



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 11:57 AM EDT

PDB ID : 4TNJ
Title : RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 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 : 4.50 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)

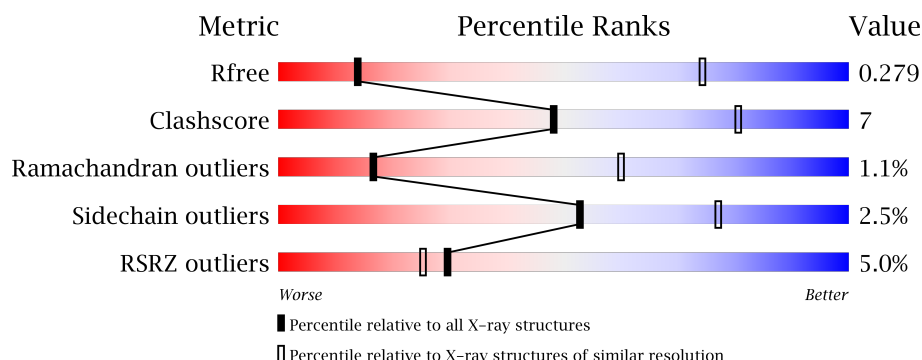
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1007 (5.30-3.64)
Clashscore	112137	1029 (5.30-3.70)
Ramachandran outliers	110173	1025 (5.30-3.66)
Sidechain outliers	110143	1006 (5.30-3.66)
RSRZ outliers	101464	1015 (5.30-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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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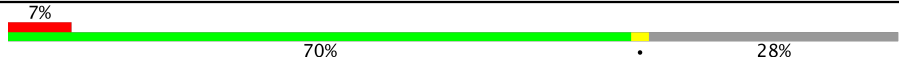

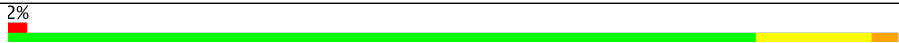
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

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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	-	-	X
22	CLA	A	405	X	-	-	X
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	X
22	CLA	B	604	X	-	-	X
22	CLA	B	605	X	-	-	X
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	X
22	CLA	B	608	X	-	-	X
22	CLA	B	609	X	-	-	X
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
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	-	-	-
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	X
22	CLA	C	504	X	-	-	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	408	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	X
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	X
22	CLA	b	618	X	-	-	X
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	X
22	CLA	c	506	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	X
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	X
22	CLA	d	405	X	-	-	X
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	j	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	618	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	513	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	521	-	-	-	X
24	BCR	D	411	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	J	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	622	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	513	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	521	-	-	-	X
24	BCR	f	102	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	D	409	-	-	-	X
25	DGD	a	411	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	408	-	-	-	X
26	LHG	C	519	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	a	413	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	m	101	-	-	-	X
28	CL	A	411	-	-	-	X
29	OEX	A	412	-	-	-	X
29	OEX	a	414	-	-	-	X
30	SQD	A	414	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	D	403	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	d	402	-	-	-	X
30	SQD	f	103	-	-	-	X
31	LMT	B	623	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	102	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	M	103	-	-	-	X
31	LMT	b	603	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	409	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	D	401	-	-	-	X
32	PHO	d	401	-	-	-	X
33	BCT	d	403	-	-	-	X
34	HEM	F	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	v	201	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

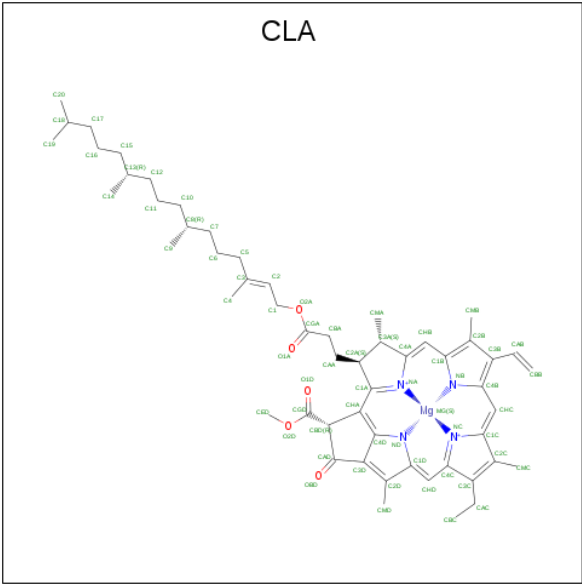
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: 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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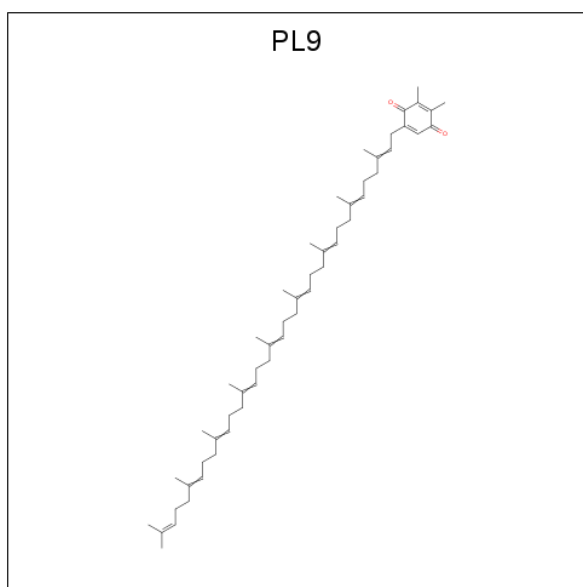
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 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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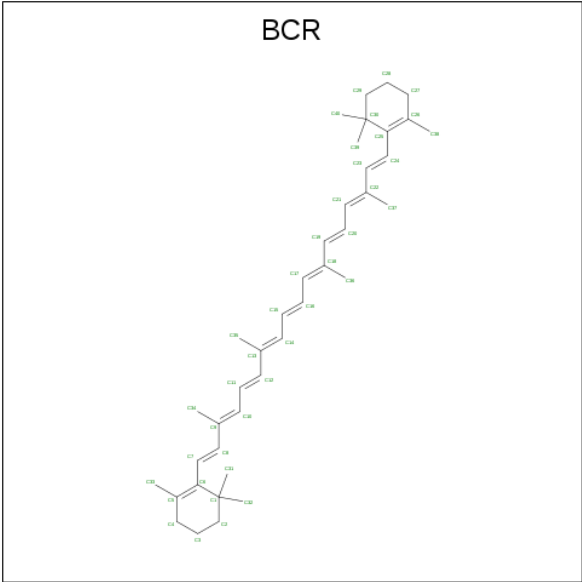
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: $C_{53}H_{80}O_2$).



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: $C_{40}H_{56}$).



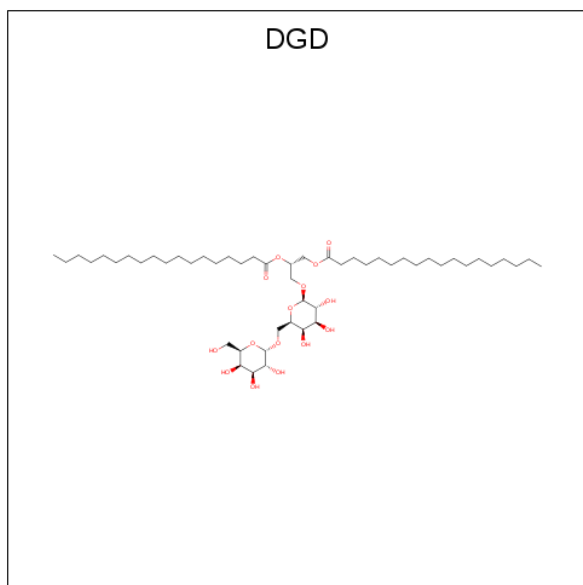
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	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: $C_{51}H_{96}O_{15}$).



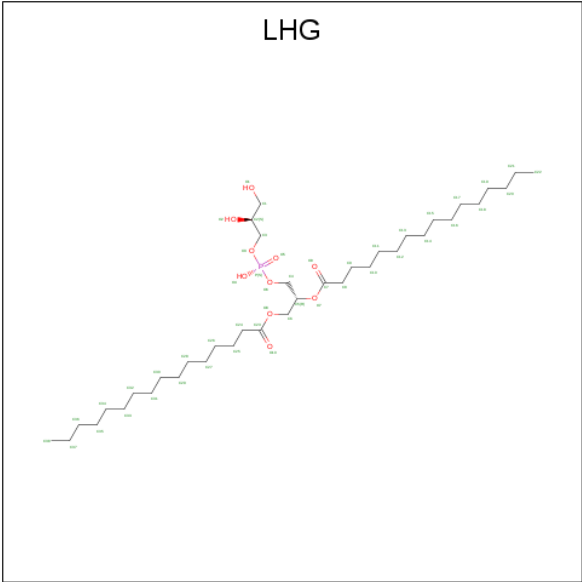
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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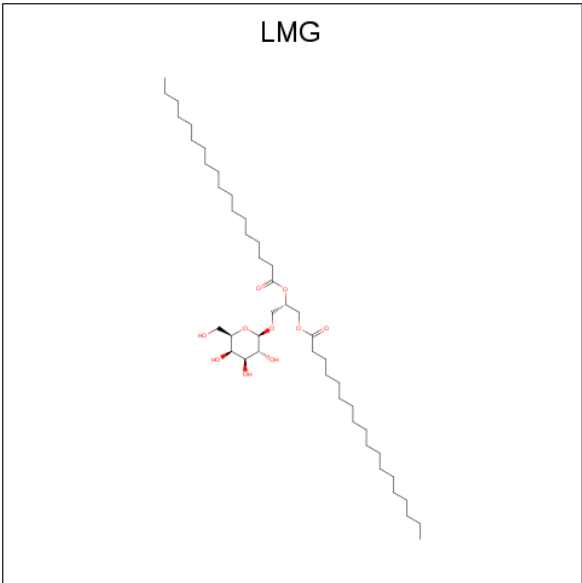
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

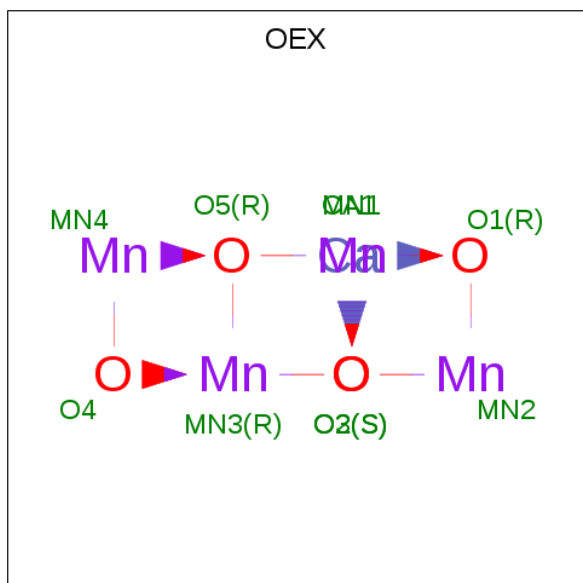


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	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	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
			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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

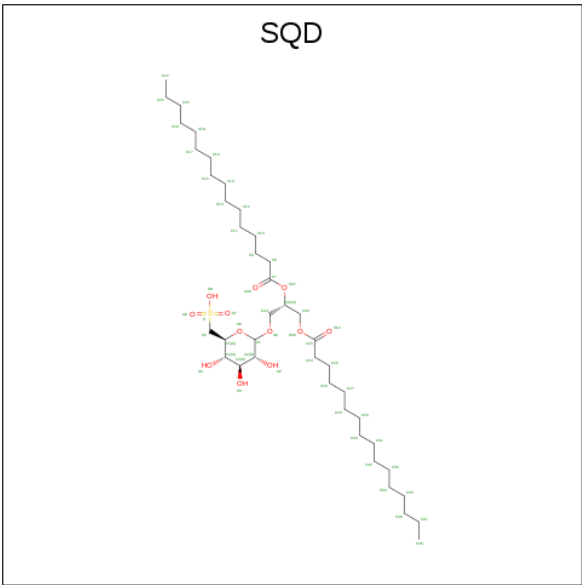
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

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



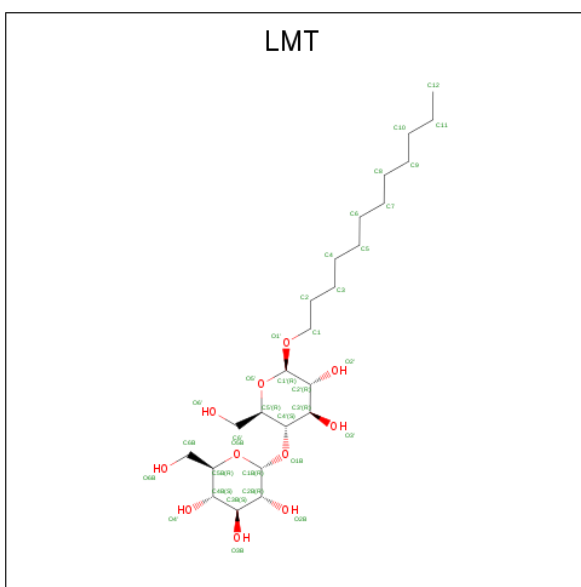
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



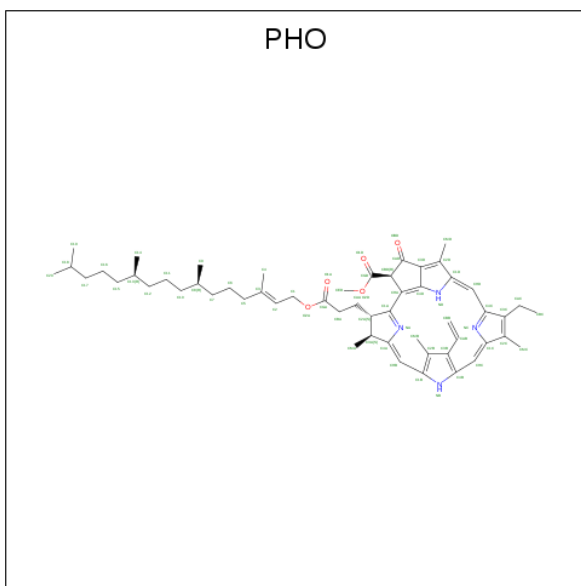
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0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

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



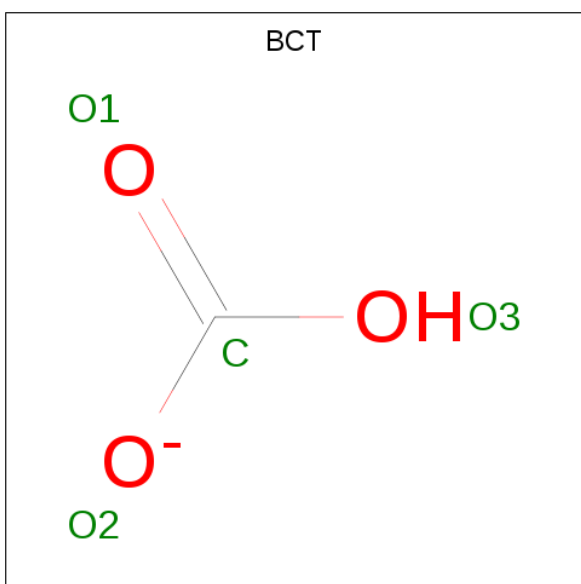
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	D	1	Total 31	C 20	O 11	0	0
31	I	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	b	1	Total 35	C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

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



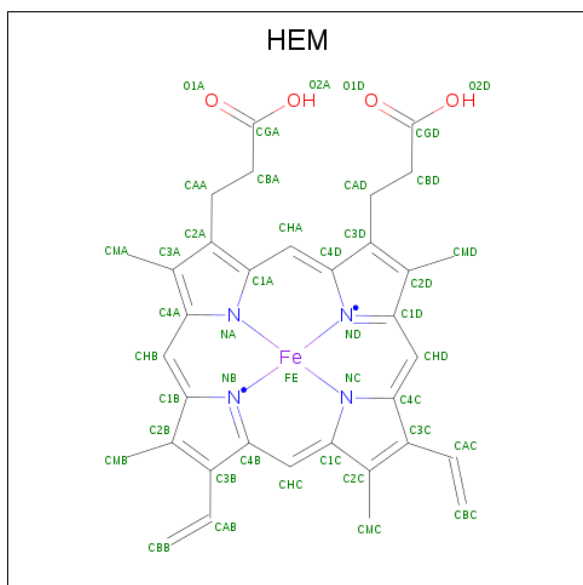
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

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



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

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

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

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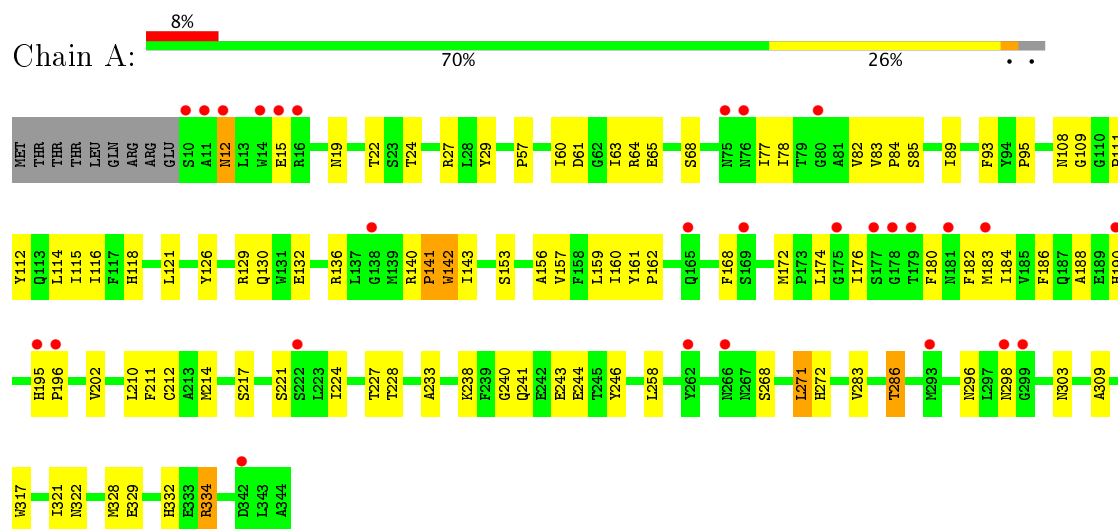
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	k	1	Total	Ca	0	0
			1	1		

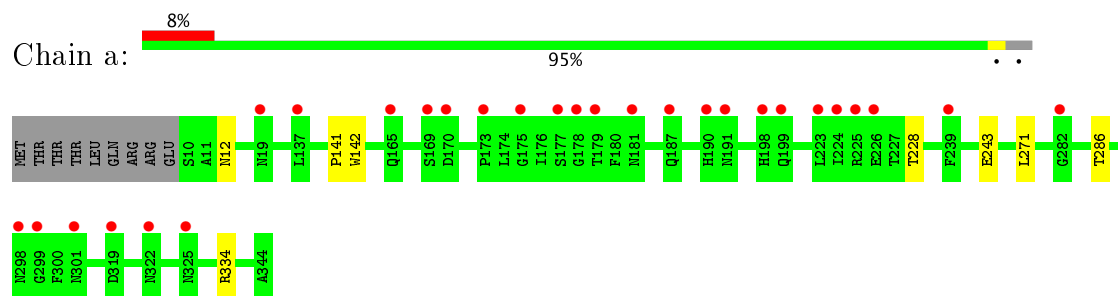
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

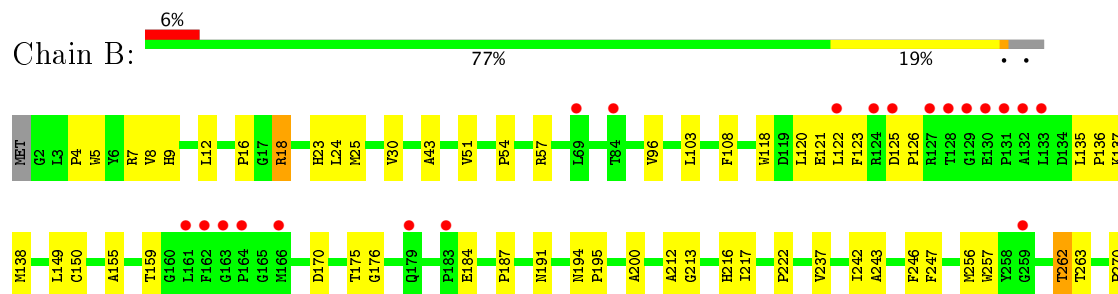
- Molecule 1: Photosystem Q(B) protein 1

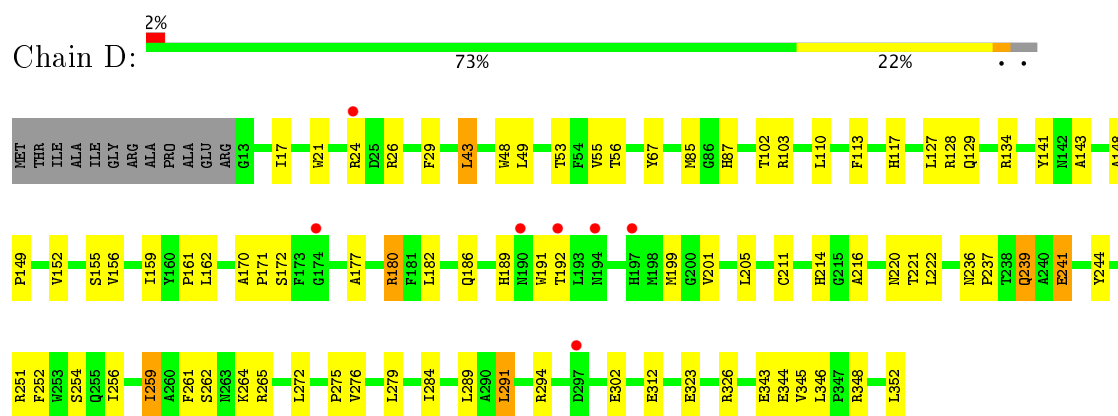


- Molecule 1: Photosystem Q(B) protein 1

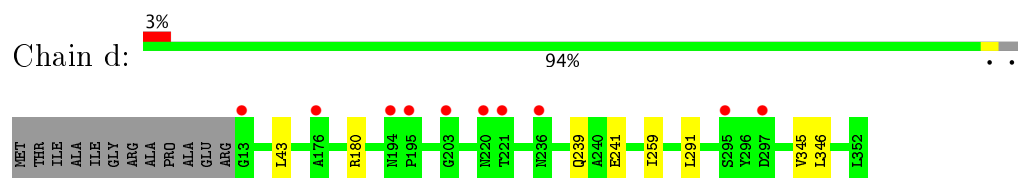


- Molecule 2: Photosystem II core light harvesting protein

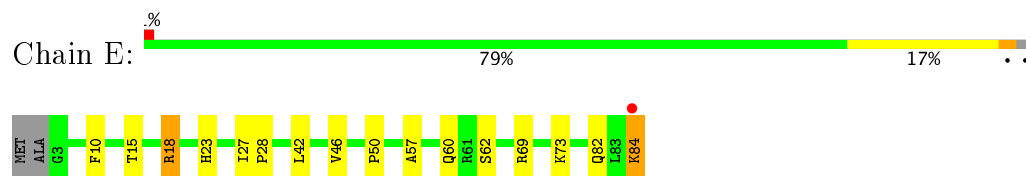




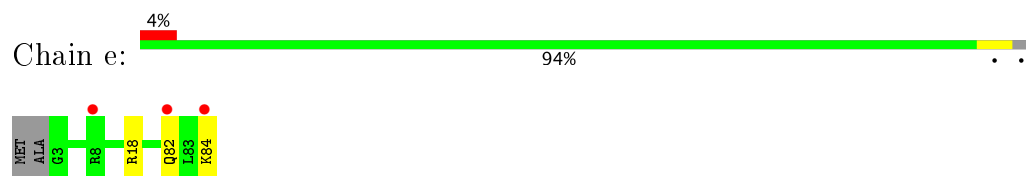
- Molecule 4: Photosystem II D2 protein



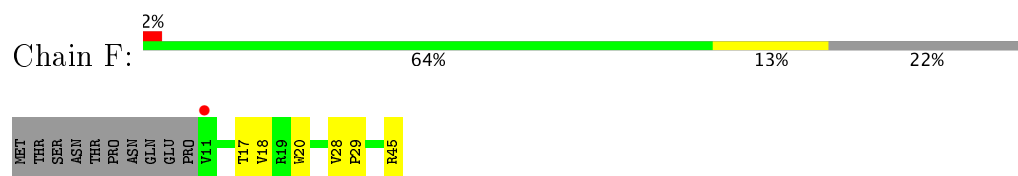
- Molecule 5: Cytochrome b559 subunit alpha



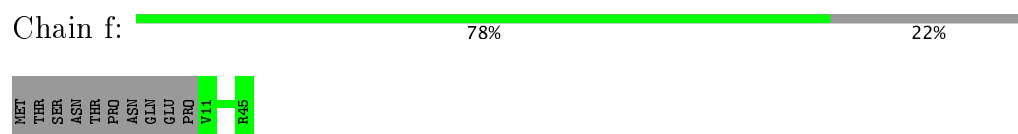
- Molecule 5: Cytochrome b559 subunit alpha



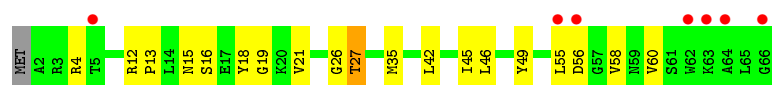
- Molecule 6: Cytochrome b559 subunit beta



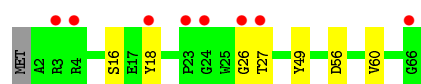
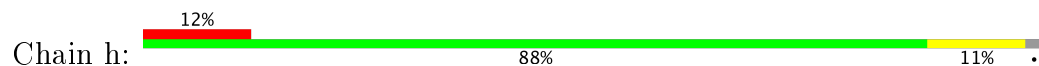
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



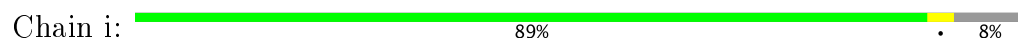
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



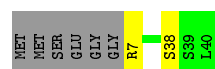
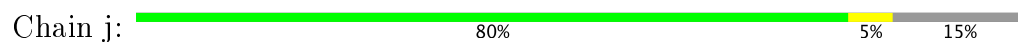
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

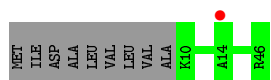


- Molecule 10: Photosystem II reaction center protein K

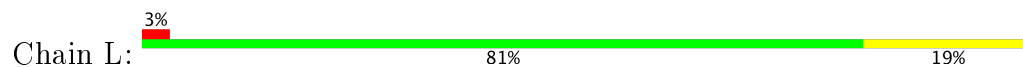


- Molecule 10: Photosystem II reaction center protein K

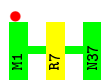




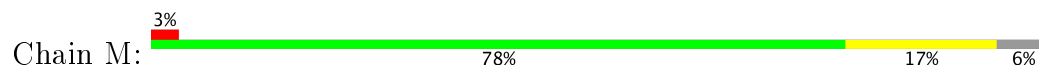
- Molecule 11: Photosystem II reaction center protein L



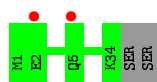
- Molecule 11: Photosystem II reaction center protein L



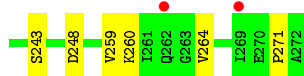
- Molecule 12: Photosystem II reaction center protein M



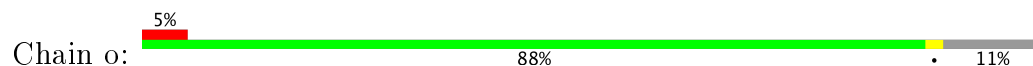
- Molecule 12: Photosystem II reaction center protein M

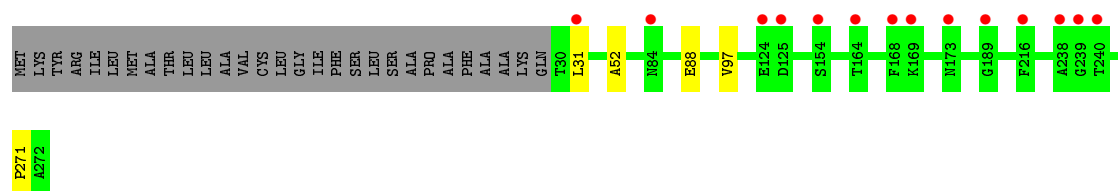


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

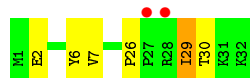
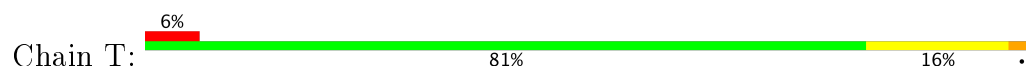


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

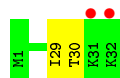
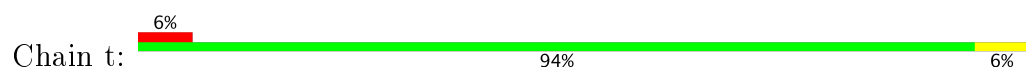




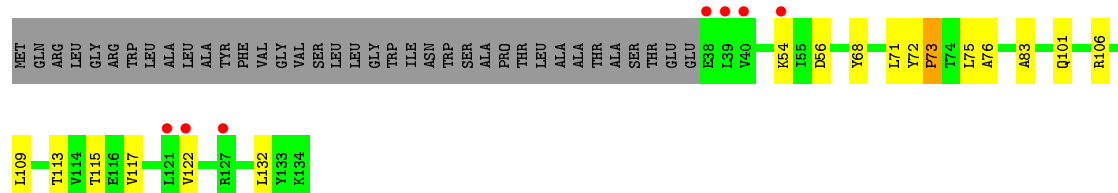
- Molecule 14: Photosystem II reaction center protein T



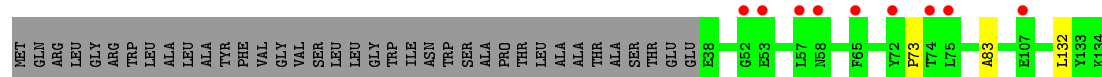
- Molecule 14: Photosystem II reaction center protein T



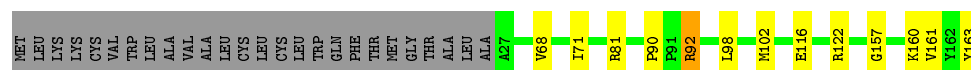
- Molecule 15: Photosystem II 12 kDa extrinsic protein



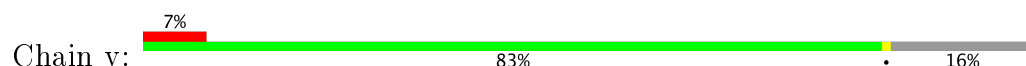
- Molecule 15: Photosystem II 12 kDa extrinsic protein

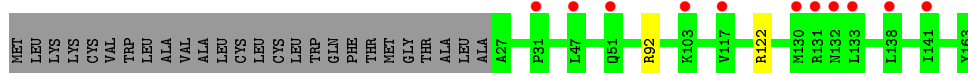


- Molecule 16: Cytochrome c-550

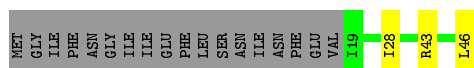


- Molecule 16: Cytochrome c-550





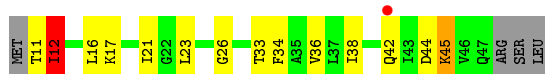
- Molecule 17: Photosystem II reaction center protein Ycf12



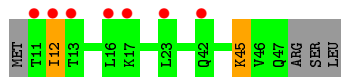
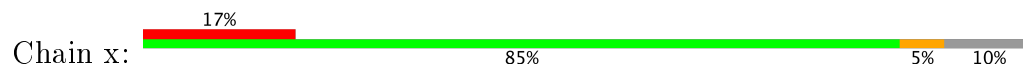
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



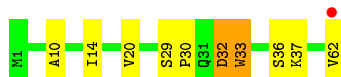
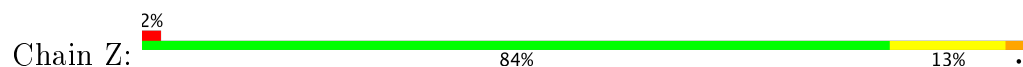
There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

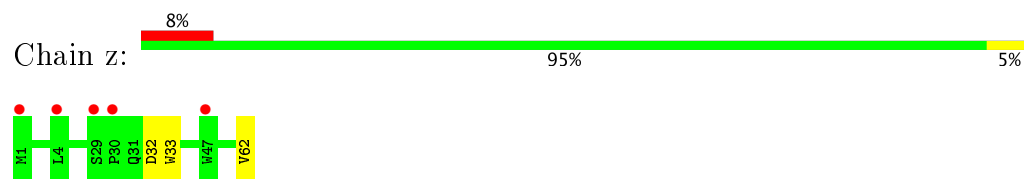


There are no outlier residues recorded for this chain.

- 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	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 4.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.276 , 0.284 0.273 , 0.279	Depositor DCC
R_{free} test set	2667 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	153.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.23	0/3556	0.41	0/4842
3	c	0.23	0/3556	0.41	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.43	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.46	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.25	0/293	0.43	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.25	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.44	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.26	0/273	0.44	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.25	0/490	0.44	0/669
All	All	0.23	0/41950	0.42	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	79	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	87	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	71	0
4	d	2706	0	2608	0	0
5	E	666	0	651	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	18	0
7	h	507	0	521	0	0
8	I	286	0	308	4	0
8	i	286	0	308	0	0
9	J	249	0	262	8	0
9	j	249	0	262	0	0
10	K	293	0	305	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	6	0
11	l	304	0	316	0	0
12	M	267	0	289	6	0
12	m	267	0	289	0	0
13	O	1845	0	1801	29	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	13	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	92	0
22	C	845	0	936	49	0
22	D	130	0	144	14	0
22	H	65	0	72	11	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	3	0
23	D	55	0	80	8	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	11	0
24	C	120	0	168	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	40	0	56	3	0
24	H	40	0	56	1	0
24	J	40	0	56	2	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	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	98	0	136	6	0
27	C	93	0	126	7	0
27	D	94	0	128	7	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	1	0
27	a	93	0	126	0	0
27	b	98	0	136	0	0
27	c	93	0	126	0	0
27	d	94	0	128	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	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	47	0	61	3	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	1	0
31	M	70	0	92	0	0
31	b	140	0	184	0	0
31	d	31	0	35	0	0
31	i	35	0	46	0	0
32	D	128	0	148	16	0
32	a	64	0	74	0	0
32	d	64	0	74	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	586	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 (586) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.56	0.87
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.60	0.82
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.61	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.50	0.80
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.77
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.71	0.72
22:B:605:CLA:H72	24:B:619:BCR:H311	1.71	0.72
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.74	0.71
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.71	0.71
4:D:199:MET:HG2	23:D:407:PL9:H322	1.73	0.71
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.73	0.71
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.73	0.71
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.56	0.70
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.74	0.70
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.74	0.69
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.69
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.69
22:C:506:CLA:H112	24:C:514:BCR:H362	1.75	0.68
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.67
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.75	0.67
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.76	0.67
4:D:29:PHE:O	4:D:128:ARG:NH2	2.29	0.67
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.30	0.67
4:D:236:ASN:ND2	4:D:239:GLN:O	2.29	0.67
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.67
3:C:250:TRP:O	3:C:254:THR:OG1	2.11	0.67
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.77	0.67
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.67
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.77	0.67
22:B:611:CLA:H42	4:D:127:LEU:HD11	29.92	0.66
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.66
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.77	0.65
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.77	0.65
4:D:259:ILE:HG12	27:D:408:LMG:H292	1.78	0.65
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.69	0.65
22:B:607:CLA:HBA2	30:D:403:SQD:H101	1.79	0.65
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.78	0.65
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
12:M:31:SER:HA	27:M:101:LMG:HC1	1.83	0.65
2:B:271:THR:HG22	2:B:273:TYR:H	1.64	0.64
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.79	0.64
1:A:174:LEU:HD22	32:D:401:PHO:H151	1.80	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.79	0.64
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.80	0.64
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.81	0.64
30:D:403:SQD:H171	30:D:403:SQD:H301	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:HB3	22:A:404:CLA:HBC2	14.89	0.63
22:A:404:CLA:H142	22:D:405:CLA:H151	1.80	0.63
1:A:183:MET:HA	22:A:404:CLA:HMD2	12.58	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	1.80	0.63
1:A:329:GLU:O	1:A:332:HIS:ND1	2.35	0.62
3:C:406:SER:O	3:C:418:ASN:ND2	2.33	0.62
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
3:C:297:TYR:O	3:C:423:ARG:NH2	2.32	0.62
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.82	0.62
22:A:404:CLA:HHC	22:A:404:CLA:HBB1	3.83	0.62
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.65	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.33	0.61
2:B:149:LEU:HG	22:B:606:CLA:HBC1	27.90	0.61
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.90	0.61
2:B:327:THR:HG21	27:B:621:LMG:H111	1.83	0.60
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.82	0.60
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.60
22:A:404:CLA:H71	22:A:405:CLA:HAB	47.01	0.60
3:C:49:LEU:O	3:C:53:HIS:ND1	2.34	0.60
2:B:12:LEU:HB2	22:B:615:CLA:HMC2	13.41	0.59
4:D:216:ALA:O	4:D:220:ASN:ND2	2.34	0.59
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.85	0.59
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.68	0.59
22:B:612:CLA:HMD1	7:H:27:THR:HB	39.55	0.59
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.88	0.59
22:A:403:CLA:H203	32:D:401:PHO:H71	1.84	0.59
30:A:413:SQD:H172	26:C:519:LHG:H172	1.85	0.59
2:B:262:THR:OG1	22:B:606:CLA:O1D	22.22	0.59
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.85	0.59
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.84	0.59
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.84	0.58
13:O:83:LYS:HG2	13:O:84:ASN:H	1.68	0.58
22:B:611:CLA:H151	22:B:612:CLA:H203	19.93	0.58
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.69	0.58
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.84	0.58
22:H:101:CLA:HBD	22:H:101:CLA:H2	1.88	0.58
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.86	0.58
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.85	0.58
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.33	0.58
12:M:25:LEU:O	12:M:28:GLN:HG3	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:404:CLA:H122	32:D:401:PHO:H3A	32.55	0.58
22:B:606:CLA:H193	7:H:42:LEU:HD12	33.85	0.58
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.91	0.58
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.89	0.57
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.86	0.57
1:A:64:ARG:O	13:O:178:ARG:NH2	2.39	0.57
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.90	0.57
4:D:24:ARG:NH2	18:X:44:ASP:O	2.37	0.57
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.89	0.57
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.57
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.33	0.57
27:D:408:LMG:O6	11:L:15:THR:HG21	2.05	0.57
22:C:501:CLA:HMB3	24:C:514:BCR:H403	1.87	0.57
5:E:84:LYS:HB2	5:E:84:LYS:HZ2	1.70	0.57
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.36	0.56
2:B:256:MET:O	2:B:448:ARG:NH1	2.34	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.23	0.56
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
22:B:607:CLA:H151	22:B:608:CLA:H203	1.88	0.56
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.95	0.56
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.87	0.56
22:C:510:CLA:HMB2	24:C:513:BCR:H382	1.87	0.56
3:C:118:HIS:CE1	27:C:518:LMG:H192	2.41	0.56
1:A:217:SER:HA	4:D:272:LEU:HD12	1.90	0.56
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.24	0.56
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.35	0.55
32:D:402:PHO:H151	22:D:405:CLA:H172	1.88	0.55
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.55
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.87	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.55
2:B:103:LEU:HD21	22:B:608:CLA:HMC3	26.63	0.55
22:D:406:CLA:H43	18:X:23:LEU:HA	1.89	0.55
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.90	0.55
22:A:404:CLA:H93	22:D:405:CLA:H152	1.89	0.55
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.89	0.55
27:D:408:LMG:HO4	27:D:408:LMG:HO5	1.52	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.89	0.55
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.55
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.89	0.55
22:B:606:CLA:C2D	22:B:608:CLA:H2	40.01	0.55
22:A:405:CLA:H203	32:D:401:PHO:H71	33.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.54
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.54
1:A:268:SER:O	1:A:272:HIS:ND1	2.37	0.54
1:A:153:SER:HB3	22:A:404:CLA:HED1	19.22	0.54
2:B:262:THR:HG22	2:B:263:THR:HG23	1.89	0.54
24:A:407:BCR:H321	30:A:414:SQD:H321	1.90	0.54
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.40	0.54
27:A:410:LMG:H231	23:D:407:PL9:H352	1.90	0.54
22:D:405:CLA:H42	18:X:26:GLY:HA3	26.54	0.54
2:B:458:PHE:HB3	22:B:607:CLA:HBC2	12.96	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
30:B:626:SQD:H1	30:B:626:SQD:H462	1.89	0.54
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.80	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.54
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.34	0.54
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.47	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.92	0.54
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.89	0.54
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.43	0.54
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.90	0.54
1:A:244:GLU:HG3	1:A:246:TYR:H	1.73	0.53
22:B:607:CLA:HBD	22:B:608:CLA:H43	4.16	0.53
25:B:625:DGD:O2D	25:B:625:DGD:O1B	2.26	0.53
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.46	0.53
2:B:155:ALA:O	2:B:159:THR:OG1	2.22	0.53
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.89	0.53
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.98	0.53
2:B:122:LEU:O	7:H:15:ASN:ND2	2.38	0.53
22:A:402:CLA:H122	32:D:401:PHO:H3A	1.90	0.53
24:A:407:BCR:H342	30:A:414:SQD:H311	1.91	0.53
1:A:85:SER:HA	1:A:109:GLY:HA3	1.95	0.53
1:A:29:TYR:O	1:A:129:ARG:NH1	2.52	0.53
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.39	0.53
30:A:413:SQD:H311	22:C:507:CLA:H71	1.91	0.53
22:D:406:CLA:H42	18:X:26:GLY:HA3	1.91	0.53
4:D:214:HIS:ND1	23:D:407:PL9:O2	2.29	0.53
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.92	0.53
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.91	0.52
26:C:519:LHG:H271	26:C:519:LHG:H101	1.89	0.52
2:B:212:ALA:HB2	22:B:612:CLA:HMC3	27.34	0.52
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.90	0.52
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
2:B:474:LEU:O	4:D:134:ARG:NH1	2.48	0.52
22:B:606:CLA:C3D	22:B:608:CLA:H2	40.25	0.52
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.92	0.52
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.91	0.52
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.91	0.52
3:C:85:GLY:N	25:C:516:DGD:HE4	2.25	0.52
22:B:608:CLA:H202	22:B:612:CLA:HBB2	21.92	0.52
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.92	0.52
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.76	0.52
22:B:605:CLA:OBD	31:B:622:LMT:O6'	2.21	0.51
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.51
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.86	0.51
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.75	0.51
1:A:211:PHE:HA	1:A:214:MET:HB2	1.91	0.51
30:A:413:SQD:H223	25:C:517:DGD:HAE1	1.91	0.51
4:D:275:PRO:O	4:D:279:LEU:HD23	2.13	0.51
1:A:132:GLU:O	1:A:136:ARG:HG2	2.10	0.51
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.74	0.51
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.44	0.51
13:O:73:PRO:HG2	13:O:102:THR:HB	1.92	0.51
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.03	0.51
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.93	0.51
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.51
2:B:150:CYS:HA	22:B:606:CLA:HBC2	29.82	0.50
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.93	0.50
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.44	0.50
22:C:504:CLA:HBD	22:C:504:CLA:HBA1	1.93	0.50
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.94	0.50
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.93	0.50
22:A:403:CLA:HED1	23:D:407:PL9:H372	1.93	0.50
24:D:411:BCR:H383	27:D:412:LMG:H171	1.92	0.50
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.50
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.47	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.46	0.50
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.93	0.50
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.98	0.50
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.42	0.50
22:A:403:CLA:HMA2	23:D:407:PL9:H411	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.50
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.56	0.50
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.96	0.50
2:B:271:THR:HB	2:B:274:GLN:HG3	1.94	0.49
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.94	0.49
22:A:404:CLA:H161	23:A:406:PL9:H253	1.93	0.49
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.49
2:B:150:CYS:HB2	22:B:606:CLA:HMC3	24.92	0.49
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.28	0.49
27:A:415:LMG:H112	2:B:43:ALA:HA	42.24	0.49
22:C:501:CLA:H193	22:C:506:CLA:H111	2.04	0.49
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.94	0.49
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.93	0.49
30:D:403:SQD:H241	30:D:403:SQD:H111	1.95	0.49
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.97	0.49
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.94	0.49
22:B:611:CLA:H51	22:B:612:CLA:H101	18.04	0.49
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.94	0.49
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.95	0.49
22:B:612:CLA:H51	27:B:624:LMG:H231	1.95	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.12	0.49
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.95	0.48
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.94	0.48
13:O:154:SER:N	13:O:169:LYS:O	2.45	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.98	0.48
4:D:261:PHE:HB2	23:D:407:PL9:H522	1.95	0.48
13:O:118:SER:HB3	13:O:157:PRO:HA	2.00	0.48
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.71	0.48
2:B:135:LEU:HA	2:B:138:MET:HE3	2.04	0.48
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.95	0.48
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.95	0.48
31:B:627:LMT:H62	8:I:4:LEU:HD22	82.13	0.48
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.95	0.48
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.43	0.48
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.82	0.48
1:A:210:LEU:HG	32:D:402:PHO:NC	2.29	0.48
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.99	0.48
22:A:405:CLA:H162	22:A:405:CLA:H141	1.69	0.48
2:B:222:PRO:HG3	7:H:27:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.02	0.48
1:A:190:HIS:O	1:A:298:ASN:HB3	2.15	0.48
3:C:130:VAL:O	3:C:134:ILE:HG12	2.18	0.48
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.48
1:A:258:LEU:O	4:D:128:ARG:NH1	2.47	0.48
2:B:383:PHE:N	4:D:344:GLU:O	2.34	0.48
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.29	0.48
2:B:327:THR:HG22	22:B:606:CLA:H12	1.96	0.48
22:B:603:CLA:HMD2	22:B:611:CLA:H193	1.96	0.48
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.96	0.48
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.96	0.48
22:D:405:CLA:H43	18:X:23:LEU:HA	28.38	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.78	0.47
22:B:611:CLA:H171	22:B:612:CLA:HBB2	1.95	0.47
4:D:279:LEU:HG	32:D:402:PHO:HBC3	1.96	0.47
31:B:628:LMT:H122	14:T:7:VAL:HG12	34.49	0.47
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.78	0.47
22:B:615:CLA:H72	22:B:615:CLA:H12	1.96	0.47
4:D:85:MET:HA	5:E:69:ARG:HB3	2.04	0.47
1:A:78:ILE:O	1:A:176:ILE:HB	2.15	0.47
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.97	0.47
22:B:614:CLA:H172	22:B:614:CLA:H111	1.97	0.47
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.45	0.47
22:B:606:CLA:H2	22:B:608:CLA:H93	34.07	0.47
22:B:612:CLA:H171	27:B:624:LMG:H401	1.97	0.47
32:D:401:PHO:H41	32:D:401:PHO:H62	1.46	0.47
22:B:611:CLA:H18	22:B:612:CLA:H192	22.23	0.47
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.97	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	2.00	0.47
24:B:619:BCR:H361	24:B:619:BCR:H20C	1.77	0.47
1:A:298:ASN:ND2	3:C:402:GLY:O	2.48	0.47
27:I:101:LMG:H181	31:I:102:LMT:H42	2.02	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.41	0.47
30:F:102:SQD:H162	18:X:33:THR:HA	1.96	0.47
25:B:625:DGD:HD1	31:B:627:LMT:H32	1.97	0.47
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.47
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.47
1:A:224:ILE:O	4:D:265:ARG:NH2	2.52	0.46
2:B:170:ASP:OD1	2:B:175:THR:N	2.51	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:518:LMG:H292	27:C:518:LMG:H111	1.96	0.46
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.97	0.46
3:C:166:ILE:O	3:C:170:ILE:HG13	2.20	0.46
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.49	0.46
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.81	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.96	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.97	0.46
22:B:613:CLA:H51	24:B:616:BCR:H372	1.97	0.46
22:C:512:CLA:HAB	24:C:521:BCR:H24C	2.03	0.46
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.60	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.98	0.46
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.47	0.46
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.98	0.46
3:C:158:THR:O	3:C:251:HIS:HB3	2.15	0.46
27:D:408:LMG:H111	11:L:19:LEU:HD21	1.97	0.46
2:B:327:THR:HG22	22:B:610:CLA:H12	26.92	0.46
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.97	0.46
22:A:405:CLA:H62	22:A:405:CLA:H41	3.95	0.46
3:C:113:VAL:HG11	27:C:518:LMG:H132	2.02	0.46
22:C:503:CLA:H201	22:C:503:CLA:HMD2	2.02	0.46
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.46
1:A:114:LEU:O	1:A:118:HIS:ND1	2.45	0.45
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.55	0.45
22:C:510:CLA:H61	22:C:510:CLA:H93	1.82	0.45
4:D:348:ARG:NH2	4:D:352:LEU:O	2.39	0.45
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.65	0.45
22:H:101:CLA:H162	22:H:101:CLA:H122	1.51	0.45
25:B:620:DGD:HAW2	22:H:101:CLA:H152	1.99	0.45
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	2.04	0.45
24:B:616:BCR:H361	24:B:616:BCR:H20C	1.76	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.45
22:C:508:CLA:H11	22:C:508:CLA:H51	1.81	0.45
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.74	0.45
22:C:504:CLA:H11	24:C:514:BCR:H312	2.02	0.45
1:A:202:VAL:HB	22:A:404:CLA:HMB3	12.99	0.45
4:D:48:TRP:CE2	32:D:402:PHO:H161	2.52	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.15	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)
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.45
22:A:402:CLA:H51	32:D:401:PHO:C3B	2.47	0.45
27:B:621:LMG:H421	4:D:284:ILE:HD13	1.99	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.45
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.45
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.45
24:C:514:BCR:H361	24:C:514:BCR:H20C	1.84	0.45
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.45
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.80	0.45
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.45
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.04	0.45
24:B:618:BCR:H20C	24:B:618:BCR:H361	1.82	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.17	0.45
3:C:224:ILE:O	3:C:227:VAL:HG23	2.17	0.45
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.45
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.03	0.45
30:A:414:SQD:H332	22:B:609:CLA:H203	66.13	0.44
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.52	0.44
4:D:102:THR:OG1	25:D:409:DGD:HD62	2.17	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.17	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.17	0.44
22:B:605:CLA:H18	22:B:615:CLA:H121	1.99	0.44
22:B:611:CLA:H162	22:B:611:CLA:H122	1.76	0.44
5:E:60:GLN:HG2	5:E:62:SER:H	1.86	0.44
22:H:101:CLA:H62	22:H:101:CLA:H41	1.56	0.44
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.44
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.70	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	1.99	0.44
22:B:604:CLA:H62	22:B:604:CLA:H41	1.80	0.44
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.06	0.44
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.19	0.44
22:C:512:CLA:HBA2	22:C:512:CLA:H3A	1.72	0.44
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.53	0.44
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.50	0.44
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.44
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.20	0.44
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.00	0.44
1:A:202:VAL:HB	22:A:402:CLA:HMB3	2.00	0.44
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.89	0.44
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.52	0.44
22:C:512:CLA:HAB	24:C:521:BCR:H371	2.02	0.44
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.53	0.44
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.48	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.84	0.44
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.19	0.44
2:B:468:TRP:HH2	27:B:624:LMG:HO2	1.62	0.44
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.99	0.44
24:C:513:BCR:H343	24:C:513:BCR:H311	2.03	0.44
7:H:35:MET:HB2	7:H:35:MET:HE3	1.86	0.44
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.44
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.44
26:A:409:LHG:H382	22:C:509:CLA:H93	2.00	0.44
22:B:607:CLA:H51	22:B:608:CLA:H101	1.99	0.44
3:C:245:ILE:O	3:C:249:ILE:HG12	2.19	0.44
4:D:262:SER:N	27:D:408:LMG:O3	2.46	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.44
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.05	0.44
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.03	0.43
22:B:605:CLA:HBA2	22:B:605:CLA:H3A	1.27	0.43
24:C:513:BCR:H24C	24:C:513:BCR:H371	1.79	0.43
24:B:616:BCR:H383	30:B:626:SQD:H111	1.99	0.43
3:C:456:GLU:N	3:C:456:GLU:OE1	2.51	0.43
22:C:520:CLA:H112	22:C:520:CLA:H142	1.76	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.53	0.43
3:C:29:GLU:HB2	3:C:30:SER:H	1.65	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43
27:D:408:LMG:O9	27:D:408:LMG:HC1	2.18	0.43
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.43
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.01	0.43
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.04	0.43
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.01	0.43
22:B:613:CLA:H12	22:B:613:CLA:H51	4.48	0.43
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.43
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.03	0.43
32:D:401:PHO:H13	32:D:401:PHO:H102	1.82	0.43
7:H:12:ARG:HD3	7:H:12:ARG:O	2.18	0.43
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
22:B:607:CLA:H18	22:B:608:CLA:H192	2.01	0.43
2:B:108:PHE:HB2	30:B:626:SQD:H223	2.00	0.43
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.43
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
1:A:240:GLY:HA3	14:T:29:ILE:HG22	2.00	0.43
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.83	0.43
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.79	0.43
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.54	0.43
22:B:606:CLA:H41	22:B:606:CLA:H61	2.86	0.43
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.04	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.43
4:D:252:PHE:O	4:D:256:ILE:HG22	2.21	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.00	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.43
24:C:521:BCR:H361	24:C:521:BCR:H20C	1.81	0.43
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.85	0.43
31:B:628:LMT:H1B	31:B:628:LMT:H3'	1.53	0.43
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.01	0.43
24:C:521:BCR:H371	24:C:521:BCR:H24C	1.82	0.43
32:D:402:PHO:CHB	22:D:405:CLA:H101	2.49	0.43
15:U:72:TYR:O	15:U:76:ALA:HB3	2.18	0.43
22:A:405:CLA:H11	22:A:405:CLA:H51	4.35	0.42
22:C:501:CLA:H162	22:C:501:CLA:H141	1.78	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.51	0.42
16:V:98:LEU:O	16:V:102:MET:HG3	2.24	0.42
22:A:403:CLA:H202	22:A:403:CLA:H162	1.76	0.42
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.02	0.42
27:C:522:LMG:H322	10:K:27:VAL:HG23	2.08	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.04	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.42
1:A:182:PHE:O	1:A:186:PHE:HB2	2.20	0.42
22:D:405:CLA:H62	22:D:405:CLA:H92	1.80	0.42
22:A:404:CLA:H143	22:A:404:CLA:H161	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.85	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42
2:B:25:MET:HG2	24:B:616:BCR:H23C	2.00	0.42
22:B:605:CLA:C3D	31:B:622:LMT:H11	2.50	0.42
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.01	0.42
3:C:402:GLY:HA3	3:C:420:VAL:HG22	2.01	0.42
22:C:511:CLA:H61	22:C:511:CLA:H13	2.01	0.42
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.03	0.42
32:D:401:PHO:H202	32:D:401:PHO:H162	1.86	0.42
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.79	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.65	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.85	0.42
22:C:520:CLA:O2D	27:C:522:LMG:O2	2.40	0.42
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.19	0.42
22:A:405:CLA:H162	22:A:405:CLA:H202	3.78	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.92	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.94	0.42
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.02	0.42
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.42
25:D:409:DGD:O5E	25:D:409:DGD:O4E	2.25	0.42
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.20	0.42
1:A:238:LYS:O	1:A:241:GLN:HG3	2.20	0.42
22:B:615:CLA:H162	22:B:615:CLA:H122	5.17	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.02	0.42
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.84	0.42
22:A:404:CLA:H151	32:D:401:PHO:H72	40.46	0.42
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.42
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.42
2:B:212:ALA:O	2:B:216:HIS:ND1	2.51	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.74	0.42
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.88	0.42
27:C:522:LMG:H112	24:J:102:BCR:H373	2.01	0.42
4:D:155:SER:HA	4:D:159:ILE:HB	2.07	0.42
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.01	0.42
11:L:4:ASN:OD1	11:L:6:ASN:ND2	2.52	0.42
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.42
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.42
18:X:12:ILE:HA	18:X:16:LEU:HD12	2.06	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.02	0.42
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.87	0.42
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.02	0.41
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.95	0.41
24:D:411:BCR:H361	24:D:411:BCR:H20C	1.81	0.41
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.41
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.06	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
1:A:303:ASN:O	3:C:415:ASN:ND2	2.41	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.87	0.41
18:X:17:LYS:O	18:X:21:ILE:HG13	2.20	0.41
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.02	0.41
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.60	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
6:F:45:ARG:NH2	9:J:40:LEU:O	2.53	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.57	0.41
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.41
24:C:521:BCR:H15C	24:C:521:BCR:H351	1.84	0.41
24:D:411:BCR:H11C	24:D:411:BCR:H341	1.94	0.41
1:A:24:THR:O	4:D:251:ARG:NH2	2.44	0.41
1:A:61:ASP:HB2	1:A:63:ILE:HG12	2.09	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
22:B:602:CLA:H162	22:B:602:CLA:H192	1.77	0.41
3:C:119:LEU:HG	24:C:513:BCR:H10C	2.18	0.41
22:A:403:CLA:H42	23:D:407:PL9:H162	2.02	0.41
13:O:192:SER:OG	13:O:193:GLY:N	2.53	0.41
22:A:403:CLA:H41	22:A:403:CLA:H62	1.78	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.95	0.41
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.35	0.41
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.50	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.21	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.43	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.04	0.41
22:B:604:CLA:H141	22:B:604:CLA:H161	1.90	0.41
22:B:606:CLA:H92	22:B:606:CLA:HBB2	11.33	0.41
3:C:420:VAL:H	25:C:516:DGD:HE62	1.85	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.78	0.41
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.09	0.41
1:A:22:THR:HG21	8:I:30:ARG:HD3	2.08	0.41
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:402:CLA:CBB	22:A:402:CLA:HHC	2.50	0.41
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.02	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.98	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.31	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	2.27	0.41
22:A:404:CLA:HMD3	4:D:182:LEU:HD11	2.02	0.41
22:B:602:CLA:H161	22:B:602:CLA:H141	1.82	0.41
22:B:602:CLA:H61	22:B:602:CLA:H41	1.67	0.41
3:C:257:PHE:HB3	3:C:258:GLY:H	1.63	0.41
22:C:508:CLA:H92	22:C:508:CLA:H62	1.72	0.41
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.02	0.41
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.07	0.40
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.86	0.40
3:C:377:LEU:O	3:C:381:LYS:HB2	2.21	0.40
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.90	0.40
3:C:57:ALA:O	3:C:61:VAL:HG23	2.20	0.40
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.58	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	2.51	0.40
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.03	0.40
22:D:405:CLA:HBA1	22:D:405:CLA:H3A	1.86	0.40
1:A:317:TRP:O	1:A:321:ILE:HG13	2.22	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
22:B:604:CLA:H162	22:B:604:CLA:H202	1.88	0.40
4:D:49:LEU:O	4:D:53:THR:HG23	2.22	0.40
22:H:101:CLA:H62	22:H:101:CLA:H93	1.88	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:140:ARG:HH22	26:A:409:LHG:P	2.44	0.40
1:A:141:PRO:O	1:A:143:ILE:N	2.53	0.40
1:A:180:PHE:O	1:A:184:ILE:HG13	2.24	0.40
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.03	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.89	0.40
22:B:607:CLA:H172	22:D:406:CLA:H3A	2.03	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.21	0.40
22:C:508:CLA:H142	22:C:508:CLA:H112	1.84	0.40
4:D:201:VAL:O	4:D:205:LEU:HB2	2.22	0.40
7:H:46:LEU:HB2	22:H:101:CLA:H61	2.03	0.40
1:A:176:ILE:HD12	22:A:405:CLA:HED3	23.91	0.40
22:A:404:CLA:H51	32:D:401:PHO:C3B	21.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:404:CLA:HAB	22:D:405:CLA:H72	2.04	0.40
2:B:137:LYS:HB2	2:B:137:LYS:HE3	1.96	0.40
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.05	0.40
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.40
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.04	0.40
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	15	58
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	15	58
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	22	66
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	28	71
3	C	445/461 (96%)	405 (91%)	36 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	39
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	39
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
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%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4	34
17	y	26/46 (56%)	20 (77%)	5 (19%)	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%)	4673 (91%)	410 (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

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Mol	Chain	Res	Type
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
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	12	ILE
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
7	h	26	GLY
9	j	38	SER
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
2	b	489	GLU
4	d	239	GLN
13	o	88	GLU
1	A	142	TRP
2	B	489	GLU
3	C	32	GLY
5	E	82	GLN
1	a	334	ARG
3	c	32	GLY
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
3	C	144	SER
7	H	16	SER
15	U	73	PRO

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Mol	Chain	Res	Type
1	a	142	TRP
3	c	144	SER
7	h	16	SER
15	u	73	PRO
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY

5.3.2 Protein sidechains ⓘ

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%)	268 (98%)	7 (2%)	53	77
4	d	275/283 (97%)	268 (98%)	7 (2%)	53	77
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	70
14	t	29/29 (100%)	28 (97%)	1 (3%)	42	70
15	U	84/112 (75%)	83 (99%)	1 (1%)	75	88
15	u	84/112 (75%)	83 (99%)	1 (1%)	75	88
16	V	116/138 (84%)	114 (98%)	2 (2%)	66	84
16	v	116/138 (84%)	114 (98%)	2 (2%)	66	84
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%)	4140 (98%)	104 (2%)	53	77

All (104) 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

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Mol	Chain	Res	Type
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG
5	E	84	LYS
7	H	27	THR
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

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Mol	Chain	Res	Type
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	472	LEU
4	d	43	LEU
4	d	180	ARG
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	345	VAL
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

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Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CLA	A	402	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	A	403	-	56,73,73	1.09	4 (7%)	65,113,113	1.26	8 (12%)
22	CLA	A	404	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	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	0.96	4 (8%)	57,57,69	1.50	8 (14%)
24	BCR	A	407	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	6 (10%)
25	DGD	A	408	-	57,57,67	0.93	0	71,71,81	1.43	8 (11%)
26	LHG	A	409	-	38,38,48	0.67	0	39,44,54	1.21	3 (7%)
27	LMG	A	410	-	51,51,55	0.74	1 (1%)	59,59,63	1.38	6 (10%)
29	OEX	A	412	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	A	413	-	50,51,54	0.97	4 (8%)	60,62,65	1.95	11 (18%)
30	SQD	A	414	-	53,54,54	0.96	5 (9%)	63,65,65	1.79	10 (15%)
27	LMG	A	415	-	42,42,55	0.84	0	50,50,63	1.28	6 (12%)
22	CLA	B	601	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	8 (12%)
22	CLA	B	602	-	56,73,73	1.10	4 (7%)	65,113,113	1.26	9 (13%)
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	1.12	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	1.25	9 (13%)
22	CLA	B	608	-	56,73,73	1.12	4 (7%)	65,113,113	1.23	8 (12%)
22	CLA	B	609	-	56,73,73	1.11	4 (7%)	65,113,113	1.26	9 (13%)
22	CLA	B	610	-	56,73,73	1.15	5 (8%)	65,113,113	1.33	9 (13%)
22	CLA	B	611	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	B	612	-	56,73,73	1.09	4 (7%)	65,113,113	1.28	8 (12%)
22	CLA	B	613	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	8 (12%)
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	1.23	8 (14%)
24	BCR	B	617	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	7 (12%)
24	BCR	B	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	8 (14%)
24	BCR	B	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)
25	DGD	B	620	-	59,59,67	0.90	0	73,73,81	1.37	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	B	621	-	49,49,55	0.78	1 (2%)	57,57,63	1.35	6 (10%)
31	LMT	B	622	-	36,36,36	1.13	5 (13%)	47,47,47	0.99	1 (2%)
31	LMT	B	623	-	36,36,36	1.11	5 (13%)	47,47,47	1.04	2 (4%)
27	LMG	B	624	-	49,49,55	0.77	0	57,57,63	1.33	5 (8%)
25	DGD	B	625	-	53,53,67	1.07	3 (5%)	67,67,81	1.34	8 (11%)
30	SQD	B	626	-	46,47,54	1.02	5 (10%)	56,58,65	1.94	10 (17%)
31	LMT	B	627	-	36,36,36	1.13	5 (13%)	47,47,47	0.98	1 (2%)
31	LMT	B	628	-	36,36,36	1.14	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	1.27	7 (10%)
22	CLA	C	503	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	7 (10%)
22	CLA	C	504	-	56,73,73	1.12	4 (7%)	65,113,113	1.26	8 (12%)
22	CLA	C	505	-	56,73,73	1.10	4 (7%)	65,113,113	1.28	8 (12%)
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	1.11	4 (7%)	65,113,113	1.20	8 (12%)
22	CLA	C	509	-	56,73,73	1.11	4 (7%)	65,113,113	1.21	9 (13%)
22	CLA	C	510	3	56,73,73	1.11	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	1.26	10 (15%)
24	BCR	C	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	10 (17%)
24	BCR	C	514	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	9 (16%)
25	DGD	C	515	-	54,54,67	0.98	2 (3%)	68,68,81	1.31	7 (10%)
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	0.89	2 (2%)	81,81,81	1.44	12 (14%)
27	LMG	C	518	-	45,45,55	0.78	0	53,53,63	1.30	6 (11%)
26	LHG	C	519	-	36,36,48	0.69	0	37,42,54	1.28	3 (8%)
22	CLA	C	520	-	56,73,73	1.09	4 (7%)	65,113,113	1.23	9 (13%)
24	BCR	C	521	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	9 (16%)
27	LMG	C	522	-	48,48,55	0.77	0	56,56,63	1.34	6 (10%)
32	PHO	D	401	-	67,69,69	1.22	8 (11%)	87,99,99	1.01	6 (6%)
32	PHO	D	402	-	67,69,69	1.24	8 (11%)	87,99,99	1.01	6 (6%)
30	SQD	D	403	-	42,43,54	1.04	3 (7%)	52,54,65	1.98	11 (21%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	405	-	56,73,73	1.14	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	D	406	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	7 (10%)
23	PL9	D	407	-	55,55,55	1.01	3 (5%)	69,69,69	1.47	11 (15%)
27	LMG	D	408	-	48,48,55	0.77	0	56,56,63	1.41	5 (8%)
25	DGD	D	409	-	64,64,67	0.92	0	78,78,81	1.34	9 (11%)
31	LMT	D	410	-	32,32,36	1.19	5 (15%)	43,43,47	1.05	2 (4%)
24	BCR	D	411	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	7 (12%)
27	LMG	D	412	-	46,46,55	0.79	2 (4%)	54,54,63	1.33	5 (9%)
27	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.33	5 (9%)
34	HEM	F	101	5,6	28,50,50	2.23	6 (21%)	17,82,82	1.44	3 (17%)
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	54,56,65	1.84	11 (20%)
22	CLA	H	101	-	56,73,73	1.12	4 (7%)	65,113,113	1.23	8 (12%)
24	BCR	H	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.18	3 (5%)
27	LMG	I	101	-	43,43,55	0.81	0	51,51,63	1.29	5 (9%)
31	LMT	I	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	2 (4%)
23	PL9	J	101	-	35,35,55	1.00	1 (2%)	45,45,69	1.51	7 (15%)
24	BCR	J	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.57	12 (21%)
27	LMG	M	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.28	4 (8%)
31	LMT	M	102	-	36,36,36	1.16	5 (13%)	47,47,47	1.03	2 (4%)
31	LMT	M	103	-	36,36,36	1.15	5 (13%)	47,47,47	1.02	2 (4%)
34	HEM	V	201	16	28,50,50	2.25	6 (21%)	17,82,82	1.44	2 (11%)
30	SQD	a	401	-	53,54,54	0.96	5 (9%)	63,65,65	1.76	10 (15%)
27	LMG	a	402	-	42,42,55	0.84	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%)
32	PHO	a	407	-	67,69,69	1.24	8 (11%)	87,99,99	1.00	5 (5%)
22	CLA	a	408	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	7 (10%)
23	PL9	a	409	-	45,45,55	1.00	4 (8%)	57,57,69	1.50	10 (17%)
24	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	7 (12%)
25	DGD	a	411	-	57,57,67	0.94	1 (1%)	71,71,81	1.42	7 (9%)
26	LHG	a	412	-	38,38,48	0.67	1 (2%)	39,44,54	1.22	3 (7%)
27	LMG	a	413	-	51,51,55	0.75	1 (1%)	59,59,63	1.36	6 (10%)
29	OEX	a	414	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	60,62,65	1.97	11 (18%)
25	DGD	b	601	-	53,53,67	1.07	4 (7%)	67,67,81	1.35	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	b	602	-	46,47,54	1.02	5 (10%)	56,58,65	1.97	10 (17%)
31	LMT	b	603	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	1 (2%)
31	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	1 (2%)
22	CLA	b	605	-	56,73,73	1.11	4 (7%)	65,113,113	1.26	7 (10%)
22	CLA	b	606	-	56,73,73	1.09	4 (7%)	65,113,113	1.26	9 (13%)
22	CLA	b	607	-	56,73,73	1.13	4 (7%)	65,113,113	1.28	10 (15%)
22	CLA	b	608	-	56,73,73	1.11	4 (7%)	65,113,113	1.23	7 (10%)
22	CLA	b	609	-	56,73,73	1.10	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	b	610	-	56,73,73	1.11	4 (7%)	65,113,113	1.22	9 (13%)
22	CLA	b	611	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	7 (10%)
22	CLA	b	612	-	56,73,73	1.12	4 (7%)	65,113,113	1.22	7 (10%)
22	CLA	b	613	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	9 (13%)
22	CLA	b	614	-	56,73,73	1.16	5 (8%)	65,113,113	1.33	9 (13%)
22	CLA	b	615	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	b	616	-	56,73,73	1.10	4 (7%)	65,113,113	1.28	9 (13%)
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	1.10	4 (7%)	65,113,113	1.23	8 (12%)
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	1.10	2 (4%)	56,56,56	1.21	5 (8%)
24	BCR	b	621	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	7 (12%)
24	BCR	b	622	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	9 (16%)
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	1 (1%)	73,73,81	1.36	7 (9%)
27	LMG	b	625	-	49,49,55	0.79	1 (2%)	57,57,63	1.34	6 (10%)
31	LMT	b	626	-	36,36,36	1.13	5 (13%)	47,47,47	0.99	1 (2%)
31	LMT	b	627	-	36,36,36	1.10	5 (13%)	47,47,47	1.03	2 (4%)
27	LMG	b	628	-	49,49,55	0.77	0	57,57,63	1.32	4 (7%)
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	1.27	7 (10%)
22	CLA	c	503	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	8 (12%)
22	CLA	c	504	-	56,73,73	1.13	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	1.10	4 (7%)	65,113,113	1.26	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	1.10	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	1.11	4 (7%)	65,113,113	1.22	8 (12%)
22	CLA	c	510	3	56,73,73	1.11	4 (7%)	65,113,113	1.26	7 (10%)
22	CLA	c	511	-	56,73,73	1.11	4 (7%)	65,113,113	1.24	9 (13%)
22	CLA	c	512	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	10 (15%)
24	BCR	c	513	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	9 (16%)
24	BCR	c	514	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	8 (14%)
25	DGD	c	515	-	54,54,67	0.96	1 (1%)	68,68,81	1.31	7 (10%)
25	DGD	c	516	-	63,63,67	0.93	2 (3%)	77,77,81	1.48	14 (18%)
25	DGD	c	517	-	67,67,67	0.89	2 (2%)	81,81,81	1.43	10 (12%)
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.30	6 (11%)
26	LHG	c	519	-	36,36,48	0.72	1 (2%)	37,42,54	1.29	3 (8%)
22	CLA	c	520	-	56,73,73	1.10	4 (7%)	65,113,113	1.23	9 (13%)
24	BCR	c	521	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	7 (12%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.33	6 (10%)
32	PHO	d	401	-	67,69,69	1.22	8 (11%)	87,99,99	1.02	6 (6%)
30	SQD	d	402	-	42,43,54	1.05	3 (7%)	52,54,65	1.98	10 (19%)
33	BCT	d	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	404	-	56,73,73	1.13	4 (7%)	65,113,113	1.22	8 (12%)
22	CLA	d	405	-	56,73,73	1.11	4 (7%)	65,113,113	1.26	8 (12%)
23	PL9	d	406	-	55,55,55	1.00	3 (5%)	69,69,69	1.48	14 (20%)
27	LMG	d	407	-	48,48,55	0.77	0	56,56,63	1.41	4 (7%)
25	DGD	d	408	-	64,64,67	0.92	2 (3%)	78,78,81	1.35	10 (12%)
31	LMT	d	409	-	32,32,36	1.19	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	d	410	-	46,46,55	0.80	1 (2%)	54,54,63	1.33	6 (11%)
27	LMG	e	101	-	44,44,55	0.76	0	52,52,63	1.32	5 (9%)
34	HEM	f	101	5,6	28,50,50	2.22	6 (21%)	17,82,82	1.46	3 (17%)
24	BCR	f	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
30	SQD	f	103	-	44,45,54	1.04	5 (11%)	54,56,65	1.84	12 (22%)
24	BCR	g	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
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	0.83	0	51,51,63	1.29	4 (7%)
31	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	1 (2%)	45,45,69	1.51	7 (15%)
24	BCR	j	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.56	12 (21%)
27	LMG	m	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.28	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	v	201	16	28,50,50	2.25	6 (21%)	17,82,82	1.42	2 (11%)
24	BCR	x	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.16	2 (3%)
24	BCR	y	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	7 (12%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
31	LMT	B	622	-	-	0/21/61/61	0/2/2/2
31	LMT	B	623	-	-	0/21/61/61	0/2/2/2
27	LMG	B	624	-	-	0/44/64/70	0/1/1/1
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
30	SQD	B	626	-	-	0/42/62/69	0/1/1/1
31	LMT	B	627	-	-	0/21/61/61	0/2/2/2
31	LMT	B	628	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	C	513	-	-	0/29/63/63	0/2/2/2
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	DGD	C	515	-	-	0/42/82/95	0/2/2/2
25	DGD	C	516	-	-	1/51/91/95	0/2/2/2
25	DGD	C	517	-	-	0/55/95/95	0/2/2/2
27	LMG	C	518	-	-	0/40/60/70	0/1/1/1
26	LHG	C	519	-	-	0/41/41/53	0/0/0/0
22	CLA	C	520	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	C	521	-	-	0/29/63/63	0/2/2/2
27	LMG	C	522	-	-	0/43/63/70	0/1/1/1
32	PHO	D	401	-	-	0/53/103/103	0/1/6/6
32	PHO	D	402	-	-	0/53/103/103	0/1/6/6
30	SQD	D	403	-	-	1/38/58/69	0/1/1/1
33	BCT	D	404	21	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/43/63/70	0/1/1/1
25	DGD	D	409	-	-	0/52/92/95	0/2/2/2
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
24	BCR	D	411	-	-	0/29/63/63	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
30	SQD	F	102	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	H	102	-	-	0/29/63/63	0/2/2/2
27	LMG	I	101	-	-	0/38/58/70	0/1/1/1
31	LMT	I	102	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
24	BCR	J	102	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	-	0/37/57/70	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
30	SQD	a	401	-	-	0/49/69/69	0/1/1/1
27	LMG	a	402	-	-	0/37/57/70	0/1/1/1
22	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
32	PHO	a	407	-	-	0/53/103/103	0/1/6/6
22	CLA	a	408	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	a	409	-	-	0/41/61/73	0/1/1/1
24	BCR	a	410	-	-	0/29/63/63	0/2/2/2
25	DGD	a	411	-	-	0/45/85/95	0/2/2/2
26	LHG	a	412	-	-	0/43/43/53	0/0/0/0
27	LMG	a	413	-	-	0/46/66/70	0/1/1/1
29	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
30	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2
30	SQD	b	602	-	-	0/42/62/69	0/1/1/1
31	LMT	b	603	-	-	0/21/61/61	0/2/2/2
31	LMT	b	604	-	-	0/21/61/61	0/2/2/2
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	DGD	b	624	-	-	0/47/87/95	0/2/2/2
27	LMG	b	625	-	-	0/44/64/70	0/1/1/1
31	LMT	b	626	-	-	0/21/61/61	0/2/2/2
31	LMT	b	627	-	-	0/21/61/61	0/2/2/2
27	LMG	b	628	-	-	0/44/64/70	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	DGD	c	515	-	-	0/42/82/95	0/2/2/2
25	DGD	c	516	-	-	1/51/91/95	0/2/2/2
25	DGD	c	517	-	-	0/55/95/95	0/2/2/2
27	LMG	c	518	-	-	0/40/60/70	0/1/1/1
26	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	LMG	c	522	-	-	0/43/63/70	0/1/1/1
32	PHO	d	401	-	-	0/53/103/103	0/1/6/6
30	SQD	d	402	-	-	1/38/58/69	0/1/1/1
33	BCT	d	403	21	-	0/0/0/0	0/0/0/0
22	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	d	406	-	-	0/53/73/73	0/1/1/1
27	LMG	d	407	-	-	0/43/63/70	0/1/1/1
25	DGD	d	408	-	-	0/52/92/95	0/2/2/2
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
27	LMG	d	410	-	-	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
30	SQD	f	103	-	-	0/40/60/69	0/1/1/1
24	BCR	g	101	-	-	0/29/63/63	0/2/2/2
22	CLA	h	101	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LMG	i	101	-	-	0/38/58/70	0/1/1/1
31	LMT	i	102	-	-	0/21/61/61	0/2/2/2
23	PL9	j	101	-	-	0/29/49/73	0/1/1/1
24	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	LMG	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 (548) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	C3B-C2B	-5.10	1.33	1.40
34	F	101	HEM	C3B-C2B	-5.09	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.80	1.34	1.40
34	V	201	HEM	C3C-C2C	-4.76	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3B-C2B	-3.92	1.35	1.40
34	F	101	HEM	C3C-C2C	-3.92	1.35	1.40
34	V	201	HEM	C3B-C2B	-3.92	1.35	1.40
34	f	101	HEM	C3C-C2C	-3.86	1.35	1.40
23	d	406	PL9	C7-C3	-3.65	1.47	1.51
24	H	102	BCR	C1-C6	-3.64	1.48	1.53
24	y	101	BCR	C1-C6	-3.63	1.48	1.53
24	D	411	BCR	C1-C6	-3.57	1.48	1.53
22	b	614	CLA	CMB-C2B	-3.57	1.44	1.51
24	g	101	BCR	C1-C6	-3.54	1.48	1.53
24	f	102	BCR	C1-C6	-3.53	1.48	1.53
24	x	101	BCR	C1-C6	-3.52	1.49	1.53
22	B	610	CLA	CMB-C2B	-3.48	1.44	1.51
23	D	407	PL9	C7-C3	-3.41	1.47	1.51
24	C	513	BCR	C1-C6	-3.39	1.49	1.53
24	B	616	BCR	C1-C6	-3.35	1.49	1.53
24	b	620	BCR	C1-C6	-3.35	1.49	1.53
23	J	101	PL9	C7-C3	-3.33	1.47	1.51
24	C	514	BCR	C1-C6	-3.32	1.49	1.53
24	c	513	BCR	C1-C6	-3.31	1.49	1.53
24	c	514	BCR	C1-C6	-3.30	1.49	1.53
23	a	409	PL9	C7-C3	-3.25	1.48	1.51
24	b	622	BCR	C30-C25	-3.24	1.49	1.53
23	j	101	PL9	C7-C3	-3.22	1.48	1.51
24	y	101	BCR	C30-C25	-3.20	1.49	1.53
24	b	621	BCR	C1-C6	-3.18	1.49	1.53
24	g	101	BCR	C30-C25	-3.17	1.49	1.53
24	B	618	BCR	C30-C25	-3.16	1.49	1.53
24	B	619	BCR	C30-C25	-3.15	1.49	1.53
24	C	521	BCR	C30-C25	-3.13	1.49	1.53
24	b	623	BCR	C30-C25	-3.13	1.49	1.53
24	a	410	BCR	C1-C6	-3.12	1.49	1.53
24	b	620	BCR	C30-C25	-3.12	1.49	1.53
24	B	617	BCR	C1-C6	-3.12	1.49	1.53
24	c	521	BCR	C30-C25	-3.10	1.49	1.53
24	a	410	BCR	C30-C25	-3.10	1.49	1.53
24	A	407	BCR	C30-C25	-3.09	1.49	1.53
24	B	616	BCR	C30-C25	-3.09	1.49	1.53
24	b	623	BCR	C1-C6	-3.09	1.49	1.53
24	D	411	BCR	C30-C25	-3.09	1.49	1.53
24	B	618	BCR	C1-C6	-3.07	1.49	1.53
24	f	102	BCR	C30-C25	-3.06	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	622	BCR	C1-C6	-3.06	1.49	1.53
24	B	619	BCR	C1-C6	-3.06	1.49	1.53
24	A	407	BCR	C1-C6	-3.05	1.49	1.53
24	J	102	BCR	C30-C25	-3.03	1.49	1.53
24	j	102	BCR	C30-C25	-3.02	1.49	1.53
24	x	101	BCR	C30-C25	-3.01	1.49	1.53
24	C	513	BCR	C30-C25	-3.00	1.49	1.53
23	A	406	PL9	C7-C3	-2.98	1.48	1.51
24	j	102	BCR	C1-C6	-2.98	1.49	1.53
24	J	102	BCR	C1-C6	-2.98	1.49	1.53
24	c	514	BCR	C30-C25	-2.96	1.49	1.53
24	C	514	BCR	C30-C25	-2.95	1.49	1.53
24	C	521	BCR	C1-C6	-2.95	1.49	1.53
24	H	102	BCR	C30-C25	-2.93	1.49	1.53
24	c	521	BCR	C1-C6	-2.90	1.49	1.53
24	c	513	BCR	C30-C25	-2.78	1.50	1.53
24	B	617	BCR	C30-C25	-2.77	1.50	1.53
24	b	621	BCR	C30-C25	-2.75	1.50	1.53
22	c	507	CLA	CMB-C2B	-2.65	1.46	1.51
22	C	507	CLA	CMB-C2B	-2.65	1.46	1.51
31	b	627	LMT	O3'-C3'	-2.64	1.36	1.43
23	a	409	PL9	C3-C4	-2.63	1.45	1.49
31	M	102	LMT	O3'-C3'	-2.63	1.36	1.43
22	B	611	CLA	CMD-C2D	-2.62	1.46	1.51
31	B	623	LMT	O3'-C3'	-2.62	1.36	1.43
31	D	410	LMT	O3'-C3'	-2.61	1.36	1.43
31	d	409	LMT	O3'-C3'	-2.61	1.37	1.43
22	b	615	CLA	CMD-C2D	-2.59	1.46	1.51
31	M	103	LMT	O3'-C3'	-2.58	1.37	1.43
31	b	603	LMT	O3'-C3'	-2.57	1.37	1.43
31	I	102	LMT	O3'-C3'	-2.56	1.37	1.43
31	b	626	LMT	O3'-C3'	-2.55	1.37	1.43
22	a	404	CLA	CMB-C2B	-2.54	1.46	1.51
31	B	622	LMT	O3'-C3'	-2.54	1.37	1.43
22	A	403	CLA	CMB-C2B	-2.54	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.53	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.52	1.46	1.51
31	B	627	LMT	O3'-C3'	-2.52	1.37	1.43
22	C	505	CLA	CMB-C2B	-2.52	1.46	1.51
31	b	604	LMT	O3'-C3'	-2.52	1.37	1.43
22	B	603	CLA	CMB-C2B	-2.52	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	CMD-C2D	-2.52	1.46	1.51
31	i	102	LMT	O3'-C3'	-2.52	1.37	1.43
22	b	607	CLA	CMB-C2B	-2.52	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.52	1.46	1.51
22	A	404	CLA	CMB-C2B	-2.51	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.51	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.49	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.49	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.49	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.49	1.46	1.51
22	c	509	CLA	CMD-C2D	-2.49	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.48	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.48	1.46	1.51
22	C	504	CLA	CMD-C2D	-2.48	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.48	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.47	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.47	1.46	1.51
22	d	404	CLA	CMB-C2B	-2.47	1.46	1.51
22	h	101	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.47	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.47	1.46	1.51
22	a	408	CLA	CMB-C2B	-2.47	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.46	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.46	1.46	1.51
23	D	407	PL9	C3-C4	-2.46	1.45	1.49
22	B	614	CLA	CMB-C2B	-2.45	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.45	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.45	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.45	1.46	1.51
31	B	628	LMT	O3'-C3'	-2.45	1.37	1.43
31	I	102	LMT	O2'-C2'	-2.45	1.37	1.43
22	b	615	CLA	CMB-C2B	-2.45	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.45	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.44	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	611	CLA	CMD-C2D	-2.43	1.46	1.51
23	d	406	PL9	C3-C4	-2.43	1.45	1.49
22	D	406	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	603	CLA	CMD-C2D	-2.43	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.42	1.46	1.51
23	A	406	PL9	C3-C4	-2.42	1.45	1.49
22	c	510	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.42	1.46	1.51
25	C	515	DGD	O2G-C2G	-2.42	1.40	1.46
22	A	402	CLA	CMD-C2D	-2.42	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	613	CLA	CMB-C2B	-2.41	1.46	1.51
31	i	102	LMT	O2'-C2'	-2.41	1.37	1.43
22	a	404	CLA	CMD-C2D	-2.41	1.46	1.51
22	b	607	CLA	CMD-C2D	-2.40	1.46	1.51
31	M	102	LMT	O3B-C3B	-2.40	1.37	1.43
22	B	604	CLA	CMD-C2D	-2.38	1.46	1.51
31	B	628	LMT	O3B-C3B	-2.38	1.37	1.43
22	A	404	CLA	CMD-C2D	-2.37	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.37	1.46	1.51
22	b	608	CLA	CMD-C2D	-2.37	1.46	1.51
22	a	406	CLA	CMD-C2D	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	CMD-C2D	-2.36	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.36	1.46	1.51
22	B	602	CLA	CMD-C2D	-2.36	1.46	1.51
31	b	604	LMT	O3B-C3B	-2.36	1.37	1.43
31	b	627	LMT	O3B-C3B	-2.35	1.37	1.43
22	A	403	CLA	CMD-C2D	-2.35	1.46	1.51
22	C	503	CLA	CMD-C2D	-2.35	1.46	1.51
22	b	619	CLA	CMD-C2D	-2.35	1.46	1.51
22	a	405	CLA	CMD-C2D	-2.34	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.34	1.46	1.51
22	C	507	CLA	CMD-C2D	-2.34	1.46	1.51
30	b	602	SQD	O2-C2	-2.34	1.37	1.43
31	I	102	LMT	O2B-C2B	-2.34	1.37	1.43
22	a	408	CLA	CMD-C2D	-2.34	1.46	1.51
22	b	614	CLA	C3B-C2B	-2.34	1.37	1.40
31	M	103	LMT	O3B-C3B	-2.34	1.37	1.43
31	B	627	LMT	O2'-C2'	-2.34	1.37	1.43
22	c	507	CLA	CMD-C2D	-2.34	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.33	1.46	1.51
22	B	615	CLA	CMD-C2D	-2.33	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.33	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.33	1.46	1.51
31	b	603	LMT	O3B-C3B	-2.33	1.37	1.43
22	C	502	CLA	CMD-C2D	-2.33	1.46	1.51
22	H	101	CLA	CMD-C2D	-2.33	1.46	1.51
31	B	622	LMT	O3B-C3B	-2.32	1.37	1.43
22	b	605	CLA	CMD-C2D	-2.32	1.46	1.51
22	c	520	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.32	1.46	1.51
22	C	511	CLA	CMD-C2D	-2.32	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.32	1.46	1.51
30	B	626	SQD	O2-C2	-2.32	1.37	1.43
31	B	623	LMT	O3B-C3B	-2.32	1.37	1.43
22	B	605	CLA	CMD-C2D	-2.32	1.46	1.51
22	B	609	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.32	1.46	1.51
22	c	511	CLA	CMD-C2D	-2.32	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	606	CLA	CMD-C2D	-2.32	1.46	1.51
22	B	601	CLA	CMD-C2D	-2.31	1.46	1.51
22	c	501	CLA	CMD-C2D	-2.31	1.46	1.51
22	D	405	CLA	CMD-C2D	-2.31	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	CMD-C2D	-2.31	1.46	1.51
22	C	520	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.31	1.46	1.51
31	I	102	LMT	O3B-C3B	-2.31	1.37	1.43
22	B	613	CLA	CMD-C2D	-2.31	1.46	1.51
31	i	102	LMT	O2B-C2B	-2.31	1.37	1.43
22	b	616	CLA	CMD-C2D	-2.30	1.46	1.51
22	b	618	CLA	CMD-C2D	-2.30	1.46	1.51
22	B	612	CLA	CMD-C2D	-2.30	1.46	1.51
31	D	410	LMT	O3B-C3B	-2.30	1.37	1.43
22	c	512	CLA	CMD-C2D	-2.30	1.46	1.51
31	d	409	LMT	O3B-C3B	-2.30	1.37	1.43
22	D	406	CLA	CMD-C2D	-2.30	1.46	1.51
22	c	510	CLA	CMD-C2D	-2.30	1.46	1.51
22	h	101	CLA	CMD-C2D	-2.30	1.46	1.51
22	c	506	CLA	CMD-C2D	-2.30	1.46	1.51
22	C	506	CLA	CMD-C2D	-2.30	1.46	1.51
22	d	404	CLA	CMD-C2D	-2.30	1.46	1.51
22	d	405	CLA	CMD-C2D	-2.30	1.46	1.51
31	b	603	LMT	O2'-C2'	-2.29	1.37	1.43
31	M	102	LMT	O2'-C2'	-2.29	1.37	1.43
22	C	501	CLA	CMD-C2D	-2.29	1.46	1.51
22	c	505	CLA	CMD-C2D	-2.29	1.46	1.51
22	C	512	CLA	CMD-C2D	-2.28	1.46	1.51
22	b	613	CLA	CMD-C2D	-2.28	1.46	1.51
22	C	510	CLA	CMD-C2D	-2.28	1.46	1.51
31	b	626	LMT	O3B-C3B	-2.28	1.37	1.43
31	M	103	LMT	O2'-C2'	-2.28	1.37	1.43
31	i	102	LMT	O3B-C3B	-2.27	1.37	1.43
31	B	627	LMT	O3B-C3B	-2.27	1.37	1.43
22	B	610	CLA	C3B-C2B	-2.26	1.37	1.40
31	b	626	LMT	O2'-C2'	-2.26	1.37	1.43
31	b	604	LMT	O2'-C2'	-2.26	1.37	1.43
31	B	622	LMT	O2'-C2'	-2.26	1.37	1.43
32	D	401	PHO	C1C-NC	-2.26	1.33	1.38
23	D	407	PL9	C6-C1	-2.25	1.44	1.48
31	b	627	LMT	O2'-C2'	-2.24	1.37	1.43
31	B	628	LMT	O2'-C2'	-2.24	1.37	1.43
31	b	603	LMT	O2B-C2B	-2.24	1.37	1.43
31	B	627	LMT	O2B-C2B	-2.24	1.37	1.43
32	a	407	PHO	C1C-NC	-2.24	1.33	1.38
22	B	610	CLA	CMD-C2D	-2.24	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	402	PHO	C1C-NC	-2.22	1.33	1.38
31	M	102	LMT	O2B-C2B	-2.22	1.37	1.43
22	b	614	CLA	CMD-C2D	-2.22	1.46	1.51
31	M	103	LMT	O2B-C2B	-2.21	1.37	1.43
32	d	401	PHO	C1C-NC	-2.21	1.33	1.38
31	B	623	LMT	O2'-C2'	-2.20	1.37	1.43
25	c	515	DGD	O2G-C2G	-2.19	1.40	1.46
31	b	626	LMT	O2B-C2B	-2.18	1.37	1.43
31	M	102	LMT	O4'-C4B	-2.18	1.37	1.43
30	d	402	SQD	O2-C2	-2.18	1.37	1.43
30	b	602	SQD	O3-C3	-2.18	1.37	1.43
31	D	410	LMT	O2B-C2B	-2.17	1.38	1.43
30	B	626	SQD	O3-C3	-2.17	1.38	1.43
31	d	409	LMT	O2'-C2'	-2.17	1.38	1.43
31	B	628	LMT	O4'-C4B	-2.17	1.38	1.43
30	f	103	SQD	O2-C2	-2.17	1.38	1.43
31	B	628	LMT	O2B-C2B	-2.17	1.38	1.43
31	D	410	LMT	O2'-C2'	-2.16	1.38	1.43
31	b	603	LMT	O4'-C4B	-2.16	1.38	1.43
30	D	403	SQD	O2-C2	-2.15	1.38	1.43
30	F	102	SQD	O2-C2	-2.15	1.38	1.43
31	B	622	LMT	O2B-C2B	-2.15	1.38	1.43
30	A	413	SQD	O2-C2	-2.15	1.38	1.43
31	d	409	LMT	O2B-C2B	-2.15	1.38	1.43
23	a	409	PL9	C53-C6	-2.15	1.46	1.50
31	M	103	LMT	O4'-C4B	-2.14	1.38	1.43
31	b	604	LMT	O2B-C2B	-2.14	1.38	1.43
31	d	409	LMT	O4'-C4B	-2.14	1.38	1.43
30	a	401	SQD	O3-C3	-2.13	1.38	1.43
30	A	414	SQD	O3-C3	-2.13	1.38	1.43
31	b	604	LMT	O4'-C4B	-2.13	1.38	1.43
30	a	415	SQD	O2-C2	-2.13	1.38	1.43
23	A	406	PL9	C53-C6	-2.12	1.46	1.50
30	A	414	SQD	O2-C2	-2.11	1.38	1.43
31	B	627	LMT	O4'-C4B	-2.11	1.38	1.43
25	C	516	DGD	O2G-C2G	-2.11	1.41	1.46
31	I	102	LMT	O4'-C4B	-2.11	1.38	1.43
30	f	103	SQD	O3-C3	-2.10	1.38	1.43
30	a	401	SQD	O2-C2	-2.10	1.38	1.43
23	A	406	PL9	C6-C1	-2.10	1.44	1.48
31	B	623	LMT	O2B-C2B	-2.10	1.38	1.43
25	C	515	DGD	O1G-C1G	-2.10	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	410	LMT	O4'-C4B	-2.09	1.38	1.43
31	B	622	LMT	O4'-C4B	-2.09	1.38	1.43
31	b	626	LMT	O4'-C4B	-2.09	1.38	1.43
30	F	102	SQD	O3-C3	-2.07	1.38	1.43
31	b	627	LMT	O2B-C2B	-2.07	1.38	1.43
31	i	102	LMT	O4'-C4B	-2.06	1.38	1.43
27	D	412	LMG	O7-C8	-2.06	1.41	1.46
31	b	627	LMT	O4'-C4B	-2.06	1.38	1.43
25	d	408	DGD	O1G-C1G	-2.06	1.40	1.45
31	B	623	LMT	O4'-C4B	-2.05	1.38	1.43
30	a	415	SQD	O3-C3	-2.05	1.38	1.43
25	a	411	DGD	O1G-C1G	-2.05	1.40	1.45
30	A	413	SQD	O3-C3	-2.04	1.38	1.43
30	A	414	SQD	O4-C4	-2.04	1.38	1.43
30	F	102	SQD	O4-C4	-2.04	1.38	1.43
26	a	412	LHG	O7-C5	-2.03	1.41	1.46
30	a	401	SQD	O4-C4	-2.03	1.38	1.43
25	c	516	DGD	O2G-C2G	-2.03	1.41	1.46
25	c	516	DGD	O5D-C6D	-2.02	1.40	1.43
30	B	626	SQD	O4-C4	-2.02	1.38	1.43
23	d	406	PL9	C6-C1	-2.02	1.45	1.48
23	a	409	PL9	C6-C1	-2.02	1.45	1.48
27	d	410	LMG	O7-C8	-2.01	1.41	1.46
25	b	624	DGD	O2G-C2G	-2.01	1.41	1.46
30	b	602	SQD	O4-C4	-2.00	1.38	1.43
30	f	103	SQD	O4-C4	-2.00	1.38	1.43
27	D	412	LMG	C7-C8	2.02	1.56	1.50
26	c	519	LHG	P-O6	2.04	1.67	1.59
27	A	410	LMG	C7-C8	2.04	1.56	1.50
32	D	402	PHO	C4B-NB	2.05	1.41	1.36
32	d	401	PHO	C4B-NB	2.05	1.41	1.36
32	a	407	PHO	C4B-NB	2.06	1.41	1.36
32	D	401	PHO	C4B-NB	2.06	1.41	1.36
25	b	601	DGD	C1G-C2G	2.08	1.56	1.50
25	d	408	DGD	C1D-C2D	2.09	1.58	1.52
25	C	517	DGD	C3G-C2G	2.10	1.56	1.50
25	c	517	DGD	C1G-C2G	2.10	1.56	1.50
27	B	621	LMG	C4-C5	2.11	1.57	1.53
27	M	101	LMG	C7-C8	2.12	1.56	1.50
25	c	517	DGD	C3G-C2G	2.15	1.56	1.50
27	m	101	LMG	C7-C8	2.15	1.56	1.50
27	a	413	LMG	C7-C8	2.16	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	517	DGD	C1G-C2G	2.17	1.56	1.50
32	D	401	PHO	CHD-C1D	2.20	1.43	1.38
25	b	601	DGD	C4D-C5D	2.20	1.57	1.53
27	b	625	LMG	C4-C5	2.21	1.57	1.53
32	d	401	PHO	CHD-C1D	2.24	1.43	1.38
32	D	401	PHO	C4C-C3C	2.27	1.49	1.45
32	D	402	PHO	C4C-C3C	2.28	1.49	1.45
32	d	401	PHO	C4C-C3C	2.31	1.49	1.45
25	b	601	DGD	C3G-C2G	2.33	1.57	1.50
25	B	625	DGD	C4D-C5D	2.34	1.58	1.53
32	D	402	PHO	CHD-C1D	2.34	1.43	1.38
34	f	101	HEM	C4D-ND	2.36	1.39	1.36
25	B	625	DGD	C3G-C2G	2.36	1.57	1.50
34	F	101	HEM	C4D-ND	2.36	1.39	1.36
32	a	407	PHO	C4C-C3C	2.37	1.49	1.45
22	b	614	CLA	CHC-C1C	2.38	1.42	1.35
32	a	407	PHO	CHD-C1D	2.41	1.43	1.38
22	B	610	CLA	CHC-C1C	2.45	1.42	1.35
32	a	407	PHO	C1A-NA	2.48	1.42	1.37
32	D	401	PHO	C1A-NA	2.49	1.42	1.37
32	D	402	PHO	C1A-NA	2.52	1.42	1.37
32	d	401	PHO	C1A-NA	2.54	1.42	1.37
22	A	405	CLA	CHC-C1C	2.57	1.42	1.35
22	a	405	CLA	CHC-C1C	2.58	1.42	1.35
22	B	611	CLA	CHC-C1C	2.58	1.42	1.35
22	c	501	CLA	CHC-C1C	2.58	1.42	1.35
22	b	605	CLA	CHC-C1C	2.60	1.42	1.35
22	b	615	CLA	CHC-C1C	2.60	1.42	1.35
22	B	615	CLA	CHC-C1C	2.60	1.42	1.35
22	b	610	CLA	CHC-C1C	2.61	1.42	1.35
22	c	506	CLA	CHC-C1C	2.61	1.42	1.35
32	D	401	PHO	C4C-NC	2.61	1.42	1.36
22	C	503	CLA	CHC-C1C	2.62	1.42	1.35
34	V	201	HEM	C4D-ND	2.62	1.39	1.36
22	b	619	CLA	CHC-C1C	2.62	1.42	1.35
22	C	501	CLA	CHC-C1C	2.62	1.42	1.35
34	v	201	HEM	C4D-ND	2.62	1.39	1.36
22	b	609	CLA	CHC-C1C	2.62	1.42	1.35
22	C	507	CLA	CHC-C1C	2.62	1.42	1.35
22	C	520	CLA	CHC-C1C	2.62	1.42	1.35
22	B	601	CLA	CHC-C1C	2.62	1.42	1.35
22	A	403	CLA	CHC-C1C	2.63	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	401	PHO	C4C-NC	2.63	1.42	1.36
22	c	520	CLA	CHC-C1C	2.63	1.42	1.35
22	B	606	CLA	CHC-C1C	2.63	1.42	1.35
22	D	406	CLA	CHC-C1C	2.63	1.42	1.35
22	c	508	CLA	CHC-C1C	2.64	1.43	1.35
22	c	503	CLA	CHC-C1C	2.64	1.43	1.35
22	B	603	CLA	CHC-C1C	2.64	1.43	1.35
22	B	612	CLA	CHC-C1C	2.64	1.43	1.35
22	A	404	CLA	CHC-C1C	2.64	1.43	1.35
22	b	608	CLA	CHC-C1C	2.65	1.43	1.35
22	b	607	CLA	CHC-C1C	2.65	1.43	1.35
22	C	502	CLA	CHC-C1C	2.65	1.43	1.35
22	B	604	CLA	CHC-C1C	2.65	1.43	1.35
22	b	613	CLA	CHC-C1C	2.65	1.43	1.35
22	c	504	CLA	CHC-C1C	2.65	1.43	1.35
22	C	506	CLA	CHC-C1C	2.65	1.43	1.35
22	B	605	CLA	CHC-C1C	2.65	1.43	1.35
22	c	510	CLA	CHC-C1C	2.66	1.43	1.35
22	a	408	CLA	CHC-C1C	2.66	1.43	1.35
22	C	508	CLA	CHC-C1C	2.66	1.43	1.35
22	b	618	CLA	CHC-C1C	2.66	1.43	1.35
22	A	402	CLA	CHC-C1C	2.66	1.43	1.35
32	D	402	PHO	C4C-NC	2.66	1.42	1.36
22	B	614	CLA	CHC-C1C	2.66	1.43	1.35
22	C	510	CLA	CHC-C1C	2.66	1.43	1.35
22	a	406	CLA	CHC-C1C	2.66	1.43	1.35
22	B	602	CLA	CHC-C1C	2.66	1.43	1.35
22	c	505	CLA	CHC-C1C	2.66	1.43	1.35
22	B	609	CLA	CHC-C1C	2.67	1.43	1.35
22	C	511	CLA	CHC-C1C	2.67	1.43	1.35
22	b	616	CLA	CHC-C1C	2.67	1.43	1.35
22	C	504	CLA	CHC-C1C	2.68	1.43	1.35
22	c	509	CLA	CHC-C1C	2.68	1.43	1.35
22	C	505	CLA	CHC-C1C	2.68	1.43	1.35
32	a	407	PHO	C4C-NC	2.68	1.42	1.36
22	C	509	CLA	CHC-C1C	2.68	1.43	1.35
22	c	511	CLA	CHC-C1C	2.68	1.43	1.35
22	b	617	CLA	CHC-C1C	2.68	1.43	1.35
22	d	404	CLA	CHC-C1C	2.69	1.43	1.35
22	c	507	CLA	CHC-C1C	2.69	1.43	1.35
22	c	512	CLA	CHC-C1C	2.70	1.43	1.35
22	b	606	CLA	CHC-C1C	2.70	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	405	CLA	CHC-C1C	2.70	1.43	1.35
22	C	512	CLA	CHC-C1C	2.70	1.43	1.35
22	d	405	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	2.71	1.43	1.35
22	b	611	CLA	CHC-C1C	2.71	1.43	1.35
22	B	607	CLA	CHC-C1C	2.71	1.43	1.35
22	H	101	CLA	CHC-C1C	2.73	1.43	1.35
22	b	612	CLA	CHC-C1C	2.73	1.43	1.35
22	B	608	CLA	CHC-C1C	2.74	1.43	1.35
22	h	101	CLA	CHC-C1C	2.75	1.43	1.35
30	f	103	SQD	O47-C7	2.76	1.42	1.34
30	B	626	SQD	O47-C7	2.76	1.42	1.34
22	B	613	CLA	CHC-C1C	2.77	1.43	1.35
30	b	602	SQD	O47-C7	2.77	1.42	1.34
30	a	415	SQD	O47-C7	2.81	1.42	1.34
30	A	413	SQD	O47-C7	2.81	1.42	1.34
30	a	401	SQD	O47-C7	2.82	1.42	1.34
30	F	102	SQD	O47-C7	2.83	1.42	1.34
30	d	402	SQD	O47-C7	2.83	1.42	1.34
25	B	625	DGD	C1E-C2E	2.84	1.60	1.52
30	D	403	SQD	O47-C7	2.85	1.42	1.34
30	A	414	SQD	O47-C7	2.86	1.42	1.34
32	d	401	PHO	CHC-C1C	2.86	1.44	1.38
32	D	401	PHO	CHC-C1C	2.89	1.44	1.38
25	b	601	DGD	C1E-C2E	2.91	1.60	1.52
32	a	407	PHO	CHC-C1C	2.94	1.44	1.38
32	D	402	PHO	CHC-C1C	3.03	1.44	1.38
30	A	413	SQD	O48-C23	3.08	1.42	1.33
30	F	102	SQD	O48-C23	3.09	1.42	1.33
32	d	401	PHO	C3B-C4B	3.09	1.49	1.43
30	D	403	SQD	O48-C23	3.10	1.42	1.33
30	a	415	SQD	O48-C23	3.10	1.42	1.33
30	B	626	SQD	O48-C23	3.11	1.42	1.33
30	f	103	SQD	O48-C23	3.11	1.42	1.33
30	b	602	SQD	O48-C23	3.13	1.42	1.33
30	d	402	SQD	O48-C23	3.15	1.42	1.33
30	a	401	SQD	O48-C23	3.15	1.42	1.33
30	A	414	SQD	O48-C23	3.15	1.42	1.33
32	D	401	PHO	C3B-C4B	3.17	1.50	1.43
32	a	407	PHO	C3B-C4B	3.23	1.50	1.43
32	D	402	PHO	C3B-C4B	3.27	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	C3B-CAB	3.63	1.55	1.47
34	F	101	HEM	C3B-CAB	3.68	1.55	1.47
34	v	201	HEM	C3C-CAC	3.88	1.55	1.47
34	V	201	HEM	C3C-CAC	3.90	1.55	1.47
34	v	201	HEM	C3B-CAB	3.91	1.55	1.47
34	V	201	HEM	C3B-CAB	3.93	1.55	1.47
22	c	505	CLA	CHB-C4A	3.94	1.38	1.33
34	F	101	HEM	C3C-CAC	3.94	1.55	1.47
22	a	404	CLA	CHB-C4A	3.96	1.38	1.33
22	B	610	CLA	CHB-C4A	3.97	1.38	1.33
22	a	405	CLA	CHB-C4A	3.98	1.38	1.33
22	A	403	CLA	CHB-C4A	3.98	1.38	1.33
22	C	505	CLA	CHB-C4A	3.99	1.38	1.33
22	b	606	CLA	CHB-C4A	4.00	1.38	1.33
22	A	402	CLA	CHB-C4A	4.00	1.38	1.33
34	f	101	HEM	C3C-CAC	4.01	1.55	1.47
22	A	404	CLA	CHB-C4A	4.01	1.38	1.33
22	C	520	CLA	CHB-C4A	4.01	1.38	1.33
22	c	507	CLA	CHB-C4A	4.02	1.38	1.33
22	b	611	CLA	CHB-C4A	4.02	1.38	1.33
22	c	506	CLA	CHB-C4A	4.03	1.38	1.33
22	B	609	CLA	CHB-C4A	4.03	1.38	1.33
22	C	506	CLA	CHB-C4A	4.04	1.38	1.33
22	b	614	CLA	CHB-C4A	4.04	1.38	1.33
22	c	509	CLA	CHB-C4A	4.04	1.38	1.33
22	C	508	CLA	CHB-C4A	4.05	1.38	1.33
22	a	406	CLA	CHB-C4A	4.06	1.38	1.33
22	D	406	CLA	CHB-C4A	4.06	1.38	1.33
22	c	508	CLA	CHB-C4A	4.07	1.38	1.33
22	d	405	CLA	CHB-C4A	4.08	1.38	1.33
22	a	408	CLA	CHB-C4A	4.09	1.38	1.33
22	B	602	CLA	CHB-C4A	4.09	1.38	1.33
22	b	608	CLA	CHB-C4A	4.10	1.38	1.33
22	B	612	CLA	CHB-C4A	4.10	1.38	1.33
22	b	610	CLA	CHB-C4A	4.10	1.38	1.33
22	h	101	CLA	CHB-C4A	4.10	1.38	1.33
22	C	509	CLA	CHB-C4A	4.11	1.38	1.33
22	c	520	CLA	CHB-C4A	4.11	1.38	1.33
22	A	405	CLA	CHB-C4A	4.12	1.38	1.33
22	B	606	CLA	CHB-C4A	4.12	1.38	1.33
22	b	612	CLA	CHB-C4A	4.13	1.38	1.33
22	B	608	CLA	CHB-C4A	4.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CHB-C4A	4.14	1.38	1.33
22	B	601	CLA	CHB-C4A	4.14	1.38	1.33
22	B	605	CLA	CHB-C4A	4.15	1.38	1.33
22	b	613	CLA	CHB-C4A	4.16	1.38	1.33
22	B	615	CLA	CHB-C4A	4.17	1.38	1.33
22	C	511	CLA	CHB-C4A	4.17	1.38	1.33
22	b	616	CLA	CHB-C4A	4.18	1.38	1.33
22	c	512	CLA	CHB-C4A	4.18	1.38	1.33
22	b	618	CLA	CHB-C4A	4.19	1.38	1.33
22	b	615	CLA	CHB-C4A	4.20	1.38	1.33
22	C	512	CLA	CHB-C4A	4.20	1.38	1.33
22	B	614	CLA	CHB-C4A	4.20	1.38	1.33
22	b	605	CLA	CHB-C4A	4.20	1.38	1.33
22	C	507	CLA	CHB-C4A	4.21	1.38	1.33
22	b	609	CLA	CHB-C4A	4.22	1.38	1.33
22	b	619	CLA	CHB-C4A	4.22	1.38	1.33
22	C	503	CLA	CHB-C4A	4.22	1.38	1.33
22	H	101	CLA	CHB-C4A	4.23	1.38	1.33
22	c	502	CLA	CHB-C4A	4.23	1.38	1.33
22	B	611	CLA	CHB-C4A	4.24	1.38	1.33
22	c	510	CLA	CHB-C4A	4.24	1.38	1.33
22	C	502	CLA	CHB-C4A	4.25	1.38	1.33
22	c	511	CLA	CHB-C4A	4.25	1.38	1.33
22	B	604	CLA	CHB-C4A	4.26	1.39	1.33
22	C	510	CLA	CHB-C4A	4.26	1.39	1.33
22	c	501	CLA	CHB-C4A	4.26	1.39	1.33
22	B	613	CLA	CHB-C4A	4.26	1.39	1.33
22	C	504	CLA	CHB-C4A	4.28	1.39	1.33
22	C	501	CLA	CHB-C4A	4.28	1.39	1.33
22	c	503	CLA	CHB-C4A	4.29	1.39	1.33
22	b	617	CLA	CHB-C4A	4.31	1.39	1.33
22	B	603	CLA	CHB-C4A	4.33	1.39	1.33
22	b	607	CLA	CHB-C4A	4.38	1.39	1.33
22	c	504	CLA	CHB-C4A	4.40	1.39	1.33
22	D	405	CLA	CHB-C4A	4.50	1.39	1.33
22	d	404	CLA	CHB-C4A	4.50	1.39	1.33
34	f	101	HEM	C3D-C2D	5.42	1.53	1.37
34	F	101	HEM	C3D-C2D	5.46	1.53	1.37
34	V	201	HEM	C3D-C2D	5.64	1.54	1.37
34	v	201	HEM	C3D-C2D	5.64	1.54	1.37

All (1222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	DGD	O3G-C3G-C2G	-4.75	99.69	110.99
25	a	411	DGD	O3G-C3G-C2G	-4.74	99.70	110.99
22	B	610	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
25	C	517	DGD	O3G-C3G-C2G	-4.47	100.36	110.99
22	b	614	CLA	CMB-C2B-C1B	-4.44	121.63	128.46
27	d	407	LMG	C1-C2-C3	-4.34	101.92	109.98
27	D	408	LMG	C1-C2-C3	-4.28	102.02	109.98
25	c	517	DGD	O3G-C3G-C2G	-4.19	101.01	110.99
22	C	507	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
22	c	507	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
25	c	516	DGD	O5D-C6D-C5D	-4.16	101.98	108.94
22	B	612	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
22	b	616	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
22	b	611	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
25	C	516	DGD	O5D-C6D-C5D	-3.86	102.48	108.94
22	B	607	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
30	D	403	SQD	O9-S-O7	-3.76	100.83	113.86
30	d	402	SQD	O9-S-O7	-3.76	100.84	113.86
30	f	103	SQD	O9-S-O7	-3.75	100.86	113.86
30	F	102	SQD	O9-S-O7	-3.74	100.89	113.86
22	c	510	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
30	A	413	SQD	O9-S-O7	-3.72	100.98	113.86
22	B	602	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
30	a	415	SQD	O9-S-O7	-3.70	101.04	113.86
22	b	617	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	B	609	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
30	b	602	SQD	O9-S-O7	-3.69	101.07	113.86
25	c	516	DGD	O3G-C3G-C2G	-3.69	102.22	110.99
22	B	613	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
30	B	626	SQD	O9-S-O7	-3.69	101.09	113.86
22	b	606	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	b	615	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
25	C	516	DGD	O3G-C3G-C2G	-3.68	102.23	110.99
25	d	408	DGD	O6D-C1D-O3G	-3.68	101.28	110.02
22	c	505	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	B	611	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
30	a	401	SQD	O9-S-O7	-3.67	101.16	113.86
22	C	512	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
22	C	506	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
25	D	409	DGD	O6D-C1D-O3G	-3.64	101.37	110.02
22	A	402	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
30	A	414	SQD	O9-S-O7	-3.63	101.27	113.86
22	c	506	CLA	CMB-C2B-C1B	-3.63	122.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	c	512	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
22	C	505	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
22	c	502	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
22	a	408	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
24	J	102	BCR	C11-C10-C9	-3.60	122.18	127.31
22	C	510	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
22	b	613	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	c	503	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
22	a	404	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
22	C	502	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	c	511	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	c	515	DGD	O3G-C3G-C2G	-3.51	102.64	110.99
25	C	515	DGD	O3G-C3G-C2G	-3.51	102.65	110.99
22	b	605	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
30	A	414	SQD	C5-C6-S	-3.50	109.47	114.34
22	B	601	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	C	520	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
24	J	102	BCR	C3-C4-C5	-3.47	107.82	113.78
22	B	614	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
22	c	520	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	c	509	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	d	405	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	b	618	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	A	403	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	C	509	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	A	404	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	B	620	DGD	O3G-C3G-C2G	-3.43	102.82	110.99
22	D	406	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
22	B	603	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
22	a	405	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	B	605	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
24	j	102	BCR	C24-C23-C22	-3.41	121.09	126.21
23	j	101	PL9	C7-C3-C2	-3.40	118.40	123.23
22	b	607	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
24	j	102	BCR	C3-C4-C5	-3.39	107.94	113.78
25	c	517	DGD	C1D-C2D-C3D	-3.39	103.68	109.98
24	j	102	BCR	C11-C10-C9	-3.39	122.48	127.31
22	b	608	CLA	CMB-C2B-C1B	-3.37	123.28	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
23	J	101	PL9	C7-C3-C2	-3.37	118.44	123.23
22	d	404	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
22	h	101	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	H	101	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
22	D	405	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
25	b	624	DGD	O3G-C3G-C2G	-3.33	103.07	110.99
22	C	508	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	b	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	C	517	DGD	C1D-C2D-C3D	-3.31	103.83	109.98
22	a	406	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
25	d	408	DGD	O3G-C3G-C2G	-3.29	103.16	110.99
25	B	625	DGD	C1D-C2D-C3D	-3.28	103.88	109.98
22	b	619	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
25	b	601	DGD	C1D-C2D-C3D	-3.26	103.91	109.98
31	B	628	LMT	C1'-O5'-C5'	-3.25	107.59	113.72
23	d	406	PL9	C7-C3-C2	-3.25	118.61	123.23
22	B	606	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	B	608	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
22	b	612	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
24	J	102	BCR	C24-C23-C22	-3.21	121.39	126.21
25	D	409	DGD	O3G-C3G-C2G	-3.19	103.40	110.99
25	b	624	DGD	O6D-C1D-O3G	-3.19	102.46	110.02
23	D	407	PL9	C7-C3-C2	-3.18	118.71	123.23
23	A	406	PL9	C7-C3-C2	-3.17	118.73	123.23
25	c	516	DGD	O6D-C1D-O3G	-3.15	102.53	110.02
22	B	603	CLA	O2D-CGD-O1D	-3.15	117.48	123.82
22	c	503	CLA	O2D-CGD-O1D	-3.14	117.50	123.82
31	b	604	LMT	C1'-O5'-C5'	-3.11	107.85	113.72
25	B	620	DGD	O6D-C1D-O3G	-3.11	102.64	110.02
22	b	606	CLA	O2D-CGD-O1D	-3.10	117.58	123.82
22	b	609	CLA	O2D-CGD-O1D	-3.09	117.60	123.82
22	B	613	CLA	O2D-CGD-O1D	-3.09	117.60	123.82
22	c	507	CLA	O2D-CGD-O1D	-3.09	117.60	123.82
25	A	408	DGD	O6D-C1D-O3G	-3.08	102.70	110.02
22	B	605	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
22	b	617	CLA	O2D-CGD-O1D	-3.06	117.66	123.82
23	a	409	PL9	C7-C3-C2	-3.06	118.88	123.23
22	C	504	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
22	c	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	BCR	C15-C14-C13	-3.05	122.96	127.31
31	B	623	LMT	C3'-C4'-C5'	-3.04	104.42	110.88
24	J	102	BCR	C7-C8-C9	-3.04	121.64	126.21
25	C	517	DGD	O5D-C6D-C5D	-3.03	103.87	108.94
25	C	516	DGD	O6D-C1D-O3G	-3.03	102.84	110.02
22	C	502	CLA	O2D-CGD-O1D	-3.03	117.73	123.82
24	g	101	BCR	C33-C5-C6	-3.02	121.13	124.51
22	C	504	CLA	O2D-CGD-O1D	-3.00	117.78	123.82
22	C	503	CLA	O2D-CGD-O1D	-3.00	117.79	123.82
24	b	622	BCR	C24-C23-C22	-3.00	121.71	126.21
24	j	102	BCR	C7-C8-C9	-2.99	121.73	126.21
22	B	604	CLA	O2D-CGD-O1D	-2.98	117.82	123.82
25	c	515	DGD	O6D-C1D-O3G	-2.98	102.94	110.02
22	C	505	CLA	O2D-CGD-O1D	-2.96	117.86	123.82
22	b	607	CLA	O2D-CGD-O1D	-2.96	117.86	123.82
31	b	627	LMT	C3'-C4'-C5'	-2.96	104.59	110.88
27	E	101	LMG	C1-C2-C3	-2.96	104.47	109.98
24	j	102	BCR	C15-C14-C13	-2.96	123.09	127.31
22	b	610	CLA	O2D-CGD-O1D	-2.96	117.87	123.82
22	c	504	CLA	O2D-CGD-O1D	-2.96	117.87	123.82
24	y	101	BCR	C33-C5-C6	-2.96	121.20	124.51
22	c	502	CLA	O2D-CGD-O1D	-2.94	117.91	123.82
22	B	606	CLA	O2D-CGD-O1D	-2.93	117.92	123.82
24	H	102	BCR	C33-C5-C6	-2.93	121.23	124.51
22	B	608	CLA	O2D-CGD-O1D	-2.92	117.94	123.82
25	C	515	DGD	O6D-C1D-O3G	-2.92	103.08	110.02
25	a	411	DGD	O6D-C1D-O3G	-2.92	103.08	110.02
22	C	507	CLA	O2D-CGD-O1D	-2.92	117.95	123.82
25	c	517	DGD	O5D-C6D-C5D	-2.92	104.06	108.94
22	b	612	CLA	O2D-CGD-O1D	-2.91	117.96	123.82
22	b	605	CLA	O2D-CGD-O1D	-2.90	117.98	123.82
22	c	505	CLA	O2D-CGD-O1D	-2.90	117.99	123.82
22	B	602	CLA	O2D-CGD-O1D	-2.90	117.99	123.82
27	b	628	LMG	O6-C1-O1	-2.90	103.14	110.02
25	b	601	DGD	O3G-C3G-C2G	-2.90	104.09	110.99
25	b	601	DGD	C3G-C2G-C1G	-2.89	105.33	111.86
22	b	611	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
30	a	415	SQD	C5-C6-S	-2.89	110.32	114.34
22	b	608	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
24	x	101	BCR	C33-C5-C6	-2.87	121.30	124.51
22	C	510	CLA	O2D-CGD-O1D	-2.86	118.07	123.82
24	B	617	BCR	C15-C16-C17	-2.86	117.37	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	101	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
24	B	617	BCR	C15-C14-C13	-2.85	123.24	127.31
25	B	625	DGD	C3G-C2G-C1G	-2.85	105.43	111.86
22	a	406	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
24	D	411	BCR	C33-C5-C6	-2.85	121.32	124.51
27	B	624	LMG	O6-C1-O1	-2.85	103.26	110.02
22	a	404	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
25	c	517	DGD	C1D-O6D-C5D	-2.84	108.36	113.72
22	c	511	CLA	O2D-CGD-O1D	-2.84	118.10	123.82
25	C	517	DGD	C1D-O6D-C5D	-2.84	108.37	113.72
22	c	501	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
22	C	501	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
22	C	506	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
27	b	625	LMG	C1-C2-C3	-2.83	104.72	109.98
25	C	517	DGD	CDB-CCB-CBB	-2.83	99.90	114.45
22	B	601	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
25	c	517	DGD	CDB-CCB-CBB	-2.82	99.92	114.45
22	B	607	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
25	B	625	DGD	O3G-C3G-C2G	-2.82	104.28	110.99
22	b	613	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
24	J	102	BCR	C15-C14-C13	-2.82	123.29	127.31
22	c	506	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
22	A	403	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
22	B	612	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
24	f	102	BCR	C33-C5-C6	-2.81	121.36	124.51
22	D	406	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
22	c	520	CLA	O2D-CGD-O1D	-2.81	118.18	123.82
22	c	512	CLA	O2D-CGD-O1D	-2.81	118.18	123.82
24	B	617	BCR	C33-C5-C6	-2.80	121.37	124.51
22	A	402	CLA	O2D-CGD-O1D	-2.80	118.18	123.82
27	M	101	LMG	C1-C2-C3	-2.80	104.77	109.98
22	b	616	CLA	O2D-CGD-O1D	-2.80	118.18	123.82
25	c	516	DGD	CDB-CCB-CBB	-2.80	100.05	114.45
22	C	501	CLA	O2D-CGD-O1D	-2.80	118.19	123.82
27	B	621	LMG	C1-C2-C3	-2.79	104.79	109.98
22	B	614	CLA	O2D-CGD-O1D	-2.78	118.22	123.82
22	c	510	CLA	O2D-CGD-O1D	-2.78	118.23	123.82
24	b	620	BCR	C33-C5-C6	-2.78	121.40	124.51
24	y	101	BCR	C7-C8-C9	-2.77	122.04	126.21
22	C	520	CLA	O2D-CGD-O1D	-2.77	118.24	123.82
24	b	621	BCR	C15-C16-C17	-2.77	117.54	123.46
22	A	404	CLA	O2D-CGD-O1D	-2.77	118.24	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	516	DGD	CDB-CCB-CBB	-2.77	100.18	114.45
22	d	405	CLA	O2D-CGD-O1D	-2.76	118.26	123.82
24	B	616	BCR	C33-C5-C6	-2.76	121.42	124.51
23	J	101	PL9	C7-C8-C9	-2.76	122.10	126.71
25	A	408	DGD	O5D-C6D-C5D	-2.75	104.33	108.94
22	C	511	CLA	O2D-CGD-O1D	-2.75	118.28	123.82
22	d	404	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
22	c	501	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
24	b	621	BCR	C33-C5-C6	-2.73	121.45	124.51
22	b	618	CLA	O2D-CGD-O1D	-2.73	118.34	123.82
22	B	609	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
22	D	405	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
22	a	408	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
32	D	402	PHO	O2D-CGD-O1D	-2.72	118.34	123.82
22	h	101	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
23	d	406	PL9	C7-C8-C9	-2.71	122.18	126.71
24	y	101	BCR	C38-C26-C25	-2.70	121.48	124.51
27	C	518	LMG	O6-C1-O1	-2.70	103.60	110.02
22	C	512	CLA	O2D-CGD-O1D	-2.70	118.39	123.82
27	A	410	LMG	C1-C2-C3	-2.70	104.96	109.98
31	M	102	LMT	C1'-O5'-C5'	-2.70	108.64	113.72
30	a	401	SQD	C5-C6-S	-2.69	110.59	114.34
22	b	614	CLA	O2D-CGD-O1D	-2.69	118.42	123.82
23	D	407	PL9	C7-C8-C9	-2.69	122.22	126.71
25	D	409	DGD	CDB-CCB-CBB	-2.68	100.62	114.45
23	j	101	PL9	C7-C8-C9	-2.68	122.23	126.71
27	c	518	LMG	O6-C1-O1	-2.68	103.66	110.02
31	b	626	LMT	C1'-O5'-C5'	-2.68	108.67	113.72
24	B	618	BCR	C24-C23-C22	-2.67	122.19	126.21
24	g	101	BCR	C38-C26-C25	-2.67	121.51	124.51
25	d	408	DGD	C3G-C2G-C1G	-2.67	105.83	111.86
22	c	509	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
24	c	514	BCR	C11-C10-C9	-2.67	123.50	127.31
22	a	405	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
25	d	408	DGD	CDB-CCB-CBB	-2.67	100.71	114.45
27	I	101	LMG	O6-C1-O1	-2.66	103.71	110.02
22	A	405	CLA	O2D-CGD-O1D	-2.66	118.47	123.82
27	e	101	LMG	C1-C2-C3	-2.66	105.04	109.98
24	b	621	BCR	C28-C27-C26	-2.66	109.21	113.78
27	m	101	LMG	O2-C2-C1	-2.66	104.47	110.03
24	g	101	BCR	C7-C8-C9	-2.65	122.22	126.21
27	D	408	LMG	O6-C1-C2	-2.65	105.18	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	622	LMT	C1'-O5'-C5'	-2.65	108.72	113.72
25	B	620	DGD	C1D-C2D-C3D	-2.65	105.06	109.98
23	D	407	PL9	C22-C23-C24	-2.65	121.03	127.68
27	i	101	LMG	O6-C1-O1	-2.64	103.76	110.02
24	b	623	BCR	C7-C8-C9	-2.64	122.25	126.21
32	D	401	PHO	O2D-CGD-O1D	-2.64	118.52	123.82
22	C	509	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
27	a	413	LMG	C1-C2-C3	-2.63	105.09	109.98
24	b	622	BCR	C11-C10-C9	-2.63	123.56	127.31
24	B	617	BCR	C28-C27-C26	-2.62	109.27	113.78
24	B	618	BCR	C11-C10-C9	-2.62	123.56	127.31
22	b	619	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
32	d	401	PHO	O2D-CGD-O1D	-2.62	118.55	123.82
31	M	102	LMT	C3'-C4'-C5'	-2.62	105.32	110.88
27	B	624	LMG	O2-C2-C1	-2.62	104.55	110.03
24	c	514	BCR	C28-C27-C26	-2.62	109.28	113.78
24	C	514	BCR	C15-C16-C17	-2.62	117.88	123.46
24	j	102	BCR	C33-C5-C6	-2.61	121.59	124.51
32	a	407	PHO	O2D-CGD-O1D	-2.61	118.58	123.82
22	B	610	CLA	O2D-CGD-O1D	-2.61	118.58	123.82
27	i	101	LMG	O2-C2-C1	-2.60	104.58	110.03
24	c	521	BCR	C15-C16-C17	-2.60	117.91	123.46
25	a	411	DGD	O5D-C6D-C5D	-2.60	104.60	108.94
24	C	514	BCR	C28-C27-C26	-2.60	109.32	113.78
23	A	406	PL9	C22-C23-C24	-2.59	121.17	127.68
34	F	101	HEM	C1D-C2D-C3D	-2.59	105.19	107.00
24	J	102	BCR	C33-C5-C6	-2.59	121.61	124.51
32	D	402	PHO	CBD-CHA-C4D	-2.59	105.62	108.54
27	D	412	LMG	C1-C2-C3	-2.58	105.17	109.98
27	m	101	LMG	C1-C2-C3	-2.58	105.18	109.98
27	C	522	LMG	O2-C2-C1	-2.58	104.63	110.03
24	C	513	BCR	C24-C23-C22	-2.58	122.34	126.21
24	c	513	BCR	C7-C8-C9	-2.57	122.35	126.21
24	J	102	BCR	C35-C13-C14	-2.57	119.33	122.92
23	a	409	PL9	C22-C23-C24	-2.57	121.23	127.68
25	C	515	DGD	C1D-C2D-C3D	-2.56	105.21	109.98
31	D	410	LMT	C1'-O5'-C5'	-2.56	108.89	113.72
31	M	103	LMT	C3'-C4'-C5'	-2.56	105.44	110.88
23	d	406	PL9	C22-C23-C24	-2.56	121.25	127.68
25	c	516	DGD	C3G-C2G-C1G	-2.56	106.09	111.86
24	c	514	BCR	C15-C14-C13	-2.56	123.66	127.31
25	d	408	DGD	C3D-C4D-C5D	-2.55	105.72	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	401	PHO	CBD-CHA-C4D	-2.55	105.66	108.54
30	A	413	SQD	C5-C6-S	-2.55	110.78	114.34
27	c	522	LMG	O2-C2-C1	-2.55	104.69	110.03
24	B	618	BCR	C15-C14-C13	-2.55	123.68	127.31
27	b	628	LMG	O2-C2-C1	-2.54	104.71	110.03
24	C	521	BCR	C15-C16-C17	-2.54	118.04	123.46
25	b	624	DGD	C1D-C2D-C3D	-2.54	105.26	109.98
24	B	619	BCR	C7-C8-C9	-2.54	122.40	126.21
27	I	101	LMG	O2-C2-C1	-2.54	104.72	110.03
25	c	516	DGD	O6E-C1E-O5D	-2.54	104.00	110.02
32	a	407	PHO	CBD-CHA-C4D	-2.53	105.69	108.54
31	b	603	LMT	C1'-O5'-C5'	-2.53	108.95	113.72
27	M	101	LMG	O2-C2-C1	-2.53	104.74	110.03
25	a	411	DGD	C1D-C2D-C3D	-2.53	105.28	109.98
23	a	409	PL9	C7-C8-C9	-2.53	122.49	126.71
23	J	101	PL9	C22-C23-C24	-2.52	121.35	127.68
31	M	103	LMT	C1'-O5'-C5'	-2.52	108.97	113.72
34	f	101	HEM	C1D-C2D-C3D	-2.52	105.24	107.00
31	d	409	LMT	C3'-C4'-C5'	-2.51	105.54	110.88
32	d	401	PHO	CBD-CHA-C4D	-2.51	105.71	108.54
25	c	515	DGD	C3G-C2G-C1G	-2.51	106.19	111.86
24	c	513	BCR	C11-C10-C9	-2.50	123.74	127.31
24	C	513	BCR	C15-C14-C13	-2.50	123.74	127.31
27	A	410	LMG	O3-C3-C2	-2.50	104.92	110.36
24	c	521	BCR	C15-C14-C13	-2.50	123.74	127.31
23	j	101	PL9	C22-C23-C24	-2.50	121.41	127.68
24	C	514	BCR	C33-C5-C6	-2.50	121.72	124.51
24	C	514	BCR	C15-C14-C13	-2.49	123.75	127.31
25	c	515	DGD	O5D-C6D-C5D	-2.49	104.77	108.94
22	B	615	CLA	O2D-CGD-O1D	-2.49	118.81	123.82
24	C	521	BCR	C15-C14-C13	-2.48	123.76	127.31
34	f	101	HEM	CBD-CAD-C3D	-2.48	107.73	112.47
25	D	409	DGD	CFB-CEB-CDB	-2.48	101.67	114.45
24	c	514	BCR	C15-C16-C17	-2.48	118.17	123.46
25	D	409	DGD	C3G-C2G-C1G	-2.48	106.26	111.86
25	C	515	DGD	C3G-C2G-C1G	-2.48	106.26	111.86
24	j	102	BCR	C15-C16-C17	-2.48	118.17	123.46
24	b	622	BCR	C15-C14-C13	-2.48	123.77	127.31
24	C	513	BCR	C8-C7-C6	-2.48	120.31	127.25
24	a	410	BCR	C33-C5-C6	-2.48	121.73	124.51
22	B	606	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
22	c	508	CLA	O2D-CGD-O1D	-2.47	118.84	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	627	LMT	C1'-O5'-C5'	-2.47	109.06	113.72
31	i	102	LMT	C1'-O5'-C5'	-2.47	109.06	113.72
27	d	410	LMG	C1-C2-C3	-2.47	105.39	109.98
25	C	516	DGD	C3G-C2G-C1G	-2.47	106.29	111.86
27	a	402	LMG	O6-C1-O1	-2.46	104.18	110.02
22	b	615	CLA	O2D-CGD-O1D	-2.46	118.87	123.82
24	c	514	BCR	C33-C5-C6	-2.46	121.76	124.51
22	c	505	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
24	c	513	BCR	C8-C7-C6	-2.46	120.37	127.25
24	c	513	BCR	C15-C14-C13	-2.46	123.81	127.31
24	C	513	BCR	C15-C16-C17	-2.45	118.22	123.46
27	d	407	LMG	O6-C1-C2	-2.45	105.56	110.30
27	C	518	LMG	O2-C2-C1	-2.45	104.90	110.03
27	d	410	LMG	C38-C37-C36	-2.45	101.83	114.45
30	f	103	SQD	C5-C6-S	-2.45	110.93	114.34
27	D	412	LMG	C38-C37-C36	-2.45	101.85	114.45
24	j	102	BCR	C35-C13-C14	-2.45	119.50	122.92
25	C	515	DGD	O5D-C6D-C5D	-2.44	104.85	108.94
22	b	606	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
27	d	407	LMG	C38-C37-C36	-2.44	101.88	114.45
25	d	408	DGD	CFB-CEB-CDB	-2.44	101.88	114.45
22	a	408	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
24	y	101	BCR	C1-C6-C5	-2.43	119.17	122.59
27	c	518	LMG	O2-C2-C1	-2.43	104.94	110.03
25	A	408	DGD	CBB-CAB-C9B	-2.43	101.94	114.45
24	B	616	BCR	C11-C10-C9	-2.43	123.84	127.31
22	a	405	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
24	b	623	BCR	C3-C4-C5	-2.43	109.61	113.78
27	A	410	LMG	C40-C39-C38	-2.43	101.96	114.45
31	D	410	LMT	C3'-C4'-C5'	-2.42	105.73	110.88
22	b	610	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	A	403	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	C	505	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	a	406	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
24	C	514	BCR	C11-C10-C9	-2.42	123.86	127.31
25	C	516	DGD	O6E-C1E-O5D	-2.42	104.28	110.02
25	a	411	DGD	CBB-CAB-C9B	-2.41	102.02	114.45
27	B	621	LMG	O2-C2-C1	-2.41	104.98	110.03
22	C	504	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
31	d	409	LMT	C1'-O5'-C5'	-2.41	109.17	113.72
22	A	404	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	b	625	LMG	O2-C2-C1	-2.41	104.99	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	O2A-CGA-O1A	-2.41	117.56	123.55
24	A	407	BCR	C33-C5-C6	-2.41	121.81	124.51
23	A	406	PL9	C7-C8-C9	-2.41	122.68	126.71
27	e	101	LMG	O6-C1-O1	-2.41	104.30	110.02
25	c	515	DGD	C1D-C2D-C3D	-2.41	105.50	109.98
30	F	102	SQD	C5-C6-S	-2.40	110.99	114.34
27	A	415	LMG	O6-C1-O1	-2.40	104.33	110.02
22	B	603	CLA	C1-C2-C3	-2.40	121.54	125.96
22	A	402	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
22	c	511	CLA	O2A-CGA-O1A	-2.40	117.60	123.55
27	D	412	LMG	O3-C3-C2	-2.40	105.14	110.36
27	D	408	LMG	C38-C37-C36	-2.39	102.12	114.45
27	c	522	LMG	O6-C1-O1	-2.39	104.34	110.02
24	B	619	BCR	C3-C4-C5	-2.39	109.67	113.78
22	b	607	CLA	C1-C2-C3	-2.39	121.55	125.96
22	a	404	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
27	C	522	LMG	C40-C39-C38	-2.39	102.15	114.45
22	B	611	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
27	c	522	LMG	C40-C39-C38	-2.38	102.17	114.45
26	c	519	LHG	C11-C10-C9	-2.38	102.17	114.45
25	A	408	DGD	C3G-C2G-C1G	-2.38	106.48	111.86
22	B	608	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
34	v	201	HEM	C1D-C2D-C3D	-2.38	105.34	107.00
22	C	508	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
25	B	620	DGD	C3G-C2G-C1G	-2.38	106.49	111.86
27	b	628	LMG	O3-C3-C2	-2.38	105.18	110.36
34	V	201	HEM	C1D-C2D-C3D	-2.38	105.34	107.00
22	C	506	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	b	612	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
27	a	413	LMG	C40-C39-C38	-2.37	102.22	114.45
25	B	620	DGD	CBB-CAB-C9B	-2.37	102.22	114.45
22	b	608	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
27	B	624	LMG	C38-C37-C36	-2.37	102.23	114.45
22	B	601	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
27	C	522	LMG	O6-C1-O1	-2.37	104.40	110.02
25	b	624	DGD	CBB-CAB-C9B	-2.37	102.26	114.45
24	b	620	BCR	C11-C10-C9	-2.37	123.93	127.31
22	b	611	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
27	B	624	LMG	O3-C3-C2	-2.36	105.21	110.36
22	c	506	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	C	516	DGD	C3D-C4D-C5D	-2.36	106.06	110.22
24	C	521	BCR	C24-C23-C22	-2.36	122.67	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	517	DGD	CFB-CEB-CDB	-2.36	102.30	114.45
22	h	101	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
25	c	516	DGD	CFB-CEB-CDB	-2.36	102.31	114.45
27	d	410	LMG	O3-C3-C2	-2.36	105.23	110.36
22	B	602	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	a	413	LMG	O2-C2-C1	-2.35	105.10	110.03
22	A	405	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
27	b	628	LMG	C38-C37-C36	-2.35	102.33	114.45
25	c	517	DGD	CFB-CEB-CDB	-2.35	102.33	114.45
22	c	507	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
27	a	413	LMG	O3-C3-C2	-2.35	105.25	110.36
22	d	405	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
24	g	101	BCR	C1-C6-C5	-2.35	119.29	122.59
31	I	102	LMT	C1'-O5'-C5'	-2.34	109.30	113.72
24	b	623	BCR	C11-C10-C9	-2.34	123.97	127.31
22	B	605	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	612	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
24	B	618	BCR	C15-C16-C17	-2.34	118.47	123.46
22	C	520	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
25	a	411	DGD	C3G-C2G-C1G	-2.33	106.59	111.86
25	D	409	DGD	C3D-C4D-C5D	-2.33	106.12	110.22
25	A	408	DGD	C1D-C2D-C3D	-2.33	105.65	109.98
25	b	601	DGD	O6D-C1D-O3G	-2.33	104.50	110.02
22	H	101	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	C	519	LHG	C11-C10-C9	-2.33	102.47	114.45
27	A	410	LMG	C38-C37-C36	-2.32	102.52	114.45
24	C	521	BCR	C33-C5-C6	-2.32	121.92	124.51
24	c	513	BCR	C3-C4-C5	-2.32	109.80	113.78
25	C	516	DGD	C1D-C2D-C3D	-2.31	105.67	109.98
24	c	513	BCR	C15-C16-C17	-2.31	118.52	123.46
27	E	101	LMG	O6-C1-O1	-2.31	104.53	110.02
27	B	621	LMG	O6-C1-O1	-2.31	104.53	110.02
24	c	513	BCR	C24-C23-C22	-2.31	122.74	126.21
24	B	616	BCR	C15-C14-C13	-2.31	124.01	127.31
24	C	513	BCR	C3-C4-C5	-2.31	109.81	113.78
27	d	410	LMG	O6-C1-O1	-2.31	104.54	110.02
27	d	410	LMG	O2-C2-C1	-2.31	105.20	110.03
25	c	516	DGD	C3D-C4D-C5D	-2.31	106.15	110.22
31	B	623	LMT	C1'-O5'-C5'	-2.31	109.37	113.72
27	m	101	LMG	C1-O6-C5	-2.30	109.37	113.72
27	a	402	LMG	O1-C7-C8	-2.30	105.51	110.99
22	b	605	CLA	C1B-CHB-C4A	-2.30	125.56	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
25	c	516	DGD	O3D-C3D-C4D	-2.30	105.35	110.36
22	B	613	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	C	522	LMG	O3-C3-C2	-2.30	105.36	110.36
25	C	516	DGD	CFB-CEB-CDB	-2.30	102.61	114.45
24	C	521	BCR	C11-C10-C9	-2.30	124.03	127.31
27	A	410	LMG	O2-C2-C1	-2.30	105.22	110.03
34	f	101	HEM	CAA-CBA-CGA	-2.30	108.74	112.66
25	C	516	DGD	O3D-C3D-C4D	-2.29	105.37	110.36
27	a	402	LMG	O3-C3-C2	-2.29	105.37	110.36
27	B	621	LMG	O3-C3-C2	-2.29	105.38	110.36
22	D	406	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	B	604	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	B	609	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	a	409	PL9	C27-C28-C29	-2.29	121.93	127.68
27	C	518	LMG	C38-C37-C36	-2.28	102.68	114.45
24	B	619	BCR	C38-C26-C25	-2.28	121.95	124.51
27	I	101	LMG	O3-C3-C2	-2.28	105.39	110.36
27	b	625	LMG	C40-C39-C38	-2.28	102.70	114.45
22	B	607	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	c	520	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	c	512	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
27	a	413	LMG	C38-C37-C36	-2.28	102.72	114.45
27	B	621	LMG	C40-C39-C38	-2.28	102.72	114.45
24	b	622	BCR	C15-C16-C17	-2.28	118.60	123.46
27	i	101	LMG	O3-C3-C2	-2.28	105.40	110.36
27	C	518	LMG	O3-C3-C2	-2.28	105.41	110.36
24	b	623	BCR	C38-C26-C25	-2.28	121.96	124.51
27	e	101	LMG	O1-C7-C8	-2.27	105.58	110.99
22	c	502	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
30	D	403	SQD	C5-C6-S	-2.27	111.17	114.34
27	c	522	LMG	O3-C3-C2	-2.27	105.41	110.36
23	D	407	PL9	C27-C28-C29	-2.27	121.98	127.68
22	C	512	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
27	c	518	LMG	C38-C37-C36	-2.27	102.77	114.45
22	c	509	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
27	b	625	LMG	O3-C3-C2	-2.27	105.42	110.36
22	B	615	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
25	b	624	DGD	C3G-C2G-C1G	-2.26	106.75	111.86
22	b	616	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	c	515	DGD	O2D-C2D-C1D	-2.26	105.30	110.03
27	D	412	LMG	O6-C1-O1	-2.26	104.66	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	625	LMG	C38-C37-C36	-2.26	102.83	114.45
24	c	521	BCR	C33-C5-C6	-2.26	121.98	124.51
24	b	623	BCR	C24-C23-C22	-2.25	122.82	126.21
27	A	415	LMG	O1-C7-C8	-2.25	105.62	110.99
27	e	101	LMG	O3-C3-C2	-2.25	105.46	110.36
27	c	518	LMG	O3-C3-C2	-2.25	105.47	110.36
22	c	504	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
27	a	402	LMG	O2-C2-C1	-2.24	105.34	110.03
24	b	622	BCR	C7-C8-C9	-2.24	122.84	126.21
27	M	101	LMG	O3-C3-C2	-2.24	105.48	110.36
22	C	509	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	b	613	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
24	b	620	BCR	C15-C14-C13	-2.23	124.12	127.31
27	c	522	LMG	C38-C37-C36	-2.23	102.95	114.45
27	A	415	LMG	O3-C3-C2	-2.23	105.50	110.36
22	B	603	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
27	b	625	LMG	O6-C1-O1	-2.23	104.72	110.02
25	B	625	DGD	O6D-C1D-O3G	-2.23	104.73	110.02
27	D	412	LMG	O2-C2-C1	-2.22	105.38	110.03
31	b	627	LMT	C1'-O5'-C5'	-2.22	109.53	113.72
27	C	522	LMG	C38-C37-C36	-2.22	103.02	114.45
22	b	618	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
24	B	618	BCR	C7-C8-C9	-2.22	122.88	126.21
22	C	501	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
24	A	407	BCR	C15-C14-C13	-2.22	124.14	127.31
22	C	511	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
27	i	101	LMG	O1-C7-C8	-2.21	105.72	110.99
22	b	617	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
23	A	406	PL9	C27-C28-C29	-2.21	122.12	127.68
22	C	502	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	D	411	BCR	C11-C10-C9	-2.21	124.16	127.31
24	a	410	BCR	C38-C26-C25	-2.21	122.03	124.51
27	B	621	LMG	C38-C37-C36	-2.21	103.09	114.45
27	A	415	LMG	O2-C2-C1	-2.21	105.42	110.03
24	g	101	BCR	C3-C2-C1	-2.21	106.66	114.59
23	D	407	PL9	C37-C38-C39	-2.20	122.14	127.68
27	e	101	LMG	O2-C2-C1	-2.20	105.42	110.03
22	C	507	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
23	D	407	PL9	C32-C33-C34	-2.20	122.15	127.68
24	J	102	BCR	C15-C16-C17	-2.20	118.77	123.46
23	d	406	PL9	C37-C38-C39	-2.20	122.15	127.68
23	d	406	PL9	C27-C28-C29	-2.20	122.16	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	E	101	LMG	O2-C2-C1	-2.20	105.43	110.03
27	E	101	LMG	O3-C3-C2	-2.20	105.57	110.36
22	c	510	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
27	m	101	LMG	O3-C3-C2	-2.20	105.58	110.36
22	C	510	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
22	B	614	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
27	D	408	LMG	O6-C1-O1	-2.19	104.82	110.02
22	b	615	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	C	508	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
25	C	516	DGD	O2D-C2D-C1D	-2.19	105.45	110.03
22	B	603	CLA	O2A-CGA-O1A	-2.19	118.12	123.55
27	a	402	LMG	C1-C2-C3	-2.19	105.91	109.98
24	C	514	BCR	C38-C26-C25	-2.19	122.06	124.51
24	A	407	BCR	C38-C26-C25	-2.19	122.06	124.51
22	D	405	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
22	b	618	CLA	O2A-CGA-O1A	-2.18	118.14	123.55
24	c	521	BCR	C11-C10-C9	-2.18	124.20	127.31
22	b	619	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
24	c	521	BCR	C24-C23-C22	-2.18	122.94	126.21
22	C	503	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
34	F	101	HEM	CAA-CBA-CGA	-2.18	108.94	112.66
22	c	501	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	d	404	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	b	607	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
25	c	516	DGD	CBB-CAB-C9B	-2.17	103.26	114.45
24	y	101	BCR	C3-C2-C1	-2.17	106.78	114.59
23	d	406	PL9	C32-C33-C34	-2.17	122.23	127.68
24	c	514	BCR	C38-C26-C25	-2.17	122.08	124.51
22	B	611	CLA	O2A-CGA-O1A	-2.17	118.16	123.55
22	c	508	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
27	C	522	LMG	C1-C2-C3	-2.17	105.95	109.98
25	C	516	DGD	CBB-CAB-C9B	-2.17	103.28	114.45
27	M	101	LMG	C1-O6-C5	-2.17	109.63	113.72
22	B	602	CLA	O2A-CGA-O1A	-2.17	118.17	123.55
23	d	406	PL9	O1-C4-C3	-2.16	118.26	120.71
24	f	102	BCR	C11-C10-C9	-2.16	124.22	127.31
22	c	506	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
24	C	514	BCR	C24-C23-C22	-2.16	122.97	126.21
22	c	509	CLA	O2A-CGA-O1A	-2.15	118.20	123.55
22	c	503	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
23	d	406	PL9	O2-C1-C2	-2.15	116.74	121.77
25	c	516	DGD	C1D-O6D-C5D	-2.15	109.67	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	101	PL9	O2-C1-C2	-2.15	116.75	121.77
24	D	411	BCR	C7-C8-C9	-2.15	122.99	126.21
24	B	619	BCR	C24-C23-C22	-2.15	122.99	126.21
25	c	516	DGD	O2D-C2D-C1D	-2.14	105.54	110.03
25	C	515	DGD	O2D-C2D-C1D	-2.14	105.55	110.03
25	C	517	DGD	CBB-CAB-C9B	-2.14	103.43	114.45
22	b	615	CLA	O2A-CGA-O1A	-2.14	118.24	123.55
22	B	611	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	c	511	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
34	F	101	HEM	CBD-CAD-C3D	-2.14	108.39	112.47
27	E	101	LMG	O1-C7-C8	-2.13	105.91	110.99
25	a	411	DGD	CAB-C9B-C8B	-2.13	103.46	114.45
22	B	614	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
25	b	601	DGD	CBB-CAB-C9B	-2.13	103.48	114.45
25	A	408	DGD	CAB-C9B-C8B	-2.13	103.49	114.45
24	C	513	BCR	C7-C8-C9	-2.13	123.02	126.21
27	d	407	LMG	O6-C1-O1	-2.12	104.98	110.02
25	C	515	DGD	O3E-C3E-C2E	-2.12	105.74	110.36
22	b	614	CLA	C1-C2-C3	-2.12	122.05	125.96
23	J	101	PL9	O2-C1-C2	-2.12	116.81	121.77
26	a	412	LHG	C27-C26-C25	-2.12	103.53	114.45
25	B	625	DGD	CBB-CAB-C9B	-2.12	103.54	114.45
24	b	622	BCR	C33-C5-C6	-2.12	122.14	124.51
25	c	517	DGD	CBB-CAB-C9B	-2.12	103.54	114.45
27	c	522	LMG	C1-C2-C3	-2.12	106.04	109.98
22	b	610	CLA	O2A-CGA-O1A	-2.12	118.30	123.55
22	B	608	CLA	C1-C2-C3	-2.12	122.06	125.96
25	C	516	DGD	CAB-C9B-C8B	-2.12	103.55	114.45
24	a	410	BCR	C15-C14-C13	-2.12	124.29	127.31
22	d	405	CLA	C1-C2-C3	-2.12	122.06	125.96
24	a	410	BCR	C24-C23-C22	-2.12	123.03	126.21
22	B	610	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
23	d	406	PL9	C36-C34-C33	-2.11	116.78	121.10
22	C	506	CLA	O2A-CGA-O1A	-2.11	118.30	123.55
24	a	410	BCR	C15-C16-C17	-2.11	118.95	123.46
24	b	623	BCR	C15-C14-C13	-2.11	124.30	127.31
24	B	619	BCR	C11-C10-C9	-2.11	124.30	127.31
22	B	601	CLA	O2A-CGA-O1A	-2.11	118.32	123.55
24	f	102	BCR	C15-C16-C17	-2.11	118.96	123.46
23	D	407	PL9	O1-C4-C3	-2.10	118.32	120.71
25	C	517	DGD	O2D-C2D-C1D	-2.10	105.63	110.03
24	c	514	BCR	C24-C23-C22	-2.10	123.05	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
22	b	614	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
24	A	407	BCR	C15-C16-C17	-2.10	118.98	123.46
24	b	621	BCR	C35-C13-C14	-2.10	119.98	122.92
22	C	501	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
32	D	401	PHO	O2A-CGA-O1A	-2.10	118.34	123.55
22	b	607	CLA	O2A-CGA-O1A	-2.09	118.35	123.55
27	A	415	LMG	C1-C2-C3	-2.09	106.09	109.98
25	b	601	DGD	CAB-C9B-C8B	-2.09	103.69	114.45
27	D	408	LMG	O3-C3-C2	-2.09	105.81	110.36
22	B	606	CLA	O2A-CGA-O1A	-2.09	118.37	123.55
25	B	620	DGD	O2D-C2D-C1D	-2.09	105.66	110.03
24	j	102	BCR	C20-C21-C22	-2.09	124.33	127.31
25	C	517	DGD	CAB-C9B-C8B	-2.09	103.70	114.45
25	C	516	DGD	C1D-O6D-C5D	-2.09	109.78	113.72
27	c	518	LMG	O7-C10-O9	-2.09	118.47	123.68
22	C	520	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
27	a	413	LMG	C1-O6-C5	-2.08	109.79	113.72
25	D	409	DGD	O3E-C3E-C2E	-2.08	105.83	110.36
22	B	612	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
22	B	610	CLA	C1-C2-C3	-2.08	122.12	125.96
32	d	401	PHO	C2B-C1B-NB	-2.08	106.74	109.82
22	c	512	CLA	O2A-CGA-O1A	-2.08	118.39	123.55
25	b	624	DGD	O2D-C2D-C1D	-2.08	105.68	110.03
24	C	514	BCR	C7-C8-C9	-2.08	123.09	126.21
22	b	606	CLA	O2A-CGA-O1A	-2.07	118.40	123.55
22	c	508	CLA	O2A-CGA-O1A	-2.07	118.40	123.55
27	C	518	LMG	O1-C7-C8	-2.07	106.06	110.99
27	c	518	LMG	O1-C7-C8	-2.07	106.07	110.99
25	B	625	DGD	CAB-C9B-C8B	-2.07	103.81	114.45
23	a	409	PL9	O1-C4-C3	-2.07	118.37	120.71
22	B	607	CLA	O2A-CGA-O1A	-2.06	118.42	123.55
22	c	501	CLA	O2A-CGA-O1A	-2.06	118.43	123.55
24	g	101	BCR	C15-C14-C13	-2.06	124.37	127.31
24	C	513	BCR	C11-C10-C9	-2.06	124.37	127.31
25	B	620	DGD	C4E-C3E-C2E	-2.06	107.20	110.84
25	c	517	DGD	CAB-C9B-C8B	-2.06	103.84	114.45
24	B	616	BCR	C38-C26-C25	-2.06	122.20	124.51
22	C	507	CLA	C1-C2-C3	-2.06	122.16	125.96
22	a	405	CLA	O2A-CGA-O1A	-2.06	118.44	123.55
24	B	618	BCR	C33-C5-C6	-2.06	122.20	124.51
26	A	409	LHG	C27-C26-C25	-2.06	103.86	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	624	DGD	CAB-C9B-C8B	-2.06	103.86	114.45
24	g	101	BCR	C15-C16-C17	-2.06	119.07	123.46
22	C	512	CLA	O2A-CGA-O1A	-2.06	118.45	123.55
25	d	408	DGD	C5B-C4B-C3B	-2.06	103.86	114.45
22	b	613	CLA	O2A-CGA-O1A	-2.05	118.45	123.55
23	D	407	PL9	O2-C1-C2	-2.05	116.97	121.77
27	C	518	LMG	O7-C10-O9	-2.05	118.56	123.68
25	c	516	DGD	CAB-C9B-C8B	-2.05	103.91	114.45
27	d	410	LMG	O1-C7-C8	-2.05	106.12	110.99
32	a	407	PHO	CMB-C2B-C1B	-2.04	121.86	125.04
22	A	403	CLA	O2A-CGA-O1A	-2.04	118.47	123.55
22	c	520	CLA	O2A-CGA-O1A	-2.04	118.47	123.55
22	a	406	CLA	O2A-CGA-O1A	-2.04	118.47	123.55
32	D	402	PHO	CMB-C2B-C1B	-2.04	121.86	125.04
24	H	102	BCR	C16-C15-C14	-2.04	119.10	123.46
32	d	401	PHO	O2A-CGA-O1A	-2.04	118.48	123.55
24	C	521	BCR	C38-C26-C25	-2.04	122.22	124.51
25	B	620	DGD	O3E-C3E-C2E	-2.04	105.92	110.36
25	c	516	DGD	C1D-C2D-C3D	-2.04	106.19	109.98
25	D	409	DGD	CAB-C9B-C8B	-2.04	103.96	114.45
32	D	401	PHO	C2B-C1B-NB	-2.04	106.80	109.82
25	D	409	DGD	C5B-C4B-C3B	-2.04	103.96	114.45
24	b	621	BCR	C24-C23-C22	-2.03	123.16	126.21
24	D	411	BCR	C15-C16-C17	-2.03	119.12	123.46
25	d	408	DGD	O3E-C3E-C2E	-2.03	105.94	110.36
24	B	616	BCR	C7-C8-C9	-2.03	123.16	126.21
24	C	513	BCR	C38-C26-C25	-2.03	122.23	124.51
27	I	101	LMG	O1-C7-C8	-2.03	106.16	110.99
24	B	616	BCR	C15-C16-C17	-2.03	119.14	123.46
25	B	625	DGD	O3E-C3E-C2E	-2.03	105.95	110.36
25	C	517	DGD	O3E-C3E-C2E	-2.03	105.95	110.36
25	b	601	DGD	O3E-C3E-C2E	-2.02	105.96	110.36
24	J	102	BCR	C34-C9-C10	-2.02	120.09	122.92
25	c	515	DGD	O3E-C3E-C2E	-2.02	105.96	110.36
24	y	101	BCR	C15-C16-C17	-2.02	119.15	123.46
27	I	101	LMG	O7-C10-O9	-2.02	118.64	123.68
23	A	406	PL9	O2-C1-C2	-2.02	117.06	121.77
23	a	409	PL9	O2-C1-C2	-2.02	117.06	121.77
22	C	508	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
25	d	408	DGD	CAB-C9B-C8B	-2.01	104.08	114.45
32	D	402	PHO	C2B-C1B-NB	-2.01	106.84	109.82
27	B	624	LMG	O1-C7-C8	-2.01	106.20	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	615	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
27	A	410	LMG	C1-O6-C5	-2.01	109.92	113.72
25	C	517	DGD	C5B-C4B-C3B	-2.01	104.09	114.45
22	B	613	CLA	O2A-CGA-O1A	-2.01	118.56	123.55
24	C	521	BCR	C7-C8-C9	-2.01	123.19	126.21
27	A	415	LMG	O7-C10-O9	-2.01	118.66	123.68
25	B	620	DGD	C3D-C4D-C5D	-2.01	106.68	110.22
23	d	406	PL9	C31-C32-C33	-2.01	105.07	111.97
22	C	510	CLA	O2A-CGA-O1A	-2.01	118.57	123.55
22	C	505	CLA	O2A-CGA-O1A	-2.01	118.57	123.55
22	C	509	CLA	O2A-CGA-O1A	-2.01	118.57	123.55
24	B	617	BCR	C24-C23-C22	-2.01	123.20	126.21
24	D	411	BCR	C24-C23-C22	-2.00	123.20	126.21
24	B	617	BCR	C38-C26-C25	-2.00	122.26	124.51
22	B	609	CLA	O2A-CGA-O1A	-2.00	118.57	123.55
25	c	517	DGD	O3E-C3E-C2E	-2.00	106.00	110.36
25	d	408	DGD	CBB-CAB-C9B	-2.00	104.14	114.45
25	A	408	DGD	O2D-C2D-C1D	-2.00	105.84	110.03
25	C	517	DGD	C3G-O3G-C1D	2.00	117.86	113.76
22	B	606	CLA	C1D-CHD-C4C	2.01	125.23	122.48
22	c	512	CLA	O1D-CGD-CBD	2.01	128.21	124.60
22	C	520	CLA	C1D-CHD-C4C	2.01	125.24	122.48
23	d	406	PL9	O2-C1-C6	2.01	124.20	120.57
22	B	602	CLA	C1D-CHD-C4C	2.02	125.24	122.48
32	a	407	PHO	C1B-NB-C4B	2.02	110.52	106.52
23	a	409	PL9	O2-C1-C6	2.02	124.21	120.57
22	b	606	CLA	O2D-CGD-CBD	2.02	114.91	111.30
24	b	622	BCR	C27-C26-C25	2.02	125.71	122.74
22	b	616	CLA	C1D-CHD-C4C	2.02	125.25	122.48
22	c	511	CLA	C1D-CHD-C4C	2.02	125.25	122.48
22	H	101	CLA	O1D-CGD-CBD	2.03	128.24	124.60
24	D	411	BCR	C27-C26-C25	2.03	125.72	122.74
22	B	610	CLA	CHB-C4A-NA	2.03	127.32	124.51
22	C	509	CLA	C1D-CHD-C4C	2.03	125.27	122.48
22	C	512	CLA	C1D-CHD-C4C	2.04	125.27	122.48
22	B	614	CLA	C1D-CHD-C4C	2.04	125.27	122.48
22	B	607	CLA	O1D-CGD-CBD	2.04	128.27	124.60
22	b	614	CLA	O1D-CGD-CBD	2.05	128.28	124.60
32	D	401	PHO	C1B-NB-C4B	2.06	110.59	106.52
22	C	510	CLA	O1D-CGD-CBD	2.06	128.30	124.60
23	J	101	PL9	O2-C1-C6	2.06	124.28	120.57
32	d	401	PHO	C1B-NB-C4B	2.06	110.60	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	O1D-CGD-CBD	2.06	128.31	124.60
24	f	102	BCR	C27-C26-C25	2.07	125.78	122.74
30	A	413	SQD	C4-C3-C2	2.07	114.49	110.84
24	H	102	BCR	C29-C30-C25	2.07	113.72	110.48
23	j	101	PL9	O2-C1-C6	2.08	124.31	120.57
22	c	520	CLA	C1D-CHD-C4C	2.08	125.33	122.48
34	V	201	HEM	CMB-C2B-C3B	2.08	128.75	124.89
25	c	517	DGD	C3G-O3G-C1D	2.08	118.02	113.76
22	b	613	CLA	C1D-CHD-C4C	2.08	125.33	122.48
22	A	403	CLA	CMD-C2D-C3D	2.09	128.76	124.89
32	D	402	PHO	C1B-NB-C4B	2.09	110.66	106.52
22	c	512	CLA	C1D-CHD-C4C	2.10	125.36	122.48
22	b	610	CLA	CMD-C2D-C3D	2.11	128.80	124.89
22	b	614	CLA	C1D-CHD-C4C	2.11	125.37	122.48
22	B	604	CLA	CMD-C2D-C3D	2.11	128.81	124.89
24	x	101	BCR	C29-C30-C25	2.13	113.81	110.48
22	c	508	CLA	CMD-C2D-C3D	2.13	128.85	124.89
22	A	402	CLA	O1D-CGD-CBD	2.14	128.44	124.60
22	B	610	CLA	C4A-NA-C1A	2.14	109.11	106.45
22	a	406	CLA	CMD-C2D-C3D	2.14	128.87	124.89
22	b	614	CLA	C4A-NA-C1A	2.15	109.11	106.45
22	a	404	CLA	CMD-C2D-C3D	2.15	128.88	124.89
34	v	201	HEM	CMB-C2B-C3B	2.15	128.89	124.89
22	C	507	CLA	C1D-CHD-C4C	2.15	125.43	122.48
23	j	101	PL9	C20-C19-C21	2.16	119.03	115.29
22	a	404	CLA	O1D-CGD-CBD	2.17	128.49	124.60
24	c	513	BCR	C27-C26-C25	2.17	125.92	122.74
22	c	510	CLA	CMD-C2D-C3D	2.17	128.92	124.89
22	C	509	CLA	CMD-C2D-C3D	2.17	128.92	124.89
22	b	610	CLA	C1D-CHD-C4C	2.17	125.45	122.48
24	C	513	BCR	C27-C26-C25	2.17	125.93	122.74
22	C	508	CLA	CMD-C2D-C3D	2.17	128.93	124.89
22	c	509	CLA	CMD-C2D-C3D	2.18	128.94	124.89
22	B	610	CLA	C1D-CHD-C4C	2.18	125.47	122.48
22	b	609	CLA	CMD-C2D-C3D	2.18	128.94	124.89
22	A	404	CLA	CMD-C2D-C3D	2.19	128.95	124.89
22	b	619	CLA	CMD-C2D-C3D	2.19	128.95	124.89
22	c	503	CLA	O2D-CGD-CBD	2.19	115.22	111.30
22	B	609	CLA	C1D-CHD-C4C	2.19	125.48	122.48
30	f	103	SQD	O48-C23-C24	2.20	118.29	111.90
22	D	405	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	B	606	CLA	CMD-C2D-C3D	2.20	128.97	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	A	402	CLA	CMD-C2D-C3D	2.21	128.99	124.89
30	a	415	SQD	C4-C3-C2	2.21	114.73	110.84
22	b	608	CLA	CMD-C2D-C3D	2.22	129.00	124.89
30	f	103	SQD	C1-O5-C5	2.22	117.89	113.72
24	b	620	BCR	C27-C26-C25	2.22	126.00	122.74
22	B	609	CLA	CMD-C2D-C3D	2.22	129.01	124.89
22	c	520	CLA	CMD-C2D-C3D	2.22	129.02	124.89
22	c	512	CLA	CMD-C2D-C3D	2.23	129.02	124.89
23	A	406	PL9	C20-C19-C21	2.23	119.16	115.29
22	C	512	CLA	CMD-C2D-C3D	2.23	129.04	124.89
22	B	615	CLA	CMD-C2D-C3D	2.24	129.04	124.89
22	C	520	CLA	CMD-C2D-C3D	2.24	129.06	124.89
22	c	507	CLA	O2D-CGD-CBD	2.25	115.31	111.30
22	b	609	CLA	O1D-CGD-CBD	2.25	128.64	124.60
22	b	616	CLA	CMD-C2D-C3D	2.25	129.06	124.89
23	D	407	PL9	C20-C19-C21	2.25	119.19	115.29
22	b	607	CLA	CMD-C2D-C3D	2.25	129.07	124.89
22	b	605	CLA	CHB-C4A-NA	2.26	127.63	124.51
24	B	616	BCR	C27-C26-C25	2.26	126.05	122.74
30	F	102	SQD	O48-C23-C24	2.26	118.47	111.90
22	C	510	CLA	CMD-C2D-C3D	2.26	129.09	124.89
23	J	101	PL9	C20-C19-C21	2.27	119.22	115.29
22	c	503	CLA	CMD-C2D-C3D	2.27	129.10	124.89
22	H	101	CLA	CMD-C2D-C3D	2.27	129.10	124.89
23	A	406	PL9	C41-C39-C40	2.27	119.90	114.60
22	c	504	CLA	O1D-CGD-CBD	2.28	128.69	124.60
30	f	103	SQD	C3-C4-C5	2.28	114.23	110.22
24	B	616	BCR	C2-C1-C6	2.28	114.05	110.48
30	F	102	SQD	C44-O6-C1	2.29	118.44	113.76
22	C	504	CLA	O1D-CGD-CBD	2.30	128.73	124.60
23	d	406	PL9	C20-C19-C21	2.30	119.28	115.29
22	B	605	CLA	CMD-C2D-C3D	2.30	129.16	124.89
22	C	503	CLA	CMD-C2D-C3D	2.30	129.16	124.89
22	B	612	CLA	CMD-C2D-C3D	2.31	129.18	124.89
22	c	506	CLA	CMD-C2D-C3D	2.31	129.19	124.89
30	b	602	SQD	O48-C23-C24	2.32	118.64	111.90
24	b	620	BCR	C2-C1-C6	2.32	114.10	110.48
22	B	601	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	b	618	CLA	CMD-C2D-C3D	2.32	129.19	124.89
22	B	613	CLA	CMD-C2D-C3D	2.32	129.20	124.89
24	a	410	BCR	C27-C26-C25	2.32	126.15	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	PL9	C20-C19-C21	2.32	119.32	115.29
22	C	501	CLA	CMB-C2B-C3B	2.32	129.20	124.89
22	B	603	CLA	CMD-C2D-C3D	2.33	129.21	124.89
22	C	505	CLA	CMD-C2D-C3D	2.33	129.21	124.89
24	J	102	BCR	C29-C30-C25	2.33	114.12	110.48
24	j	102	BCR	C29-C30-C25	2.33	114.12	110.48
22	c	501	CLA	CMD-C2D-C3D	2.33	129.22	124.89
22	C	501	CLA	CMD-C2D-C3D	2.33	129.22	124.89
22	H	101	CLA	CHB-C4A-NA	2.34	127.74	124.51
23	a	409	PL9	C41-C39-C40	2.34	120.06	114.60
24	A	407	BCR	C27-C26-C25	2.35	126.19	122.74
22	B	614	CLA	CMD-C2D-C3D	2.35	129.25	124.89
22	b	613	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	C	506	CLA	CMD-C2D-C3D	2.35	129.26	124.89
22	B	602	CLA	CMD-C2D-C3D	2.35	129.26	124.89
22	c	509	CLA	CHB-C4A-NA	2.35	127.77	124.51
22	b	605	CLA	CMD-C2D-C3D	2.35	129.26	124.89
22	c	501	CLA	CMB-C2B-C3B	2.36	129.27	124.89
22	C	507	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	C	507	CLA	CMD-C2D-C3D	2.36	129.27	124.89
22	b	613	CLA	CMD-C2D-C3D	2.36	129.27	124.89
22	b	606	CLA	CMD-C2D-C3D	2.36	129.28	124.89
22	C	509	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	b	623	BCR	C27-C26-C25	2.37	126.22	122.74
24	B	617	BCR	C29-C30-C25	2.37	114.18	110.48
24	b	621	BCR	C29-C30-C25	2.37	114.18	110.48
24	C	521	BCR	C27-C26-C25	2.37	126.23	122.74
22	D	406	CLA	CMD-C2D-C3D	2.38	129.30	124.89
22	b	617	CLA	CMD-C2D-C3D	2.38	129.30	124.89
22	h	101	CLA	CMD-C2D-C3D	2.38	129.31	124.89
22	b	612	CLA	C4A-NA-C1A	2.38	109.41	106.45
30	B	626	SQD	O48-C23-C24	2.38	118.84	111.90
22	b	612	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	b	619	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	c	509	CLA	C4A-NA-C1A	2.39	109.42	106.45
24	c	521	BCR	C27-C26-C25	2.40	126.26	122.74
22	A	405	CLA	CMD-C2D-C3D	2.40	129.34	124.89
22	A	405	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	B	619	BCR	C27-C26-C25	2.40	126.27	122.74
22	D	405	CLA	O1D-CGD-CBD	2.40	128.92	124.60
22	B	605	CLA	O1D-CGD-CBD	2.40	128.92	124.60
22	A	402	CLA	C4A-NA-C1A	2.40	109.44	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	CMD-C2D-C3D	2.41	129.36	124.89
22	a	404	CLA	C4A-NA-C1A	2.41	109.44	106.45
22	b	617	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	601	CLA	CMD-C2D-C3D	2.41	129.37	124.89
22	b	611	CLA	CMD-C2D-C3D	2.41	129.37	124.89
22	B	615	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	B	607	CLA	CMD-C2D-C3D	2.41	129.37	124.89
22	d	405	CLA	CMD-C2D-C3D	2.41	129.37	124.89
22	C	509	CLA	C4A-NA-C1A	2.42	109.45	106.45
22	C	502	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	d	404	CLA	O1D-CGD-CBD	2.43	128.96	124.60
22	c	502	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	b	606	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	c	504	CLA	CMD-C2D-C3D	2.43	129.40	124.89
22	b	613	CLA	C4A-NA-C1A	2.43	109.47	106.45
22	b	607	CLA	O1D-CGD-CBD	2.43	128.97	124.60
22	b	606	CLA	C4A-NA-C1A	2.43	109.47	106.45
22	c	507	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	b	610	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	b	605	CLA	C4A-NA-C1A	2.43	109.47	106.45
22	B	611	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	A	402	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	A	404	CLA	C4A-NA-C1A	2.44	109.48	106.45
22	B	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	C	508	CLA	CHB-C4A-NA	2.45	127.90	124.51
30	A	414	SQD	C1-O5-C5	2.45	118.33	113.72
22	a	408	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	b	612	CLA	CMD-C2D-C3D	2.46	129.46	124.89
22	B	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	h	101	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	b	611	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	D	406	CLA	C4A-NA-C1A	2.47	109.51	106.45
22	B	608	CLA	C4A-NA-C1A	2.47	109.52	106.45
22	H	101	CLA	C4A-NA-C1A	2.47	109.52	106.45
30	A	413	SQD	O48-C23-C24	2.47	119.09	111.90
22	C	502	CLA	CMD-C2D-C3D	2.47	129.48	124.89
22	B	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	b	616	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	D	406	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	C4A-NA-C1A	2.47	109.52	106.45
22	A	404	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	c	507	CLA	CMD-C2D-C3D	2.48	129.49	124.89
22	B	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	B	608	CLA	CMD-C2D-C3D	2.48	129.50	124.89
22	c	504	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	c	514	BCR	C29-C30-C25	2.49	114.36	110.48
24	C	514	BCR	C29-C30-C25	2.49	114.37	110.48
22	c	502	CLA	C4A-NA-C1A	2.49	109.54	106.45
22	C	511	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	c	501	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	508	CLA	C4A-NA-C1A	2.49	109.55	106.45
22	d	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	C	502	CLA	C4A-NA-C1A	2.49	109.55	106.45
22	d	405	CLA	C4A-NA-C1A	2.49	109.55	106.45
22	b	611	CLA	C4A-NA-C1A	2.49	109.55	106.45
22	a	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	b	610	CLA	C4A-NA-C1A	2.50	109.55	106.45
30	F	102	SQD	C3-C4-C5	2.50	114.62	110.22
22	B	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	a	415	SQD	O48-C23-C24	2.50	119.19	111.90
30	A	414	SQD	O48-C23-C24	2.51	119.19	111.90
22	b	615	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	c	503	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	b	615	CLA	CMD-C2D-C3D	2.51	129.56	124.89
22	D	405	CLA	CMD-C2D-C3D	2.52	129.57	124.89
30	a	401	SQD	C1-O5-C5	2.52	118.46	113.72
22	c	507	CLA	C4A-NA-C1A	2.52	109.58	106.45
22	B	613	CLA	C4A-NA-C1A	2.52	109.58	106.45
22	c	508	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	C	507	CLA	C4A-NA-C1A	2.53	109.59	106.45
22	c	505	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	B	602	CLA	C4A-NA-C1A	2.53	109.59	106.45
22	h	101	CLA	C4A-NA-C1A	2.53	109.59	106.45
22	a	408	CLA	CMD-C2D-C3D	2.53	129.59	124.89
22	B	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	c	511	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	a	408	CLA	C4A-NA-C1A	2.54	109.60	106.45
22	c	508	CLA	C4A-NA-C1A	2.54	109.60	106.45
22	C	503	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	c	505	CLA	C4A-NA-C1A	2.54	109.60	106.45
22	D	405	CLA	C4A-NA-C1A	2.54	109.60	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	502	CLA	CMD-C2D-C3D	2.54	129.60	124.89
22	B	607	CLA	C4A-NA-C1A	2.54	109.61	106.45
22	b	618	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	d	404	CLA	CMD-C2D-C3D	2.55	129.62	124.89
22	b	617	CLA	C4A-NA-C1A	2.55	109.61	106.45
22	c	510	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	c	504	CLA	CMB-C2B-C3B	2.55	129.62	124.89
22	C	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	609	CLA	C4A-NA-C1A	2.56	109.62	106.45
22	b	619	CLA	CMB-C2B-C3B	2.56	129.64	124.89
30	b	602	SQD	C4-C3-C2	2.56	115.35	110.84
22	A	405	CLA	C4A-NA-C1A	2.56	109.63	106.45
30	a	401	SQD	O48-C23-C24	2.56	119.35	111.90
22	B	611	CLA	CMD-C2D-C3D	2.56	129.65	124.89
30	d	402	SQD	O48-C23-C24	2.57	119.37	111.90
22	C	504	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	d	404	CLA	C4A-NA-C1A	2.57	109.65	106.45
30	D	403	SQD	C44-O6-C1	2.57	119.03	113.76
30	B	626	SQD	C4-C3-C2	2.57	115.38	110.84
22	a	406	CLA	C4A-NA-C1A	2.57	109.65	106.45
22	C	505	CLA	C4A-NA-C1A	2.58	109.65	106.45
22	C	504	CLA	CMD-C2D-C3D	2.58	129.68	124.89
22	c	506	CLA	C4A-NA-C1A	2.58	109.66	106.45
22	b	608	CLA	C4A-NA-C1A	2.58	109.66	106.45
22	B	612	CLA	C4A-NA-C1A	2.58	109.66	106.45
22	c	512	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	606	CLA	C4A-NA-C1A	2.58	109.66	106.45
22	B	603	CLA	O1D-CGD-CBD	2.59	129.25	124.60
22	C	520	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	b	619	CLA	C4A-NA-C1A	2.59	109.66	106.45
22	C	505	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	B	604	CLA	C4A-NA-C1A	2.59	109.67	106.45
22	B	614	CLA	C4A-NA-C1A	2.59	109.67	106.45
22	C	511	CLA	C4A-NA-C1A	2.59	109.67	106.45
32	D	401	PHO	O1D-CGD-CBD	2.59	129.26	124.60
22	B	610	CLA	CMD-C2D-C3D	2.60	129.71	124.89
22	a	406	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	C	506	CLA	C4A-NA-C1A	2.60	109.68	106.45
22	b	607	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	c	512	CLA	C4A-NA-C1A	2.60	109.68	106.45
22	C	512	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	c	520	CLA	CHB-C4A-NA	2.60	128.11	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	CMB-C2B-C3B	2.60	129.72	124.89
22	B	615	CLA	CMB-C2B-C3B	2.61	129.73	124.89
22	b	608	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	C	511	CLA	CMD-C2D-C3D	2.61	129.74	124.89
23	D	407	PL9	C40-C39-C41	2.61	119.82	115.29
22	c	511	CLA	CMD-C2D-C3D	2.62	129.75	124.89
22	C	512	CLA	C4A-NA-C1A	2.62	109.70	106.45
22	B	605	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	B	615	CLA	C4A-NA-C1A	2.63	109.71	106.45
22	c	506	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	B	603	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	c	511	CLA	C4A-NA-C1A	2.63	109.72	106.45
30	D	403	SQD	O48-C23-C24	2.63	119.56	111.90
24	j	102	BCR	C27-C26-C25	2.63	126.61	122.74
22	a	404	CLA	CMB-C2B-C3B	2.63	129.78	124.89
22	c	501	CLA	C4A-NA-C1A	2.64	109.72	106.45
22	B	605	CLA	C4A-NA-C1A	2.64	109.72	106.45
30	d	402	SQD	C44-O6-C1	2.64	119.17	113.76
22	C	508	CLA	CMB-C2B-C3B	2.64	129.79	124.89
22	b	618	CLA	C4A-NA-C1A	2.64	109.73	106.45
22	C	520	CLA	C4A-NA-C1A	2.64	109.73	106.45
22	a	406	CLA	CMB-C2B-C3B	2.64	129.80	124.89
22	C	506	CLA	CHB-C4A-NA	2.65	128.17	124.51
22	c	510	CLA	C4A-NA-C1A	2.65	109.74	106.45
22	b	616	CLA	C4A-NA-C1A	2.65	109.74	106.45
22	C	503	CLA	C4A-NA-C1A	2.66	109.75	106.45
24	g	101	BCR	C27-C26-C25	2.66	126.64	122.74
22	c	508	CLA	CMB-C2B-C3B	2.66	129.83	124.89
22	c	503	CLA	C4A-NA-C1A	2.66	109.76	106.45
22	C	510	CLA	CHB-C4A-NA	2.66	128.20	124.51
22	C	501	CLA	C4A-NA-C1A	2.66	109.76	106.45
22	B	606	CLA	CMB-C2B-C3B	2.67	129.84	124.89
22	a	405	CLA	CMB-C2B-C3B	2.67	129.85	124.89
22	B	601	CLA	CMB-C2B-C3B	2.67	129.85	124.89
22	B	608	CLA	CMB-C2B-C3B	2.68	129.86	124.89
32	a	407	PHO	O1D-CGD-CBD	2.68	129.41	124.60
32	d	401	PHO	O1D-CGD-CBD	2.68	129.41	124.60
22	b	614	CLA	CMD-C2D-C3D	2.68	129.86	124.89
22	c	520	CLA	C4A-NA-C1A	2.69	109.79	106.45
22	b	605	CLA	CMB-C2B-C3B	2.69	129.88	124.89
24	b	622	BCR	C29-C30-C25	2.69	114.69	110.48
31	I	102	LMT	O1'-C1'-C2'	2.70	112.63	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	101	BCR	C27-C26-C25	2.70	126.70	122.74
30	f	103	SQD	C44-O6-C1	2.70	119.29	113.76
22	b	612	CLA	CMB-C2B-C3B	2.70	129.91	124.89
22	A	402	CLA	CMB-C2B-C3B	2.71	129.91	124.89
22	a	405	CLA	CHB-C4A-NA	2.71	128.25	124.51
22	c	520	CLA	CMB-C2B-C3B	2.71	129.91	124.89
23	d	406	PL9	C40-C39-C41	2.71	119.98	115.29
32	D	402	PHO	O1D-CGD-CBD	2.71	129.47	124.60
24	B	618	BCR	C29-C30-C25	2.71	114.72	110.48
22	A	403	CLA	C4A-NA-C1A	2.72	109.83	106.45
22	C	509	CLA	CMB-C2B-C3B	2.72	129.94	124.89
22	b	610	CLA	CMB-C2B-C3B	2.72	129.94	124.89
22	a	405	CLA	C4A-NA-C1A	2.72	109.83	106.45
22	A	403	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	A	403	CLA	CMB-C2B-C3B	2.72	129.95	124.89
24	C	521	BCR	C2-C1-C6	2.72	114.74	110.48
22	b	609	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	H	101	CLA	CMB-C2B-C3B	2.73	129.96	124.89
22	b	607	CLA	C4A-NA-C1A	2.73	109.84	106.45
22	b	607	CLA	CMB-C2B-C3B	2.73	129.96	124.89
22	c	509	CLA	CMB-C2B-C3B	2.73	129.96	124.89
24	J	102	BCR	C27-C26-C25	2.74	126.76	122.74
22	h	101	CLA	CMB-C2B-C3B	2.74	129.98	124.89
22	b	615	CLA	C4A-NA-C1A	2.74	109.86	106.45
22	b	609	CLA	CMB-C2B-C3B	2.74	129.98	124.89
22	b	609	CLA	C4A-NA-C1A	2.75	109.86	106.45
31	i	102	LMT	O1'-C1'-C2'	2.75	112.73	108.23
22	C	520	CLA	CMB-C2B-C3B	2.76	130.01	124.89
22	B	611	CLA	C4A-NA-C1A	2.76	109.88	106.45
22	B	603	CLA	C4A-NA-C1A	2.76	109.88	106.45
22	A	404	CLA	CMB-C2B-C3B	2.76	130.02	124.89
22	B	603	CLA	CMB-C2B-C3B	2.77	130.03	124.89
22	B	614	CLA	CMB-C2B-C3B	2.77	130.03	124.89
22	B	605	CLA	CMB-C2B-C3B	2.78	130.05	124.89
22	C	510	CLA	C4A-NA-C1A	2.78	109.90	106.45
22	d	404	CLA	CMB-C2B-C3B	2.78	130.06	124.89
22	b	618	CLA	CMB-C2B-C3B	2.78	130.06	124.89
22	c	504	CLA	C4A-NA-C1A	2.78	109.91	106.45
25	b	601	DGD	O5D-C1E-C2E	2.79	112.78	108.23
22	D	405	CLA	CMB-C2B-C3B	2.79	130.06	124.89
26	C	519	LHG	O8-C23-C24	2.80	120.04	111.90
22	b	614	CLA	CMB-C2B-C3B	2.80	130.09	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	411	BCR	C29-C30-C25	2.80	114.86	110.48
26	c	519	LHG	O8-C23-C24	2.80	120.05	111.90
22	C	504	CLA	C4A-NA-C1A	2.81	109.94	106.45
22	B	604	CLA	CMB-C2B-C3B	2.81	130.11	124.89
22	D	406	CLA	CMB-C2B-C3B	2.82	130.13	124.89
22	b	608	CLA	CMB-C2B-C3B	2.82	130.13	124.89
22	c	511	CLA	CMB-C2B-C3B	2.84	130.16	124.89
22	d	405	CLA	CMB-C2B-C3B	2.84	130.17	124.89
24	c	521	BCR	C2-C1-C6	2.84	114.92	110.48
22	C	502	CLA	CMB-C2B-C3B	2.85	130.19	124.89
22	C	511	CLA	CMB-C2B-C3B	2.87	130.22	124.89
25	B	625	DGD	O5D-C1E-C2E	2.88	112.93	108.23
24	b	623	BCR	C2-C1-C6	2.89	114.99	110.48
24	f	102	BCR	C29-C30-C25	2.90	115.01	110.48
22	b	613	CLA	CMB-C2B-C3B	2.90	130.28	124.89
24	B	619	BCR	C2-C1-C6	2.91	115.03	110.48
22	c	503	CLA	CMB-C2B-C3B	2.92	130.30	124.89
30	b	602	SQD	C3-C4-C5	2.93	115.37	110.22
22	C	505	CLA	CMB-C2B-C3B	2.93	130.33	124.89
22	B	611	CLA	CMB-C2B-C3B	2.93	130.34	124.89
22	C	510	CLA	CMB-C2B-C3B	2.95	130.36	124.89
22	b	615	CLA	CMB-C2B-C3B	2.95	130.37	124.89
22	C	503	CLA	CMB-C2B-C3B	2.95	130.37	124.89
22	c	512	CLA	CMB-C2B-C3B	2.95	130.37	124.89
22	c	502	CLA	CMB-C2B-C3B	2.95	130.37	124.89
30	B	626	SQD	C3-C4-C5	2.96	115.43	110.22
26	A	409	LHG	O8-C23-C24	2.96	120.51	111.90
22	B	609	CLA	CMB-C2B-C3B	2.96	130.39	124.89
22	c	505	CLA	CMB-C2B-C3B	2.96	130.39	124.89
22	B	610	CLA	CMB-C2B-C3B	2.98	130.42	124.89
30	A	414	SQD	O8-S-C6	2.99	109.66	106.01
26	a	412	LHG	O8-C23-C24	2.99	120.60	111.90
22	A	405	CLA	CMB-C2B-C3B	2.99	130.44	124.89
22	C	512	CLA	CMB-C2B-C3B	3.00	130.46	124.89
24	b	622	BCR	C2-C1-C6	3.01	115.18	110.48
30	f	103	SQD	O6-C1-C2	3.01	113.15	108.23
30	A	413	SQD	O8-S-C6	3.01	109.69	106.01
22	b	617	CLA	CMB-C2B-C3B	3.02	130.49	124.89
22	a	408	CLA	CMB-C2B-C3B	3.02	130.50	124.89
30	b	602	SQD	O8-S-C6	3.03	109.70	106.01
22	c	510	CLA	CMB-C2B-C3B	3.03	130.52	124.89
30	A	414	SQD	C44-O6-C1	3.04	120.00	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	506	CLA	CMB-C2B-C3B	3.05	130.55	124.89
24	B	618	BCR	C2-C1-C6	3.05	115.24	110.48
22	B	613	CLA	CMB-C2B-C3B	3.06	130.57	124.89
22	C	506	CLA	CMB-C2B-C3B	3.06	130.58	124.89
24	a	410	BCR	C2-C1-C6	3.08	115.29	110.48
22	B	602	CLA	CMB-C2B-C3B	3.10	130.64	124.89
22	B	607	CLA	CMB-C2B-C3B	3.11	130.66	124.89
30	a	415	SQD	O8-S-C6	3.13	109.83	106.01
22	b	606	CLA	CMB-C2B-C3B	3.13	130.71	124.89
30	A	413	SQD	C3-C4-C5	3.14	115.75	110.22
22	b	611	CLA	CMB-C2B-C3B	3.15	130.75	124.89
30	a	401	SQD	O8-S-C6	3.16	109.87	106.01
30	B	626	SQD	O8-S-C6	3.17	109.88	106.01
22	C	507	CLA	CMB-C2B-C3B	3.18	130.79	124.89
30	D	403	SQD	C3-C4-C5	3.19	115.84	110.22
24	j	102	BCR	C2-C1-C6	3.21	115.50	110.48
24	J	102	BCR	C2-C1-C6	3.21	115.50	110.48
24	A	407	BCR	C2-C1-C6	3.22	115.51	110.48
30	a	415	SQD	C3-C4-C5	3.22	115.89	110.22
30	a	401	SQD	C44-O6-C1	3.23	120.38	113.76
22	c	507	CLA	CMB-C2B-C3B	3.24	130.90	124.89
30	F	102	SQD	O6-C1-C2	3.27	113.57	108.23
22	b	616	CLA	CMB-C2B-C3B	3.31	131.04	124.89
22	B	612	CLA	CMB-C2B-C3B	3.37	131.15	124.89
30	a	401	SQD	O47-C7-C8	3.37	118.56	111.55
30	d	402	SQD	C3-C4-C5	3.40	116.22	110.22
30	d	402	SQD	O47-C7-C8	3.41	118.63	111.55
30	f	103	SQD	O47-C7-C8	3.44	118.69	111.55
30	F	102	SQD	O47-C7-C8	3.48	118.77	111.55
30	D	403	SQD	O47-C7-C8	3.51	118.84	111.55
30	A	413	SQD	O5-C5-C4	3.52	116.14	109.66
30	F	102	SQD	O5-C5-C4	3.55	116.20	109.66
30	f	103	SQD	O5-C5-C4	3.58	116.25	109.66
30	A	414	SQD	O47-C7-C8	3.58	118.98	111.55
30	a	415	SQD	O5-C5-C4	3.67	116.42	109.66
24	c	513	BCR	C2-C1-C6	3.68	116.23	110.48
24	C	513	BCR	C2-C1-C6	3.71	116.28	110.48
30	a	401	SQD	O5-C5-C4	3.72	116.50	109.66
30	b	602	SQD	O47-C7-C8	3.77	119.37	111.55
30	B	626	SQD	O47-C7-C8	3.78	119.39	111.55
30	D	403	SQD	O8-S-C6	3.91	110.79	106.01
30	A	414	SQD	O5-C5-C4	3.93	116.91	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	LHG	O4-P-O5	3.96	132.80	112.28
26	c	519	LHG	O4-P-O5	3.97	132.82	112.28
26	C	519	LHG	O4-P-O5	3.97	132.83	112.28
30	B	626	SQD	O5-C5-C4	3.98	116.99	109.66
30	b	602	SQD	O5-C5-C4	3.98	116.99	109.66
26	a	412	LHG	O4-P-O5	3.99	132.92	112.28
30	a	415	SQD	O47-C7-C8	4.04	119.94	111.55
30	f	103	SQD	O9-S-C6	4.05	110.29	106.83
30	A	413	SQD	O47-C7-C8	4.06	119.99	111.55
30	d	402	SQD	O8-S-C6	4.07	110.97	106.01
30	D	403	SQD	O5-C5-C4	4.20	117.40	109.66
30	d	402	SQD	O6-C1-C2	4.28	115.22	108.23
30	d	402	SQD	O5-C5-C4	4.29	117.55	109.66
30	D	403	SQD	O6-C1-C2	4.32	115.28	108.23
30	F	102	SQD	O9-S-C6	4.46	110.64	106.83
30	f	103	SQD	O8-S-C6	4.54	111.55	106.01
30	F	102	SQD	O8-S-C6	4.55	111.57	106.01
30	A	413	SQD	O6-C1-C2	4.74	115.97	108.23
30	A	414	SQD	O9-S-C6	4.95	111.06	106.83
30	a	415	SQD	O6-C1-C2	5.03	116.45	108.23
23	a	409	PL9	C7-C3-C4	5.14	121.06	116.88
30	d	402	SQD	O7-S-C6	5.15	111.23	106.83
30	B	626	SQD	O6-C1-C2	5.18	116.68	108.23
30	A	413	SQD	O7-S-C6	5.22	111.29	106.83
23	D	407	PL9	C7-C3-C4	5.24	121.14	116.88
30	a	415	SQD	O7-S-C6	5.27	111.33	106.83
30	a	401	SQD	O9-S-C6	5.30	111.36	106.83
23	d	406	PL9	C7-C3-C4	5.31	121.19	116.88
30	b	602	SQD	O6-C1-C2	5.37	116.99	108.23
23	A	406	PL9	C7-C3-C4	5.38	121.25	116.88
30	D	403	SQD	O7-S-C6	5.44	111.47	106.83
23	J	101	PL9	C7-C3-C4	5.58	121.41	116.88
23	j	101	PL9	C7-C3-C4	5.66	121.48	116.88
30	D	403	SQD	O9-S-C6	5.73	111.72	106.83
30	d	402	SQD	O9-S-C6	5.79	111.78	106.83
30	F	102	SQD	O7-S-C6	5.84	111.82	106.83
30	B	626	SQD	O9-S-C6	5.85	111.82	106.83
30	b	602	SQD	O9-S-C6	5.89	111.86	106.83
30	B	626	SQD	O7-S-C6	6.01	111.96	106.83
30	f	103	SQD	O7-S-C6	6.13	112.06	106.83
30	a	401	SQD	O7-S-C6	6.16	112.09	106.83
30	b	602	SQD	O7-S-C6	6.28	112.20	106.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	414	SQD	O7-S-C6	6.30	112.21	106.83
30	a	415	SQD	O9-S-C6	7.31	113.08	106.83
30	A	413	SQD	O9-S-C6	7.65	113.36	106.83

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	D	406	CLA	NC
22	D	406	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	d	404	CLA	NC
22	d	404	CLA	ND
22	d	404	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	c	520	CLA	NC
22	c	520	CLA	ND
22	c	520	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA

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Mol	Chain	Res	Type	Atom
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND
22	b	619	CLA	NA
22	C	520	CLA	NC
22	C	520	CLA	ND
22	C	520	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA

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Mol	Chain	Res	Type	Atom
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	a	408	CLA	NC
22	a	408	CLA	ND
22	a	408	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA

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Mol	Chain	Res	Type	Atom
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	ND
22	d	405	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA

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Mol	Chain	Res	Type	Atom
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND
22	a	404	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA

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Mol	Chain	Res	Type	Atom
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

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
30	d	402	SQD	C45-O47-C7-C8
30	D	403	SQD	C45-O47-C7-C8

There are no ring outliers.

80 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	11	0
22	A	403	CLA	12	0
22	A	404	CLA	16	0
22	A	405	CLA	8	0
23	A	406	PL9	3	0
24	A	407	BCR	2	0
25	A	408	DGD	1	0
26	A	409	LHG	3	0
27	A	410	LMG	2	0
30	A	413	SQD	3	0
30	A	414	SQD	3	0
27	A	415	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	10	0
22	B	605	CLA	6	0
22	B	606	CLA	16	0
22	B	607	CLA	10	0
22	B	608	CLA	14	0
22	B	609	CLA	3	0
22	B	610	CLA	6	0
22	B	611	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	6	0
24	B	617	BCR	1	0
24	B	618	BCR	3	0
24	B	619	BCR	2	0
25	B	620	DGD	2	0
27	B	621	LMG	3	0
31	B	622	LMT	2	0
27	B	624	LMG	3	0
25	B	625	DGD	2	0
30	B	626	SQD	3	0
31	B	627	LMT	2	0
31	B	628	LMT	2	0
22	C	501	CLA	6	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	4	0
22	C	509	CLA	6	0
22	C	510	CLA	10	0
22	C	511	CLA	1	0
22	C	512	CLA	3	0
24	C	513	BCR	8	0
24	C	514	BCR	7	0
25	C	515	DGD	3	0
25	C	516	DGD	4	0
25	C	517	DGD	5	0
27	C	518	LMG	4	0
26	C	519	LHG	2	0
22	C	520	CLA	5	0
24	C	521	BCR	5	0
27	C	522	LMG	3	0
32	D	401	PHO	11	0
32	D	402	PHO	5	0
30	D	403	SQD	3	0
22	D	405	CLA	11	0
22	D	406	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	407	PL9	8	0
27	D	408	LMG	6	0
25	D	409	DGD	2	0
24	D	411	BCR	3	0
27	D	412	LMG	1	0
27	E	101	LMG	1	0
34	F	101	HEM	4	0
30	F	102	SQD	2	0
22	H	101	CLA	11	0
24	H	102	BCR	1	0
27	I	101	LMG	1	0
31	I	102	LMT	1	0
24	J	102	BCR	2	0
27	M	101	LMG	1	0
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%)	0.42	28 (8%) 12 12	172, 174, 175, 176	0
1	a	335/344 (97%)	0.45	28 (8%) 12 12	172, 174, 175, 176	0
2	B	490/510 (96%)	0.22	31 (6%) 21 18	172, 174, 175, 176	0
2	b	490/510 (96%)	0.28	16 (3%) 47 39	172, 174, 175, 176	0
3	C	447/461 (96%)	0.25	24 (5%) 26 23	172, 174, 175, 176	0
3	c	447/461 (96%)	0.13	16 (3%) 43 36	173, 174, 175, 176	0
4	D	340/352 (96%)	0.17	7 (2%) 64 56	171, 174, 175, 176	0
4	d	340/352 (96%)	0.17	10 (2%) 52 44	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.06	1 (1%) 79 72	172, 174, 175, 175	0
5	e	82/84 (97%)	0.02	3 (3%) 42 35	173, 174, 175, 177	0
6	F	35/45 (77%)	-0.14	1 (2%) 52 44	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.45	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.41	7 (10%) 6 8	173, 174, 175, 176	0
7	h	65/66 (98%)	0.71	8 (12%) 5 7	173, 174, 175, 176	0
8	I	35/38 (92%)	0.24	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	-0.12	0 100 100	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.11	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	-0.43	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.31	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	0.15	1 (2%) 55 46	174, 174, 175, 176	0
11	L	37/37 (100%)	0.34	1 (2%) 55 46	172, 174, 175, 175	0
11	l	37/37 (100%)	0.15	1 (2%) 55 46	173, 174, 175, 176	0
12	M	34/36 (94%)	0.21	1 (2%) 52 44	172, 174, 174, 176	0
12	m	34/36 (94%)	0.10	2 (5%) 23 19	173, 173, 174, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.47	16 (6%) 19 16	172, 174, 175, 176	0
13	o	243/272 (89%)	0.47	14 (5%) 24 20	172, 174, 175, 176	0
14	T	32/32 (100%)	0.25	2 (6%) 21 18	173, 174, 176, 176	0
14	t	32/32 (100%)	0.35	2 (6%) 21 18	173, 174, 175, 176	0
15	U	97/134 (72%)	0.47	7 (7%) 16 14	172, 174, 174, 175	0
15	u	97/134 (72%)	0.62	9 (9%) 9 10	173, 174, 175, 175	0
16	V	137/163 (84%)	0.05	0 100 100	172, 174, 175, 175	0
16	v	137/163 (84%)	0.49	11 (8%) 13 13	173, 174, 175, 176	0
17	g	28/46 (60%)	0.32	1 (3%) 43 36	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.05	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	0.33	1 (2%) 55 46	173, 174, 175, 176	0
18	x	37/41 (90%)	0.85	7 (18%) 1 4	173, 175, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.25	1 (1%) 72 64	173, 174, 175, 176	0
20	z	62/62 (100%)	0.88	5 (8%) 13 12	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.27	262 (5%) 30 25	171, 174, 175, 177	0

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.4
1	a	224	ILE	5.3
5	e	84	LYS	5.0
15	U	38	GLU	4.9
3	C	135	ARG	4.6
13	O	90	GLU	4.4
3	C	332	GLN	4.3
5	E	84	LYS	4.3
14	t	31	LYS	4.3
1	a	165	GLN	4.3
1	a	191	ASN	4.2
7	h	66	GLY	4.1
4	d	295	SER	4.1
7	h	23	PRO	3.9
14	t	32	LYS	3.9
1	A	299	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
7	h	26	GLY	3.8
2	b	217	ILE	3.8
1	A	175	GLY	3.8
3	c	200	THR	3.7
1	a	225	ARG	3.7
13	o	169	LYS	3.7
7	H	56	ASP	3.7
18	x	42	GLN	3.7
20	z	1	MET	3.7
2	B	69	LEU	3.7
10	k	14	ALA	3.6
15	U	39	LEU	3.6
18	x	12	ILE	3.6
15	u	53	GLU	3.5
3	C	136	GLY	3.4
3	C	184	GLY	3.4
1	A	190	HIS	3.4
2	B	162	PHE	3.4
5	e	82	GLN	3.4
3	C	147	PHE	3.4
1	a	175	GLY	3.3
1	A	293	MET	3.3
15	u	58	ASN	3.3
3	C	137	PRO	3.3
1	a	282	GLY	3.3
2	B	295	GLY	3.3
3	C	140	LEU	3.3
7	H	66	GLY	3.2
14	T	28	ARG	3.2
7	h	4	ARG	3.2
1	A	177	SER	3.2
3	c	201	ASN	3.2
2	B	309	LEU	3.1
7	H	5	THR	3.1
1	a	223	LEU	3.1
1	a	190	HIS	3.1
4	D	190	ASN	3.1
1	A	15	GLU	3.1
3	c	372	PRO	3.1
3	C	402	GLY	3.1
16	v	51	GLN	3.1
2	B	259	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	b	411	PHE	3.1
3	c	202	PRO	3.1
1	A	266	ASN	3.0
1	a	325	ASN	3.0
13	o	124	GLU	3.0
2	b	379	ALA	3.0
7	h	24	GLY	3.0
1	a	178	GLY	3.0
1	A	179	THR	3.0
7	H	63	LYS	3.0
2	B	179	GLN	3.0
2	b	303	SER	3.0
15	u	74	THR	3.0
14	T	27	PRO	3.0
16	v	47	LEU	2.9
1	a	226	GLU	2.9
18	X	42	GLN	2.9
13	o	31	LEU	2.9
15	U	40	VAL	2.9
2	B	474	LEU	2.9
1	A	298	ASN	2.9
13	o	240	THR	2.9
18	x	17	LYS	2.9
3	C	149	TYR	2.8
1	A	138	GLY	2.8
2	b	301	ALA	2.8
16	v	131	ARG	2.8
7	H	64	ALA	2.8
15	u	107	GLU	2.8
2	b	218	LEU	2.8
3	c	403	SER	2.8
1	A	196	PRO	2.8
1	A	181	ASN	2.8
15	u	65	PHE	2.8
2	B	132	ALA	2.8
7	h	3	ARG	2.8
1	A	195	HIS	2.8
13	O	222	GLN	2.8
2	b	482	ILE	2.8
1	a	299	GLY	2.8
2	B	164	PRO	2.8
4	D	24	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
13	O	79	LYS	2.7
4	d	221	THR	2.7
12	m	5	GLN	2.7
13	O	170	GLY	2.7
13	O	218	LEU	2.7
13	O	262	GLN	2.7
1	a	181	ASN	2.6
13	o	173	ASN	2.6
2	B	294	SER	2.6
3	C	44	ASN	2.6
16	v	133	LEU	2.6
15	u	57	LEU	2.6
3	c	329	GLY	2.6
1	a	19	ASN	2.6
1	a	239	PHE	2.6
15	u	72	TYR	2.6
3	C	266	TRP	2.5
3	C	473	ASP	2.5
13	O	46	PRO	2.5
4	D	174	GLY	2.5
13	O	269	ILE	2.5
3	C	151	TRP	2.5
1	a	198	HIS	2.5
6	F	11	VAL	2.5
1	a	187	GLN	2.5
1	A	10	SER	2.5
4	d	236	ASN	2.5
3	c	260	ALA	2.5
13	O	84	ASN	2.5
2	B	127	ARG	2.5
2	b	120	LEU	2.5
2	B	477	ASP	2.5
2	b	490	GLN	2.4
11	L	33	SER	2.4
18	x	16	LEU	2.4
2	B	402	TYR	2.4
7	h	18	TYR	2.4
13	o	154	SER	2.4
13	o	239	GLY	2.4
2	B	161	LEU	2.4
20	z	4	LEU	2.4
2	b	119	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
13	O	195	ASP	2.4
13	O	91	PHE	2.4
16	v	138	LEU	2.4
13	O	58	ILE	2.4
1	A	222	SER	2.4
3	C	148	GLY	2.4
3	C	183	GLY	2.4
1	A	178	GLY	2.4
4	d	195	PRO	2.4
13	o	168	PHE	2.4
20	z	47	TRP	2.4
1	A	14	TRP	2.3
16	v	31	PRO	2.3
2	B	129	GLY	2.3
15	u	52	GLY	2.3
1	a	170	ASP	2.3
16	v	130	MET	2.3
3	c	203	THR	2.3
1	a	319	ASP	2.3
12	M	2	GLU	2.3
7	h	27	THR	2.3
3	C	144	SER	2.3
17	g	27	MET	2.3
2	B	128	THR	2.3
3	c	373	ASN	2.3
2	B	293	ALA	2.3
2	b	302	TRP	2.3
2	b	402	TYR	2.3
15	u	75	LEU	2.3
3	c	180	MET	2.3
13	o	189	GLY	2.3
1	a	137	LEU	2.3
2	b	133	LEU	2.3
4	d	194	ASN	2.3
15	U	121	LEU	2.3
2	B	397	VAL	2.3
13	O	169	LYS	2.3
13	o	84	ASN	2.3
1	A	165	GLN	2.3
12	m	2	GLU	2.3
15	U	127	ARG	2.3
3	c	259	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	a	199	GLN	2.2
2	b	339	ALA	2.2
16	v	103	LYS	2.2
1	A	80	GLY	2.2
4	d	13	GLY	2.2
2	b	420	TYR	2.2
3	C	261	ARG	2.2
4	d	176	ALA	2.2
2	B	130	GLU	2.2
3	C	134	ILE	2.2
3	C	154	LYS	2.2
1	a	169	SER	2.2
4	d	203	GLY	2.2
1	A	262	TYR	2.2
1	a	301	ASN	2.2
2	B	125	ASP	2.2
13	o	238	ALA	2.2
15	U	122	VAL	2.2
3	C	141	GLU	2.2
3	c	191	PRO	2.2
2	B	411	PHE	2.2
18	x	13	THR	2.2
3	C	336	GLY	2.2
1	A	169	SER	2.2
1	A	16	ARG	2.2
1	A	75	ASN	2.2
5	e	8	ARG	2.2
4	d	220	ASN	2.2
2	B	122	LEU	2.2
3	C	46	SER	2.2
2	B	84	THR	2.2
2	b	216	HIS	2.2
20	Z	62	VAL	2.2
1	a	298	ASN	2.2
1	a	177	SER	2.2
7	H	55	LEU	2.2
1	A	76	ASN	2.2
20	z	30	PRO	2.1
3	C	403	SER	2.1
13	O	119	LEU	2.1
3	C	212	TYR	2.1
2	B	354	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	297	ASP	2.1
3	c	365	TRP	2.1
15	U	54	LYS	2.1
4	D	192	THR	2.1
2	B	133	LEU	2.1
4	D	194	ASN	2.1
13	O	171	GLU	2.1
20	z	29	SER	2.1
3	c	212	TYR	2.1
11	l	1	MET	2.1
16	v	132	ASN	2.1
4	d	297	ASP	2.1
7	H	62	TRP	2.1
18	x	23	LEU	2.1
2	B	124	ARG	2.1
1	A	183	MET	2.1
2	B	163	GLY	2.1
1	A	11	ALA	2.1
3	c	388	GLN	2.1
1	a	173	PRO	2.1
1	a	322	ASN	2.1
2	B	183	PRO	2.1
13	o	216	PHE	2.1
1	a	179	THR	2.1
2	B	166	MET	2.1
4	D	197	HIS	2.1
16	v	117	VAL	2.0
13	O	50	ASP	2.0
3	c	405	ASN	2.0
16	v	141	ILE	2.0
1	A	12	ASN	2.0
13	o	164	THR	2.0
1	A	342	ASP	2.0
13	o	125	ASP	2.0
2	B	131	PRO	2.0
2	B	326	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
31	LMT	i	102	35/35	0.52	1.30	9.06	173,175,176,177	0
24	BCR	B	619	40/40	0.80	0.83	7.14	172,173,174,175	0
25	DGD	D	409	63/66	0.70	0.81	6.82	172,174,176,178	0
24	BCR	y	101	40/40	0.78	0.99	6.67	173,173,174,175	0
31	LMT	D	410	31/35	0.63	0.93	6.54	174,175,176,176	0
24	BCR	b	623	40/40	0.80	0.76	6.35	171,173,174,174	0
27	LMG	c	518	45/55	0.72	1.00	6.01	172,174,176,176	0
25	DGD	d	408	63/66	0.66	0.77	5.36	172,175,177,178	0
24	BCR	c	521	40/40	0.81	1.26	5.31	172,174,175,175	0
27	LMG	C	518	45/55	0.61	1.09	5.29	171,174,175,175	0
33	BCT	d	403	4/4	0.91	0.92	5.20	174,174,175,176	0
31	LMT	I	102	35/35	0.41	0.92	4.70	173,175,176,178	0
31	LMT	b	627	35/35	0.54	1.22	4.57	173,175,177,177	0
22	CLA	a	408	65/65	0.74	0.81	4.42	173,174,175,175	0
24	BCR	a	410	40/40	0.73	0.67	4.33	172,173,174,175	0
24	BCR	C	513	40/40	0.87	0.77	4.10	172,173,174,174	0
22	CLA	A	405	65/65	0.83	0.62	3.75	172,174,175,176	0
22	CLA	b	605	65/65	0.60	1.14	3.53	172,175,176,176	0
22	CLA	D	406	65/65	0.88	0.63	3.26	172,174,175,176	0
24	BCR	f	102	40/40	0.64	0.47	3.20	171,173,175,175	0
23	PL9	J	101	35/55	0.44	0.53	3.05	172,175,176,176	0
23	PL9	j	101	35/55	0.50	0.37	3.04	173,175,175,176	0
24	BCR	J	102	40/40	0.50	0.44	3.02	172,174,176,177	0
24	BCR	g	101	40/40	0.63	0.78	2.98	173,174,175,175	0
24	BCR	c	513	40/40	0.83	0.87	2.93	172,173,175,175	0
30	SQD	a	401	54/54	0.84	0.58	2.92	172,174,176,178	0
30	SQD	d	402	43/54	0.74	0.84	2.91	172,174,176,178	0
31	LMT	B	623	35/35	0.78	0.50	2.84	173,174,177,177	0
27	LMG	M	101	42/55	0.73	0.53	2.74	173,174,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	LMG	A	415	42/55	0.62	0.53	2.64	171,174,176,177	0
25	DGD	B	625	52/66	0.76	0.57	2.59	172,175,177,177	0
24	BCR	H	102	40/40	0.68	0.94	2.58	173,174,175,176	0
25	DGD	b	601	52/66	0.72	0.47	2.48	172,174,176,177	0
24	BCR	B	617	40/40	0.75	0.44	2.48	172,173,174,174	0
22	CLA	B	601	65/65	0.62	0.85	2.43	172,175,176,177	0
24	BCR	B	618	40/40	0.83	0.32	2.41	171,172,174,174	0
24	BCR	C	514	40/40	0.78	0.83	2.36	172,173,175,175	0
30	SQD	f	103	45/54	0.84	0.52	2.31	172,174,176,178	0
22	CLA	c	512	65/65	0.77	0.69	2.30	172,174,176,176	0
22	CLA	b	607	65/65	0.82	0.43	2.22	172,173,175,176	0
22	CLA	c	508	65/65	0.84	0.56	2.21	172,174,175,175	0
22	CLA	b	606	65/65	0.85	0.61	2.20	172,173,174,174	0
24	BCR	C	521	40/40	0.78	0.82	2.06	172,174,175,176	0
24	BCR	b	622	40/40	0.77	0.37	2.00	171,172,173,173	0
22	CLA	b	613	65/65	0.81	0.67	1.79	172,174,175,175	0
31	LMT	B	627	35/35	0.75	0.55	1.78	172,175,177,177	0
24	BCR	D	411	40/40	0.67	0.44	1.72	171,173,174,175	0
22	CLA	b	609	65/65	0.81	0.55	1.70	172,174,175,175	0
22	CLA	B	611	65/65	0.92	0.36	1.70	171,173,174,174	0
22	CLA	B	603	65/65	0.81	0.49	1.68	171,173,175,175	0
27	LMG	D	412	46/55	0.77	0.39	1.65	172,174,175,175	0
22	CLA	b	608	65/65	0.88	0.50	1.64	172,173,175,176	0
22	CLA	c	511	65/65	0.89	0.61	1.62	172,174,175,176	0
22	CLA	C	508	65/65	0.88	0.86	1.61	172,174,175,175	0
22	CLA	c	503	65/65	0.82	0.56	1.61	172,174,175,175	0
22	CLA	B	604	65/65	0.87	0.68	1.59	172,173,175,175	0
22	CLA	c	506	65/65	0.86	0.55	1.53	173,174,175,175	0
22	CLA	C	506	65/65	0.77	0.72	1.51	172,174,175,175	0
22	CLA	C	502	65/65	0.69	0.53	1.51	173,174,174,175	0
27	LMG	a	402	42/55	0.66	0.49	1.49	171,174,176,176	0
24	BCR	c	514	40/40	0.68	0.70	1.42	172,173,175,175	0
22	CLA	b	615	65/65	0.92	0.40	1.39	172,173,174,175	0
31	LMT	b	603	35/35	0.80	0.44	1.39	172,174,175,176	0
22	CLA	h	101	65/65	0.78	0.54	1.39	171,174,175,175	0
31	LMT	d	409	31/35	0.53	0.66	1.36	172,175,177,177	0
24	BCR	B	616	40/40	0.71	0.43	1.31	172,173,174,175	0
22	CLA	C	511	65/65	0.90	0.91	1.30	172,174,175,175	0
30	SQD	F	102	45/54	0.78	0.69	1.28	172,175,177,178	0
31	LMT	b	604	35/35	0.69	0.48	1.26	172,174,176,176	0
30	SQD	B	626	47/54	0.79	0.46	1.25	170,174,176,178	0
25	DGD	b	624	58/66	0.76	0.41	1.24	171,173,174,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	CLA	c	501	65/65	0.85	0.45	1.22	172,174,175,175	0
25	DGD	A	408	56/66	0.71	0.45	1.22	172,174,175,176	0
22	CLA	B	609	65/65	0.86	0.53	1.20	172,174,175,175	0
22	CLA	c	510	65/65	0.86	0.53	1.19	173,174,175,176	0
27	LMG	C	522	48/55	0.73	0.36	1.14	172,174,174,175	0
24	BCR	A	407	40/40	0.79	0.47	1.13	171,173,174,174	0
22	CLA	b	619	65/65	0.64	0.77	1.12	172,174,175,175	0
22	CLA	b	612	65/65	0.84	0.66	1.09	171,174,175,176	0
24	BCR	j	102	40/40	0.62	0.34	1.08	173,175,177,178	0
27	LMG	E	101	44/55	0.62	0.57	1.08	170,174,176,177	0
27	LMG	a	413	51/55	0.69	0.42	1.04	172,173,175,176	0
22	CLA	B	608	65/65	0.90	0.50	1.01	172,174,175,175	0
22	CLA	c	502	65/65	0.66	0.54	1.00	173,174,175,175	0
23	PL9	a	409	45/55	0.76	0.38	0.97	171,173,174,175	0
30	SQD	A	414	54/54	0.85	0.41	0.96	171,174,176,179	0
22	CLA	d	405	65/65	0.86	0.45	0.95	172,174,175,175	0
24	BCR	x	101	40/40	0.71	0.86	0.93	173,174,175,175	0
25	DGD	a	411	56/66	0.74	0.43	0.92	173,174,175,176	0
22	CLA	C	512	65/65	0.83	0.88	0.91	172,174,176,177	0
22	CLA	B	614	65/65	0.89	0.62	0.87	172,174,175,175	0
34	HEM	F	101	43/43	0.91	0.48	0.86	173,174,175,176	0
22	CLA	b	618	65/65	0.82	0.67	0.86	172,174,175,175	0
31	LMT	B	628	35/35	0.67	0.46	0.85	172,174,177,178	0
34	HEM	V	201	43/43	0.88	0.45	0.81	172,173,175,175	0
27	LMG	m	101	42/55	0.79	0.44	0.80	170,174,175,175	0
22	CLA	B	605	65/65	0.86	0.72	0.78	172,173,175,176	0
30	SQD	b	602	47/54	0.80	0.38	0.73	171,174,176,178	0
22	CLA	C	503	65/65	0.85	0.41	0.71	172,174,175,176	0
22	CLA	C	505	65/65	0.79	0.45	0.68	172,174,175,176	0
22	CLA	B	602	65/65	0.92	0.52	0.62	171,173,174,175	0
22	CLA	B	615	65/65	0.85	0.66	0.57	172,174,175,175	0
22	CLA	B	613	65/65	0.76	0.45	0.56	172,174,174,175	0
27	LMG	e	101	44/55	0.75	0.39	0.54	171,174,175,176	0
22	CLA	C	501	65/65	0.87	0.40	0.53	172,174,174,175	0
22	CLA	c	504	65/65	0.89	0.33	0.53	172,174,175,175	0
22	CLA	b	617	65/65	0.82	0.45	0.47	173,173,175,176	0
22	CLA	B	607	65/65	0.85	0.42	0.43	172,174,174,175	0
34	HEM	f	101	43/43	0.93	0.34	0.41	173,174,175,175	0
22	CLA	A	404	65/65	0.87	0.46	0.41	170,173,174,175	0
22	CLA	a	405	65/65	0.84	0.58	0.39	170,172,174,175	0
22	CLA	b	616	65/65	0.95	0.29	0.39	171,173,174,175	0
25	DGD	C	515	53/66	0.83	0.36	0.38	172,173,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	CLA	C	510	65/65	0.83	0.47	0.37	172,173,175,175	0
34	HEM	v	201	43/43	0.90	0.55	0.37	171,174,175,175	0
22	CLA	C	507	65/65	0.77	0.40	0.33	173,174,175,177	0
22	CLA	c	505	65/65	0.85	0.45	0.33	172,174,175,175	0
22	CLA	C	509	65/65	0.85	0.34	0.33	173,173,174,174	0
22	CLA	C	504	65/65	0.84	0.41	0.32	171,173,175,175	0
22	CLA	A	403	65/65	0.93	0.54	0.29	171,173,174,175	0
23	PL9	A	406	45/55	0.70	0.43	0.29	172,174,175,175	0
22	CLA	H	101	65/65	0.85	0.35	0.28	172,174,175,175	0
30	SQD	D	403	43/54	0.82	0.41	0.26	172,174,177,180	0
25	DGD	c	515	53/66	0.86	0.37	0.25	171,174,175,177	0
32	PHO	D	402	64/64	0.79	0.37	0.20	171,173,175,175	0
27	LMG	A	410	51/55	0.79	0.35	0.19	171,173,174,175	0
22	CLA	a	404	65/65	0.88	0.55	0.17	172,173,174,176	0
30	SQD	A	413	51/54	0.73	0.37	0.13	172,174,175,176	0
28	CL	A	411	1/1	0.75	0.46	0.09	172,172,172,172	0
24	BCR	b	621	40/40	0.86	0.33	0.09	171,173,174,174	0
32	PHO	D	401	64/64	0.84	0.40	0.09	171,173,174,175	0
31	LMT	M	103	35/35	0.77	0.47	0.07	172,173,175,176	0
26	LHG	c	519	37/49	0.75	0.35	0.05	172,174,178,181	0
22	CLA	B	610	65/65	0.84	0.34	0.04	172,174,174,175	0
32	PHO	d	401	64/64	0.72	0.42	0.04	172,173,174,174	0
22	CLA	b	611	65/65	0.92	0.31	0.02	172,174,175,175	0
24	BCR	b	620	40/40	0.90	0.32	0.01	172,173,174,175	0
27	LMG	D	408	48/55	0.86	0.28	0.01	170,173,175,175	0
23	PL9	D	407	55/55	0.68	0.39	-0.02	171,173,174,175	0
27	LMG	d	410	46/55	0.91	0.23	-0.07	172,173,175,175	0
22	CLA	d	404	65/65	0.84	0.46	-0.08	172,173,174,174	0
22	CLA	b	614	65/65	0.88	0.30	-0.11	172,173,174,175	0
22	CLA	A	402	65/65	0.90	0.43	-0.12	172,173,174,175	0
27	LMG	c	522	48/55	0.81	0.30	-0.14	172,174,175,176	0
23	PL9	d	406	55/55	0.69	0.38	-0.16	172,173,175,175	0
25	DGD	B	620	58/66	0.84	0.33	-0.16	171,173,175,176	0
30	SQD	a	415	51/54	0.85	0.29	-0.18	173,174,175,176	0
22	CLA	C	520	65/65	0.82	0.33	-0.19	172,174,175,176	0
22	CLA	c	509	65/65	0.88	0.32	-0.21	172,173,175,175	0
27	LMG	b	625	49/55	0.78	0.34	-0.23	172,174,175,175	0
26	LHG	C	519	37/49	0.64	0.48	-0.24	172,174,179,183	0
22	CLA	c	520	65/65	0.87	0.35	-0.27	173,174,174,175	0
22	CLA	b	610	65/65	0.90	0.33	-0.34	172,173,175,175	0
31	LMT	M	102	35/35	0.77	0.46	-0.36	172,174,175,175	0
22	CLA	a	406	65/65	0.85	0.36	-0.38	172,174,175,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	DGD	c	517	66/66	0.79	0.35	-0.45	172,173,175,176	0
26	LHG	A	409	39/49	0.85	0.28	-0.46	172,173,175,176	0
22	CLA	B	606	65/65	0.88	0.34	-0.47	172,173,174,175	0
22	CLA	D	405	65/65	0.89	0.37	-0.49	172,173,174,175	0
27	LMG	d	407	48/55	0.87	0.27	-0.50	171,173,175,175	0
25	DGD	C	517	66/66	0.77	0.34	-0.54	172,173,174,175	0
26	LHG	a	412	39/49	0.83	0.28	-0.56	171,174,176,177	0
22	CLA	c	507	65/65	0.91	0.25	-0.58	172,174,175,176	0
22	CLA	B	612	65/65	0.91	0.28	-0.60	171,173,175,175	0
27	LMG	B	624	49/55	0.78	0.30	-0.66	171,173,174,175	0
29	OEX	A	412	10/10	0.93	0.43	-0.70	165,169,172,173	0
32	PHO	a	407	64/64	0.86	0.26	-0.72	173,174,175,175	0
29	OEX	a	414	10/10	0.96	0.45	-0.77	168,171,173,177	0
25	DGD	C	516	62/66	0.84	0.29	-0.78	171,174,175,176	0
33	BCT	D	404	4/4	0.95	0.25	-0.92	173,174,174,174	0
25	DGD	c	516	62/66	0.87	0.30	-0.94	172,174,175,175	0
27	LMG	b	628	49/55	0.93	0.23	-1.28	172,174,175,175	0
27	LMG	B	621	49/55	0.88	0.26	-1.49	172,173,174,174	0
28	CL	a	416	1/1	0.91	0.34	-2.14	173,173,173,173	0
21	FE2	A	401	1/1	0.91	0.19	-2.52	170,170,170,170	0
21	FE2	a	403	1/1	0.85	0.18	-3.12	175,175,175,175	0
35	CA	K	101	1/1	0.81	0.35	-	177,177,177,177	0
35	CA	O	301	1/1	0.53	0.38	-	177,177,177,177	0
35	CA	k	101	1/1	0.78	0.20	-	172,172,172,172	0
27	LMG	i	101	43/55	0.75	0.80	-	172,174,177,178	0
27	LMG	I	101	43/55	0.65	1.04	-	172,174,177,177	0
31	LMT	b	626	35/35	0.59	0.69	-	172,175,176,177	0
31	LMT	B	622	35/35	0.65	0.86	-	171,175,177,177	0
35	CA	o	301	1/1	0.31	0.73	-	180,180,180,180	0

6.5 Other polymers ⓘ

There are no such residues in this entry.