b	616	CLA	C4A-NA-C1A	2.68	109.78	106.45
22	a	405	CLA	C4A-NA-C1A	2.68	109.78	106.45
22	b	605	CLA	CMB-C2B-C3B	2.68	129.87	124.89
22	B	603	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	g	101	BCR	C27-C26-C25	2.69	126.69	122.74
22	c	503	CLA	C4A-NA-C1A	2.69	109.80	106.45
22	B	603	CLA	CMB-C2B-C3B	2.70	129.89	124.89
22	A	403	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	D	407	PL9	C40-C39-C41	2.70	119.97	115.29
22	A	403	CLA	C4A-NA-C1A	2.70	109.80	106.45
22	A	404	CLA	CMB-C2B-C3B	2.70	129.91	124.89
22	c	509	CLA	CMB-C2B-C3B	2.71	129.92	124.89
22	c	520	CLA	CMB-C2B-C3B	2.71	129.92	124.89
22	b	609	CLA	CMB-C2B-C3B	2.71	129.93	124.89
22	a	405	CLA	CMB-C2B-C3B	2.71	129.93	124.89
25	b	601	DGD	O5D-C1E-C2E	2.72	112.67	108.23
22	C	501	CLA	C4A-NA-C1A	2.72	109.83	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	CMB-C2B-C3B	2.72	129.94	124.89
31	D	402	PHO	O1D-CGD-CBD	2.72	129.49	124.60
24	K	102	BCR	C2-C1-C6	2.73	114.74	110.48
30	i	102	LMT	O1'-C1'-C2'	2.73	112.68	108.23
31	d	402	PHO	O1D-CGD-CBD	2.73	129.50	124.60
22	C	509	CLA	CMB-C2B-C3B	2.73	129.96	124.89
22	h	101	CLA	CMB-C2B-C3B	2.73	129.96	124.89
24	y	101	BCR	C27-C26-C25	2.73	126.75	122.74
22	b	610	CLA	CMB-C2B-C3B	2.74	129.97	124.89
22	b	607	CLA	C4A-NA-C1A	2.74	109.85	106.45
22	C	510	CLA	C4A-NA-C1A	2.74	109.86	106.45
22	H	101	CLA	CMB-C2B-C3B	2.75	129.99	124.89
22	C	520	CLA	CMB-C2B-C3B	2.75	129.99	124.89
22	b	609	CLA	C4A-NA-C1A	2.75	109.87	106.45
22	b	607	CLA	CMB-C2B-C3B	2.76	130.01	124.89
22	b	615	CLA	C4A-NA-C1A	2.76	109.88	106.45
22	b	618	CLA	CMB-C2B-C3B	2.76	130.02	124.89
23	d	407	PL9	C40-C39-C41	2.76	120.08	115.29
24	f	102	BCR	C29-C30-C25	2.77	114.80	110.48
30	I	102	LMT	O1'-C1'-C2'	2.77	112.76	108.23
22	B	614	CLA	CMB-C2B-C3B	2.78	130.05	124.89
26	c	519	LHG	O8-C23-C24	2.79	120.03	111.90
26	C	519	LHG	O8-C23-C24	2.80	120.04	111.90
24	b	623	BCR	C2-C1-C6	2.80	114.86	110.48
24	B	619	BCR	C2-C1-C6	2.80	114.86	110.48
22	b	608	CLA	CMB-C2B-C3B	2.81	130.10	124.89
22	B	603	CLA	C4A-NA-C1A	2.81	109.94	106.45
22	B	605	CLA	CMB-C2B-C3B	2.81	130.11	124.89
22	d	406	CLA	CMB-C2B-C3B	2.82	130.12	124.89
24	j	102	BCR	C27-C26-C25	2.82	126.88	122.74
22	c	504	CLA	C4A-NA-C1A	2.82	109.95	106.45
22	d	405	CLA	CMB-C2B-C3B	2.83	130.15	124.89
22	B	604	CLA	CMB-C2B-C3B	2.84	130.15	124.89
22	B	611	CLA	C4A-NA-C1A	2.85	109.99	106.45
22	C	504	CLA	C4A-NA-C1A	2.86	110.00	106.45
25	B	625	DGD	O5D-C1E-C2E	2.86	112.90	108.23
22	C	511	CLA	CMB-C2B-C3B	2.87	130.21	124.89
22	C	502	CLA	CMB-C2B-C3B	2.87	130.23	124.89
22	c	502	CLA	CMB-C2B-C3B	2.88	130.23	124.89
29	B	622	SQD	C3-C4-C5	2.88	115.29	110.22
29	a	415	SQD	C3-C4-C5	2.88	115.30	110.22
22	D	406	CLA	CMB-C2B-C3B	2.88	130.24	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	521	BCR	C2-C1-C6	2.89	114.99	110.48
24	J	102	BCR	C27-C26-C25	2.89	126.98	122.74
22	D	405	CLA	CMB-C2B-C3B	2.90	130.26	124.89
22	B	609	CLA	CMB-C2B-C3B	2.90	130.27	124.89
22	c	503	CLA	CMB-C2B-C3B	2.90	130.27	124.89
22	c	511	CLA	CMB-C2B-C3B	2.90	130.27	124.89
22	C	512	CLA	CMB-C2B-C3B	2.92	130.30	124.89
29	A	412	SQD	C3-C4-C5	2.93	115.38	110.22
22	B	611	CLA	CMB-C2B-C3B	2.93	130.34	124.89
22	C	503	CLA	CMB-C2B-C3B	2.93	130.34	124.89
22	A	405	CLA	CMB-C2B-C3B	2.94	130.34	124.89
26	a	411	LHG	O8-C23-C24	2.94	120.46	111.90
22	c	505	CLA	CMB-C2B-C3B	2.96	130.38	124.89
22	C	510	CLA	CMB-C2B-C3B	2.96	130.39	124.89
22	b	613	CLA	CMB-C2B-C3B	2.96	130.39	124.89
22	c	512	CLA	CMB-C2B-C3B	2.97	130.41	124.89
22	b	615	CLA	CMB-C2B-C3B	2.98	130.43	124.89
26	A	409	LHG	O8-C23-C24	2.98	120.58	111.90
22	b	614	CLA	CMB-C2B-C3B	2.99	130.44	124.89
22	a	407	CLA	CMB-C2B-C3B	2.99	130.44	124.89
22	b	617	CLA	CMB-C2B-C3B	3.00	130.46	124.89
29	d	403	SQD	C3-C4-C5	3.00	115.51	110.22
22	C	505	CLA	CMB-C2B-C3B	3.00	130.47	124.89
29	A	413	SQD	C44-O6-C1	3.01	119.94	113.76
24	b	622	BCR	C2-C1-C6	3.02	115.20	110.48
22	c	510	CLA	CMB-C2B-C3B	3.02	130.50	124.89
29	f	103	SQD	O6-C1-C2	3.03	113.17	108.23
22	B	613	CLA	CMB-C2B-C3B	3.05	130.55	124.89
22	c	506	CLA	CMB-C2B-C3B	3.06	130.56	124.89
22	C	506	CLA	CMB-C2B-C3B	3.06	130.57	124.89
22	B	607	CLA	CMB-C2B-C3B	3.07	130.59	124.89
24	B	618	BCR	C2-C1-C6	3.07	115.28	110.48
22	b	606	CLA	CMB-C2B-C3B	3.09	130.63	124.89
22	B	602	CLA	CMB-C2B-C3B	3.10	130.65	124.89
22	B	610	CLA	CMB-C2B-C3B	3.10	130.65	124.89
24	a	409	BCR	C2-C1-C6	3.11	115.34	110.48
22	C	507	CLA	CMB-C2B-C3B	3.13	130.70	124.89
22	b	611	CLA	CMB-C2B-C3B	3.15	130.73	124.89
29	b	602	SQD	C3-C4-C5	3.16	115.78	110.22
29	B	626	SQD	C3-C4-C5	3.19	115.85	110.22
29	F	103	SQD	O6-C1-C2	3.22	113.48	108.23
24	A	407	BCR	C2-C1-C6	3.23	115.53	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CMB-C2B-C3B	3.29	130.99	124.89
29	a	401	SQD	O47-C7-C8	3.31	118.42	111.55
29	A	412	SQD	O8-S-C6	3.31	110.06	106.01
29	a	401	SQD	C44-O6-C1	3.32	120.57	113.76
22	b	616	CLA	CMB-C2B-C3B	3.33	131.07	124.89
22	B	612	CLA	CMB-C2B-C3B	3.34	131.09	124.89
29	a	415	SQD	O8-S-C6	3.37	110.12	106.01
29	A	413	SQD	O47-C7-C8	3.44	118.70	111.55
29	f	103	SQD	O47-C7-C8	3.45	118.71	111.55
29	b	602	SQD	O8-S-C6	3.50	110.28	106.01
29	A	413	SQD	O8-S-C6	3.52	110.31	106.01
29	F	103	SQD	O47-C7-C8	3.53	118.88	111.55
29	A	412	SQD	O5-C5-C4	3.57	116.23	109.66
29	B	622	SQD	O47-C7-C8	3.57	118.96	111.55
29	d	403	SQD	O47-C7-C8	3.57	118.96	111.55
29	F	103	SQD	O5-C5-C4	3.59	116.27	109.66
24	j	102	BCR	C2-C1-C6	3.61	116.12	110.48
29	B	626	SQD	O8-S-C6	3.61	110.42	106.01
24	J	102	BCR	C2-C1-C6	3.62	116.13	110.48
29	a	401	SQD	O8-S-C6	3.62	110.43	106.01
29	f	103	SQD	O5-C5-C4	3.62	116.33	109.66
29	a	415	SQD	O5-C5-C4	3.66	116.41	109.66
24	c	513	BCR	C2-C1-C6	3.69	116.25	110.48
29	B	626	SQD	O47-C7-C8	3.70	119.24	111.55
29	b	602	SQD	O47-C7-C8	3.70	119.24	111.55
24	C	513	BCR	C2-C1-C6	3.72	116.29	110.48
29	A	412	SQD	O47-C7-C8	3.75	119.33	111.55
29	b	602	SQD	O5-C5-C4	3.78	116.61	109.66
29	a	401	SQD	O5-C5-C4	3.82	116.70	109.66
29	B	626	SQD	O5-C5-C4	3.83	116.72	109.66
29	a	415	SQD	O47-C7-C8	3.84	119.53	111.55
29	B	622	SQD	O8-S-C6	3.88	110.74	106.01
29	A	413	SQD	O5-C5-C4	3.88	116.81	109.66
26	A	409	LHG	O4-P-O5	3.98	132.89	112.28
26	a	411	LHG	O4-P-O5	4.01	133.03	112.28
26	C	519	LHG	O4-P-O5	4.01	133.04	112.28
26	c	519	LHG	O4-P-O5	4.01	133.05	112.28
29	B	622	SQD	O6-C1-C2	4.02	114.79	108.23
29	d	403	SQD	O6-C1-C2	4.03	114.81	108.23
29	d	403	SQD	O8-S-C6	4.06	110.96	106.01
29	f	103	SQD	O8-S-C6	4.15	111.08	106.01
29	F	103	SQD	O8-S-C6	4.31	111.27	106.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	622	SQD	O5-C5-C4	4.41	117.79	109.66
29	d	403	SQD	O5-C5-C4	4.49	117.94	109.66
29	F	103	SQD	O9-S-C6	4.75	110.89	106.83
29	A	413	SQD	O9-S-C6	4.84	110.96	106.83
29	a	401	SQD	O9-S-C6	4.86	110.98	106.83
29	f	103	SQD	O9-S-C6	4.91	111.02	106.83
29	d	403	SQD	O7-S-C6	5.08	111.17	106.83
29	B	626	SQD	O6-C1-C2	5.08	116.53	108.23
29	B	622	SQD	O9-S-C6	5.10	111.19	106.83
23	a	408	PL9	C7-C3-C4	5.18	121.08	116.88
29	b	602	SQD	O6-C1-C2	5.21	116.74	108.23
23	D	407	PL9	C7-C3-C4	5.22	121.12	116.88
23	d	407	PL9	C7-C3-C4	5.27	121.16	116.88
29	a	415	SQD	O7-S-C6	5.29	111.35	106.83
29	d	403	SQD	O9-S-C6	5.30	111.36	106.83
29	A	412	SQD	O6-C1-C2	5.31	116.91	108.23
29	B	626	SQD	O7-S-C6	5.34	111.39	106.83
29	B	622	SQD	O7-S-C6	5.38	111.42	106.83
29	A	412	SQD	O7-S-C6	5.39	111.44	106.83
23	A	406	PL9	C7-C3-C4	5.44	121.30	116.88
29	a	415	SQD	O6-C1-C2	5.45	117.13	108.23
29	b	602	SQD	O7-S-C6	5.54	111.56	106.83
23	J	101	PL9	C7-C3-C4	5.59	121.42	116.88
23	j	101	PL9	C7-C3-C4	5.69	121.50	116.88
29	B	626	SQD	O9-S-C6	5.77	111.75	106.83
29	b	602	SQD	O9-S-C6	5.77	111.76	106.83
29	A	413	SQD	O7-S-C6	5.79	111.78	106.83
29	a	401	SQD	O7-S-C6	5.83	111.81	106.83
29	F	103	SQD	O7-S-C6	6.00	111.95	106.83
29	f	103	SQD	O7-S-C6	6.04	111.99	106.83
29	a	415	SQD	O9-S-C6	6.99	112.81	106.83
29	A	412	SQD	O9-S-C6	7.13	112.92	106.83

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA

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Mol	Chain	Res	Type	Atom
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	c	520	CLA	NC
22	c	520	CLA	ND
22	c	520	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA

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Mol	Chain	Res	Type	Atom
22	d	405	CLA	NC
22	d	405	CLA	ND
22	d	405	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	D	406	CLA	NC
22	D	406	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	d	406	CLA	NC
22	d	406	CLA	ND
22	d	406	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	b	617	CLA	NC

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Mol	Chain	Res	Type	Atom
22	b	617	CLA	ND
22	b	617	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA
22	c	511	CLA	NC

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Mol	Chain	Res	Type	Atom
22	c	511	CLA	ND
22	c	511	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND
22	b	619	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	C	520	CLA	NC
22	C	520	CLA	ND
22	C	520	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	a	404	CLA	NC

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Mol	Chain	Res	Type	Atom
22	a	404	CLA	ND
22	a	404	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	h	101	CLA	NC
22	h	101	CLA	ND
22	h	101	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	a	407	CLA	NC
22	a	407	CLA	ND
22	a	407	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA

All (4) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
29	B	622	SQD	C45-O47-C7-C8

There are no ring outliers.

79 monomers are involved in 296 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	10	0
22	A	403	CLA	13	0
22	A	404	CLA	15	0
22	A	405	CLA	9	0
23	A	406	PL9	4	0
24	A	407	BCR	3	0
25	A	408	DGD	1	0
26	A	409	LHG	3	0
27	A	410	LMG	2	0
29	A	412	SQD	3	0
29	A	413	SQD	3	0
27	A	414	LMG	1	0
22	B	601	CLA	1	0
22	B	602	CLA	11	0
22	B	603	CLA	3	0
22	B	604	CLA	7	0
22	B	605	CLA	7	0
22	B	606	CLA	16	0
22	B	607	CLA	9	0
22	B	608	CLA	13	0
22	B	609	CLA	3	0
22	B	610	CLA	6	0
22	B	611	CLA	11	0
22	B	612	CLA	10	0
22	B	613	CLA	4	0
22	B	614	CLA	2	0
22	B	615	CLA	6	0
24	B	616	BCR	4	0
24	B	617	BCR	2	0
24	B	618	BCR	4	0
24	B	619	BCR	1	0
25	B	620	DGD	2	0
27	B	621	LMG	3	0
29	B	622	SQD	3	0
30	B	623	LMT	2	0
25	B	625	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	626	SQD	1	0
30	B	627	LMT	2	0
30	B	628	LMT	2	0
22	C	501	CLA	7	0
22	C	503	CLA	5	0
22	C	504	CLA	4	0
22	C	505	CLA	2	0
22	C	506	CLA	6	0
22	C	507	CLA	4	0
22	C	508	CLA	2	0
22	C	509	CLA	6	0
22	C	510	CLA	10	0
22	C	511	CLA	2	0
22	C	512	CLA	3	0
24	C	513	BCR	7	0
24	C	514	BCR	7	0
25	C	515	DGD	3	0
25	C	516	DGD	3	0
25	C	517	DGD	5	0
27	C	518	LMG	4	0
26	C	519	LHG	2	0
22	C	520	CLA	4	0
31	D	401	PHO	10	0
31	D	402	PHO	5	0
22	D	405	CLA	8	0
22	D	406	CLA	3	0
23	D	407	PL9	12	0
27	D	408	LMG	4	0
27	D	409	LMG	6	0
25	D	410	DGD	2	0
27	D	412	LMG	1	0
27	E	101	LMG	1	0
34	F	101	HEM	4	0
24	F	102	BCR	4	0
29	F	103	SQD	3	0
22	H	101	CLA	9	0
24	H	102	BCR	2	0
27	I	101	LMG	1	0
30	I	102	LMT	1	0
24	J	102	BCR	1	0
24	K	102	BCR	3	0
27	M	101	LMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	V	201	HEM	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.43	28 (8%) 12 12	178, 179, 180, 181	0
1	a	335/344 (97%)	0.38	29 (8%) 11 11	178, 179, 180, 181	0
2	B	490/510 (96%)	0.19	22 (4%) 34 29	178, 179, 180, 181	0
2	b	490/510 (96%)	0.31	29 (5%) 23 20	178, 179, 180, 181	0
3	C	447/461 (96%)	0.26	28 (6%) 21 18	178, 179, 180, 181	0
3	c	447/461 (96%)	0.10	15 (3%) 46 39	178, 180, 180, 181	0
4	D	340/352 (96%)	0.18	10 (2%) 52 44	177, 179, 180, 181	0
4	d	340/352 (96%)	0.16	7 (2%) 64 56	177, 179, 180, 181	0
5	E	82/84 (97%)	0.07	2 (2%) 59 52	178, 180, 180, 181	0
5	e	82/84 (97%)	-0.03	3 (3%) 42 36	178, 180, 181, 181	0
6	F	35/45 (77%)	-0.19	1 (2%) 52 44	179, 179, 180, 180	0
6	f	35/45 (77%)	-0.47	0 100 100	179, 180, 181, 181	0
7	H	65/66 (98%)	0.38	8 (12%) 5 7	179, 180, 180, 181	0
7	h	65/66 (98%)	0.49	8 (12%) 5 7	179, 180, 181, 181	0
8	I	35/38 (92%)	0.45	2 (5%) 24 21	178, 179, 180, 181	0
8	i	35/38 (92%)	-0.07	0 100 100	179, 179, 181, 181	0
9	J	34/40 (85%)	-0.02	1 (2%) 52 44	178, 179, 180, 180	0
9	j	34/40 (85%)	-0.42	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	-0.06	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.44	4 (10%) 6 8	179, 180, 181, 181	0
11	L	37/37 (100%)	0.49	1 (2%) 55 47	178, 179, 180, 181	0
11	l	37/37 (100%)	0.12	0 100 100	178, 179, 180, 181	0
12	M	34/36 (94%)	0.28	1 (2%) 52 44	178, 179, 180, 181	0
12	m	34/36 (94%)	0.06	1 (2%) 52 44	178, 179, 180, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.55	20 (8%) 12 13	177, 179, 180, 181	0
13	o	243/272 (89%)	0.56	19 (7%) 14 13	177, 179, 181, 181	0
14	T	32/32 (100%)	0.17	2 (6%) 21 18	178, 179, 181, 181	0
14	t	32/32 (100%)	0.32	4 (12%) 4 7	178, 179, 180, 181	0
15	U	97/134 (72%)	0.52	7 (7%) 16 15	178, 179, 180, 181	0
15	u	97/134 (72%)	0.74	11 (11%) 6 8	178, 179, 180, 181	0
16	V	137/163 (84%)	0.11	2 (1%) 74 66	178, 179, 180, 181	0
16	v	137/163 (84%)	0.45	7 (5%) 29 25	178, 180, 181, 181	0
17	g	28/46 (60%)	0.39	2 (7%) 17 15	179, 180, 181, 182	0
17	y	28/46 (60%)	0.15	0 100 100	178, 180, 181, 181	0
18	X	37/41 (90%)	0.45	2 (5%) 26 23	179, 179, 181, 181	0
18	x	37/41 (90%)	0.75	6 (16%) 2 5	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.28	0 100 100	179, 180, 181, 181	0
20	z	62/62 (100%)	0.85	3 (4%) 31 27	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.29	285 (5%) 26 22	177, 179, 180, 182	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	84	LYS	7.1
15	U	38	GLU	6.4
13	o	169	LYS	6.3
1	A	10	SER	5.5
7	H	66	GLY	5.5
3	C	148	GLY	5.2
5	e	82	GLN	4.8
3	C	149	TYR	4.8
1	A	299	GLY	4.5
3	c	201	ASN	4.3
2	b	490	GLN	4.2
5	E	84	LYS	4.2
18	x	11	THR	4.1
16	v	132	ASN	4.1
4	D	24	ARG	4.0
2	B	69	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
4	d	295	SER	3.9
1	A	179	THR	3.9
13	O	84	ASN	3.9
3	c	202	PRO	3.9
13	o	168	PHE	3.8
3	c	372	PRO	3.8
13	O	90	GLU	3.8
1	A	11	ALA	3.8
4	d	13	GLY	3.7
1	a	175	GLY	3.7
15	U	39	LEU	3.6
17	g	27	MET	3.6
13	o	31	LEU	3.6
1	a	137	LEU	3.6
3	C	140	LEU	3.5
15	u	53	GLU	3.5
3	C	141	GLU	3.5
13	o	124	GLU	3.5
3	C	184	GLY	3.5
3	C	147	PHE	3.5
3	c	200	THR	3.4
1	A	175	GLY	3.4
2	B	411	PHE	3.4
4	D	190	ASN	3.4
2	B	295	GLY	3.4
1	a	19	ASN	3.4
1	a	224	ILE	3.3
1	a	190	HIS	3.3
2	b	218	LEU	3.3
1	A	195	HIS	3.3
3	C	266	TRP	3.2
2	B	83	GLU	3.2
3	c	260	ALA	3.2
4	D	174	GLY	3.1
13	o	154	SER	3.1
13	O	91	PHE	3.1
9	J	7	ARG	3.1
1	a	239	PHE	3.1
3	C	143	TYR	3.1
14	t	31	LYS	3.1
1	A	294	ALA	3.1
3	C	183	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	12	ASN	3.1
1	a	165	GLN	3.0
1	a	179	THR	3.0
3	C	139	THR	3.0
2	b	338	GLN	3.0
1	A	198	HIS	3.0
13	O	170	GLY	3.0
1	A	177	SER	3.0
14	t	30	THR	3.0
2	b	229	LEU	3.0
2	b	302	TRP	3.0
14	t	32	LYS	3.0
1	a	187	GLN	2.9
4	d	191	TRP	2.9
1	a	178	GLY	2.9
13	O	50	ASP	2.9
15	u	52	GLY	2.9
14	T	28	ARG	2.9
7	H	6	TRP	2.9
15	u	58	ASN	2.9
13	O	223	ILE	2.9
15	U	40	VAL	2.8
1	a	282	GLY	2.8
1	a	299	GLY	2.8
20	z	4	LEU	2.8
3	c	203	THR	2.8
13	O	243	SER	2.8
2	b	301	ALA	2.8
3	C	142	GLU	2.8
3	C	473	ASP	2.8
2	b	339	ALA	2.8
13	o	153	ALA	2.8
2	B	84	THR	2.8
2	b	303	SER	2.7
1	a	183	MET	2.7
2	B	183	PRO	2.7
3	c	403	SER	2.7
1	A	138	GLY	2.7
20	z	1	MET	2.7
2	B	378	LYS	2.7
10	k	14	ALA	2.7
2	B	294	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	196	PRO	2.7
15	u	72	TYR	2.7
18	x	12	ILE	2.7
2	B	161	LEU	2.7
13	o	32	THR	2.7
1	A	298	ASN	2.7
3	C	332	GLN	2.7
1	A	137	LEU	2.6
2	b	119	ASP	2.6
1	A	293	MET	2.6
1	A	80	GLY	2.6
1	a	325	ASN	2.6
3	C	137	PRO	2.6
2	b	485	GLU	2.6
1	a	298	ASN	2.6
1	a	138	GLY	2.6
1	A	178	GLY	2.6
2	B	185	TRP	2.6
2	b	340	TRP	2.6
3	c	402	GLY	2.6
2	b	402	TYR	2.6
3	C	144	SER	2.6
7	h	66	GLY	2.6
4	d	197	HIS	2.5
14	t	29	ILE	2.5
7	h	2	ALA	2.5
1	A	165	GLN	2.5
18	x	16	LEU	2.5
1	A	191	ASN	2.5
3	C	212	TYR	2.5
15	U	121	LEU	2.5
18	x	47	GLN	2.5
4	d	194	ASN	2.5
3	C	145	SER	2.5
7	H	63	LYS	2.5
3	C	464	GLU	2.5
4	D	197	HIS	2.5
13	o	35	ASP	2.5
13	O	169	LYS	2.5
7	H	56	ASP	2.5
13	o	215	ARG	2.5
13	O	46	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
16	v	133	LEU	2.5
7	H	5	THR	2.5
1	a	177	SER	2.4
2	B	164	PRO	2.4
6	F	11	VAL	2.4
7	h	14	LEU	2.4
15	U	42	VAL	2.4
2	b	487	SER	2.4
2	B	293	ALA	2.4
16	v	47	LEU	2.4
8	I	30	ARG	2.4
2	b	133	LEU	2.4
2	b	298	LEU	2.4
1	A	15	GLU	2.4
2	b	482	ILE	2.4
13	O	195	ASP	2.4
13	O	268	SER	2.4
7	h	3	ARG	2.4
13	O	58	ILE	2.4
13	o	229	LYS	2.4
8	I	34	ARG	2.4
3	C	261	ARG	2.4
3	C	27	ASP	2.4
3	C	136	GLY	2.4
10	k	17	ILE	2.4
18	X	42	GLN	2.4
2	B	410	THR	2.4
15	u	47	LEU	2.4
2	B	165	GLY	2.4
13	o	213	VAL	2.4
1	a	198	HIS	2.4
3	C	135	ARG	2.4
2	b	412	THR	2.4
16	v	131	ARG	2.4
15	u	131	GLY	2.4
15	u	51	TYR	2.3
12	m	1	MET	2.3
15	u	107	GLU	2.3
1	a	199	GLN	2.3
7	h	56	ASP	2.3
1	a	286	THR	2.3
3	c	209	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
13	O	225	LEU	2.3
4	D	194	ASN	2.3
3	C	258	GLY	2.3
17	g	30	ILE	2.3
2	B	326	ARG	2.3
15	u	57	LEU	2.3
7	h	26	GLY	2.3
1	A	183	MET	2.3
16	V	47	LEU	2.3
2	b	393	GLU	2.3
13	O	269	ILE	2.3
13	o	224	SER	2.3
16	v	138	LEU	2.3
15	u	54	LYS	2.3
10	k	43	VAL	2.3
15	u	65	PHE	2.3
1	A	19	ASN	2.3
3	c	411	ALA	2.3
2	B	474	LEU	2.2
4	D	199	MET	2.2
13	o	62	GLN	2.2
4	D	171	PRO	2.2
1	a	201	GLY	2.2
16	V	94	ASN	2.2
12	M	5	GLN	2.2
2	b	120	LEU	2.2
2	b	379	ALA	2.2
5	E	17	VAL	2.2
13	o	63	THR	2.2
2	b	219	VAL	2.2
2	b	397	VAL	2.2
1	A	262	TYR	2.2
3	C	44	ASN	2.2
13	o	123	GLU	2.2
2	b	398	THR	2.2
4	d	241	GLU	2.2
18	x	42	GLN	2.2
1	A	169	SER	2.2
2	B	412	THR	2.2
13	O	68	ARG	2.2
4	D	176	ALA	2.2
1	a	301	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
7	H	62	TRP	2.2
2	B	127	ARG	2.2
4	D	170	ALA	2.2
7	H	9	ASP	2.2
13	O	262	GLN	2.2
13	O	222	GLN	2.2
11	L	33	SER	2.2
16	v	142	ALA	2.2
18	X	45	LYS	2.2
3	c	371	GLY	2.2
7	h	4	ARG	2.2
3	C	201	ASN	2.2
16	v	51	GLN	2.2
13	o	269	ILE	2.2
2	b	122	LEU	2.2
20	z	17	PHE	2.1
2	B	379	ALA	2.1
2	b	488	PRO	2.1
7	H	8	GLY	2.1
13	O	224	SER	2.1
1	a	240	GLY	2.1
1	a	225	ARG	2.1
10	k	10	LYS	2.1
4	D	295	SER	2.1
2	B	129	GLY	2.1
2	b	420	TYR	2.1
3	c	180	MET	2.1
1	a	172	MET	2.1
2	b	431	GLU	2.1
15	U	69	ARG	2.1
1	A	181	ASN	2.1
1	a	191	ASN	2.1
15	U	65	PHE	2.1
1	A	342	ASP	2.1
2	b	228	ALA	2.1
13	o	167	ASP	2.1
3	C	151	TRP	2.1
7	h	54	ILE	2.1
2	B	8	VAL	2.1
3	c	211	GLY	2.1
13	O	126	GLY	2.1
1	A	192	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
13	o	237	ILE	2.1
2	B	353	GLU	2.1
1	a	181	ASN	2.0
13	O	113	VAL	2.0
18	x	15	SER	2.0
1	a	26	ASN	2.0
1	A	300	PHE	2.0
3	C	402	GLY	2.0
4	d	200	GLY	2.0
2	b	217	ILE	2.0
3	C	262	ARG	2.0
5	e	83	LEU	2.0
3	c	207	ARG	2.0
3	c	373	ASN	2.0
14	T	27	PRO	2.0
1	a	303	ASN	2.0
13	o	120	THR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	LMT	i	102	35/35	0.51	1.11	7.54	178,181,183,183	0
30	LMT	I	102	35/35	0.48	1.09	7.13	178,180,182,183	0
27	LMG	C	518	45/55	0.65	1.11	5.83	178,179,180,181	0
24	BCR	c	521	40/40	0.85	1.25	5.60	178,179,181,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	LMG	c	518	45/55	0.74	1.01	5.58	178,180,181,181	0
24	BCR	y	101	40/40	0.76	1.00	5.52	177,179,180,180	0
25	DGD	D	410	63/66	0.74	0.87	5.39	178,181,182,183	0
24	BCR	B	619	40/40	0.73	0.82	5.25	178,179,180,180	0
25	DGD	d	410	63/66	0.64	0.84	5.06	178,180,183,183	0
24	BCR	b	623	40/40	0.73	0.73	4.61	177,178,180,180	0
22	CLA	A	405	65/65	0.80	0.70	4.44	177,179,180,181	0
30	LMT	b	627	35/35	0.67	1.10	4.35	178,180,182,182	0
24	BCR	C	513	40/40	0.88	0.74	4.14	177,179,180,180	0
23	PL9	J	101	35/55	0.25	0.59	4.10	177,180,181,181	0
22	CLA	b	605	65/65	0.59	1.12	3.73	179,180,182,183	0
30	LMT	D	411	31/35	0.66	0.87	3.33	179,180,182,182	0
22	CLA	c	512	65/65	0.76	0.80	3.26	178,180,181,182	0
22	CLA	B	603	65/65	0.78	0.53	3.16	176,179,180,180	0
24	BCR	H	102	40/40	0.67	1.01	3.15	178,180,181,182	0
22	CLA	D	406	65/65	0.89	0.67	2.96	177,179,180,181	0
23	PL9	j	101	35/55	0.52	0.35	2.92	179,180,181,181	0
24	BCR	a	409	40/40	0.69	0.69	2.84	177,178,180,180	0
22	CLA	a	407	65/65	0.77	0.71	2.71	178,179,180,181	0
24	BCR	c	513	40/40	0.76	0.89	2.71	178,179,180,180	0
22	CLA	B	601	65/65	0.61	0.95	2.70	177,180,181,182	0
24	BCR	g	101	40/40	0.57	0.89	2.67	178,179,180,180	0
25	DGD	b	601	52/66	0.71	0.55	2.57	178,180,181,182	0
22	CLA	c	511	65/65	0.87	0.68	2.52	178,180,181,182	0
30	LMT	d	411	31/35	0.49	0.79	2.46	178,181,182,183	0
25	DGD	B	625	52/66	0.76	0.59	2.43	177,180,182,182	0
27	LMG	M	101	42/55	0.69	0.55	2.36	178,180,181,182	0
30	LMT	B	624	35/35	0.80	0.50	2.32	178,180,182,183	0
24	BCR	B	617	40/40	0.67	0.50	2.31	177,179,180,180	0
24	BCR	K	102	40/40	0.71	0.89	2.27	178,180,181,182	0
24	BCR	J	102	40/40	0.53	0.37	2.26	178,180,181,181	0
30	LMT	B	627	35/35	0.64	0.64	2.25	178,180,182,182	0
29	SQD	f	103	45/54	0.86	0.57	2.12	177,179,181,182	0
24	BCR	C	514	40/40	0.81	0.77	2.10	178,179,180,181	0
24	BCR	F	102	40/40	0.61	0.53	2.09	177,179,180,180	0
22	CLA	b	606	65/65	0.88	0.59	2.07	177,179,180,181	0
22	CLA	c	503	65/65	0.82	0.56	2.04	177,179,180,181	0
30	LMT	b	604	35/35	0.71	0.57	2.04	177,179,181,182	0
24	BCR	f	102	40/40	0.78	0.33	2.02	177,179,181,181	0
27	LMG	e	101	44/55	0.77	0.37	1.97	177,179,181,181	0
22	CLA	B	611	65/65	0.92	0.41	1.95	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
29	SQD	B	626	47/54	0.74	0.56	1.95	175,179,181,183	0
22	CLA	b	613	65/65	0.86	0.76	1.94	178,179,180,181	0
24	BCR	A	407	40/40	0.76	0.53	1.92	177,179,180,180	0
27	LMG	a	402	42/55	0.64	0.49	1.82	177,180,181,182	0
22	CLA	c	508	65/65	0.86	0.46	1.80	177,179,180,181	0
22	CLA	c	501	65/65	0.86	0.49	1.79	177,179,180,181	0
22	CLA	C	506	65/65	0.81	0.75	1.75	177,179,180,180	0
22	CLA	C	502	65/65	0.68	0.54	1.70	178,179,180,180	0
22	CLA	B	604	65/65	0.89	0.72	1.70	177,179,180,180	0
22	CLA	d	406	65/65	0.83	0.56	1.68	177,179,180,181	0
24	BCR	c	514	40/40	0.73	0.78	1.65	177,179,180,180	0
22	CLA	b	609	65/65	0.85	0.64	1.65	178,179,180,181	0
29	SQD	a	401	54/54	0.84	0.65	1.64	178,180,181,183	0
29	SQD	d	403	43/54	0.67	0.86	1.59	178,180,182,186	0
22	CLA	c	502	65/65	0.55	0.64	1.59	178,179,180,181	0
22	CLA	C	508	65/65	0.83	0.85	1.58	177,179,180,180	0
22	CLA	c	506	65/65	0.88	0.58	1.58	178,179,180,181	0
22	CLA	b	607	65/65	0.82	0.43	1.48	177,179,180,181	0
30	LMT	b	603	35/35	0.68	0.50	1.47	178,179,181,182	0
25	DGD	b	624	58/66	0.72	0.43	1.47	177,178,180,180	0
22	CLA	B	608	65/65	0.86	0.58	1.44	177,179,180,180	0
22	CLA	b	608	65/65	0.88	0.52	1.41	178,179,180,181	0
24	BCR	B	618	40/40	0.87	0.32	1.41	177,178,179,179	0
27	LMG	A	414	42/55	0.62	0.52	1.39	177,179,182,182	0
22	CLA	c	510	65/65	0.80	0.56	1.38	178,179,181,181	0
24	BCR	B	616	40/40	0.68	0.47	1.36	176,178,180,180	0
22	CLA	B	614	65/65	0.85	0.67	1.32	177,179,180,181	0
22	CLA	B	609	65/65	0.90	0.51	1.29	178,179,180,181	0
27	LMG	E	101	44/55	0.63	0.61	1.24	176,179,181,182	0
22	CLA	C	501	65/65	0.86	0.47	1.22	178,179,180,180	0
22	CLA	h	101	65/65	0.84	0.46	1.19	176,179,180,181	0
24	BCR	x	101	40/40	0.74	0.86	1.16	178,179,180,181	0
22	CLA	b	619	65/65	0.67	0.76	1.16	177,179,180,181	0
22	CLA	C	512	65/65	0.81	0.91	1.12	177,180,181,182	0
22	CLA	b	615	65/65	0.88	0.40	1.12	177,179,180,180	0
29	SQD	b	602	47/54	0.80	0.42	1.08	176,179,182,185	0
22	CLA	C	511	65/65	0.90	0.88	1.05	178,179,180,181	0
24	BCR	b	622	40/40	0.75	0.37	1.03	176,178,179,179	0
25	DGD	a	410	56/66	0.71	0.41	0.97	178,180,181,182	0
22	CLA	B	605	65/65	0.87	0.69	0.93	178,179,180,180	0
22	CLA	B	615	65/65	0.83	0.73	0.93	176,179,180,181	0
29	SQD	A	413	54/54	0.87	0.38	0.91	178,180,182,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
29	SQD	F	103	45/54	0.82	0.64	0.90	178,180,182,182	0
22	CLA	C	510	65/65	0.77	0.54	0.88	177,179,180,181	0
25	DGD	A	408	56/66	0.73	0.42	0.88	178,179,181,182	0
22	CLA	b	612	65/65	0.84	0.63	0.85	176,179,181,181	0
27	LMG	m	101	42/55	0.79	0.42	0.83	175,179,181,181	0
27	LMG	a	412	51/55	0.78	0.36	0.81	177,179,180,180	0
34	HEM	f	101	43/43	0.89	0.35	0.80	178,180,180,181	0
24	BCR	b	621	40/40	0.79	0.38	0.79	178,178,179,179	0
22	CLA	C	505	65/65	0.81	0.47	0.74	177,179,180,181	0
30	LMT	B	628	35/35	0.57	0.49	0.74	177,180,182,183	0
22	CLA	b	618	65/65	0.81	0.68	0.72	177,179,180,180	0
34	HEM	F	101	43/43	0.94	0.42	0.70	178,180,181,182	0
22	CLA	C	503	65/65	0.86	0.40	0.69	177,179,180,180	0
23	PL9	a	408	45/55	0.81	0.30	0.67	176,179,180,180	0
34	HEM	V	201	43/43	0.91	0.39	0.61	176,178,180,180	0
23	PL9	A	406	45/55	0.72	0.41	0.59	177,179,180,180	0
22	CLA	B	602	65/65	0.92	0.50	0.59	176,178,180,180	0
22	CLA	c	505	65/65	0.81	0.51	0.59	177,179,180,181	0
25	DGD	c	515	53/66	0.83	0.40	0.56	176,179,181,182	0
22	CLA	C	504	65/65	0.87	0.39	0.46	177,179,180,180	0
34	HEM	v	201	43/43	0.91	0.53	0.45	177,179,180,180	0
24	BCR	b	620	40/40	0.85	0.37	0.44	177,179,179,180	0
22	CLA	c	504	65/65	0.89	0.31	0.42	177,179,180,180	0
22	CLA	b	616	65/65	0.94	0.30	0.41	177,179,180,180	0
22	CLA	a	404	65/65	0.76	0.61	0.41	177,178,180,180	0
22	CLA	b	617	65/65	0.83	0.42	0.41	178,179,180,182	0
27	LMG	C	521	48/55	0.77	0.31	0.33	177,179,180,181	0
29	SQD	B	622	43/54	0.85	0.43	0.31	177,180,182,185	0
22	CLA	a	405	65/65	0.80	0.58	0.29	174,178,179,180	0
22	CLA	B	607	65/65	0.89	0.38	0.27	178,179,180,181	0
22	CLA	C	509	65/65	0.85	0.36	0.27	177,179,180,180	0
22	CLA	B	613	65/65	0.74	0.44	0.24	177,179,180,180	0
27	LMG	d	412	46/55	0.92	0.24	0.24	177,178,180,180	0
27	LMG	D	412	46/55	0.80	0.32	0.19	178,179,180,181	0
22	CLA	b	611	65/65	0.86	0.35	0.18	177,179,180,180	0
22	CLA	C	507	65/65	0.84	0.36	0.14	178,179,180,181	0
23	PL9	d	407	55/55	0.60	0.41	0.11	177,179,180,181	0
31	PHO	d	401	64/64	0.73	0.42	0.08	178,179,180,180	0
23	PL9	D	407	55/55	0.71	0.40	0.08	177,178,179,180	0
31	PHO	D	402	64/64	0.79	0.36	0.06	177,179,180,181	0
29	SQD	a	415	51/54	0.79	0.31	0.04	178,179,181,182	0
27	LMG	A	410	51/55	0.81	0.32	0.03	177,178,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	CLA	H	101	65/65	0.87	0.32	0.02	177,179,180,181	0
25	DGD	B	620	58/66	0.83	0.33	0.02	176,179,181,182	0
24	BCR	j	102	40/40	0.69	0.30	0.00	179,180,182,183	0
27	LMG	D	409	48/55	0.88	0.28	-0.03	175,178,180,181	0
26	LHG	A	409	39/49	0.86	0.30	-0.04	178,179,181,181	0
22	CLA	b	614	65/65	0.91	0.28	-0.08	178,179,180,180	0
32	CL	a	413	1/1	0.94	0.54	-0.09	177,177,177,177	0
22	CLA	A	403	65/65	0.92	0.50	-0.09	177,179,179,180	0
25	DGD	C	517	66/66	0.74	0.41	-0.13	177,179,180,181	0
22	CLA	C	520	65/65	0.85	0.33	-0.16	178,179,180,181	0
27	LMG	d	409	48/55	0.84	0.30	-0.17	177,179,180,180	0
29	SQD	A	412	51/54	0.80	0.31	-0.18	178,179,180,181	0
31	PHO	D	401	64/64	0.87	0.35	-0.20	177,179,180,180	0
26	LHG	c	519	37/49	0.73	0.31	-0.21	178,180,183,187	0
22	CLA	B	610	65/65	0.87	0.36	-0.22	177,179,180,180	0
27	LMG	c	522	48/55	0.85	0.28	-0.25	178,180,180,181	0
22	CLA	A	402	65/65	0.92	0.41	-0.26	178,179,180,181	0
22	CLA	d	405	65/65	0.88	0.44	-0.30	177,178,179,180	0
25	DGD	C	515	53/66	0.87	0.31	-0.31	177,178,179,180	0
22	CLA	D	405	65/65	0.91	0.39	-0.32	177,179,180,180	0
22	CLA	c	509	65/65	0.86	0.32	-0.38	177,179,180,180	0
22	CLA	c	507	65/65	0.90	0.27	-0.44	177,179,180,181	0
27	LMG	D	408	49/55	0.78	0.32	-0.44	177,178,180,180	0
30	LMT	M	103	35/35	0.80	0.46	-0.44	177,179,180,180	0
22	CLA	B	606	65/65	0.86	0.34	-0.45	177,179,180,180	0
22	CLA	A	404	65/65	0.81	0.36	-0.52	176,178,180,181	0
26	LHG	C	519	37/49	0.77	0.34	-0.55	176,180,184,188	0
25	DGD	c	517	66/66	0.78	0.32	-0.58	177,179,181,181	0
22	CLA	c	520	65/65	0.90	0.30	-0.60	177,179,180,181	0
28	OEX	A	411	10/10	0.92	0.42	-0.60	172,175,178,178	0
26	LHG	a	411	39/49	0.85	0.26	-0.62	177,179,180,181	0
33	BCT	D	404	4/4	0.90	0.26	-0.64	178,179,179,179	0
22	CLA	b	610	65/65	0.89	0.28	-0.67	177,179,180,180	0
22	CLA	B	612	65/65	0.92	0.26	-0.76	176,178,180,181	0
27	LMG	b	625	49/55	0.86	0.29	-0.80	178,179,180,180	0
22	CLA	a	406	65/65	0.84	0.30	-0.88	177,179,180,181	0
31	PHO	d	402	64/64	0.86	0.24	-0.94	178,179,180,181	0
25	DGD	C	516	62/66	0.86	0.25	-1.02	177,179,180,181	0
27	LMG	d	408	49/55	0.94	0.20	-1.16	178,179,180,180	0
27	LMG	B	621	49/55	0.91	0.26	-1.22	177,179,180,180	0
30	LMT	M	102	35/35	0.73	0.36	-1.27	178,179,181,182	0
28	OEX	a	414	10/10	0.94	0.41	-1.36	174,177,179,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	CL	D	403	1/1	0.79	0.28	-1.56	180,180,180,180	0
25	DGD	c	516	62/66	0.88	0.27	-1.57	178,179,180,181	0
33	BCT	d	404	4/4	0.95	0.18	-1.88	178,180,180,180	0
21	FE2	A	401	1/1	0.92	0.20	-2.13	176,176,176,176	0
21	FE2	a	403	1/1	0.88	0.07	-3.50	182,182,182,182	0
30	LMT	b	626	35/35	0.65	0.67	-	178,180,182,183	0
30	LMT	B	623	35/35	0.69	0.86	-	177,181,182,183	0
27	LMG	I	101	43/55	0.59	1.02	-	178,180,181,182	0
35	CA	O	301	1/1	0.62	0.42	-	182,182,182,182	0
35	CA	k	101	1/1	0.87	0.27	-	180,180,180,180	0
35	CA	K	101	1/1	0.67	0.52	-	184,184,184,184	0
35	CA	o	301	1/1	0.77	0.56	-	184,184,184,184	0
27	LMG	i	101	43/55	0.77	0.79	-	177,180,182,184	0

6.5 Other polymers [i](#)

There are no such residues in this entry.