



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:45 PM GMT

PDB ID : 4IXR
Title : RT fs X-ray diffraction of Photosystem II, first illuminated state
Authors : Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on : 2013-01-27
Resolution : 5.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

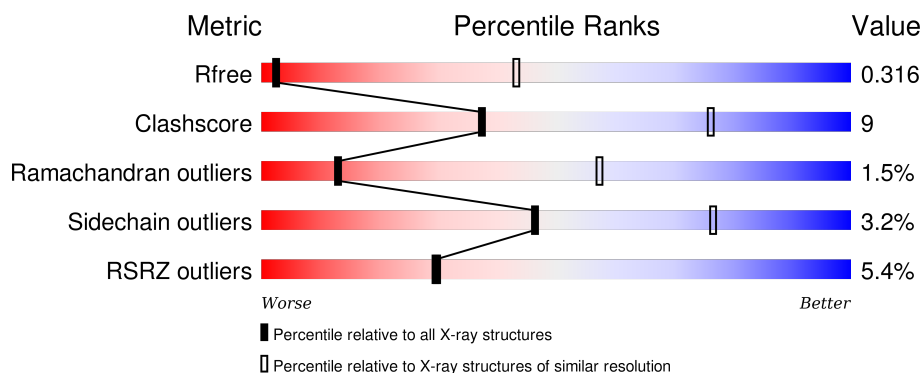
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1000 (8.00-3.66)
Clashscore	102246	1048 (8.00-3.70)
Ramachandran outliers	100387	1021 (8.00-3.66)
Sidechain outliers	100360	1010 (8.00-3.64)
RSRZ outliers	91569	1015 (8.00-3.64)

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	360	<div> <div>3%</div> <div>61%</div> <div>31%</div> <div>7%</div> </div>
1	a	360	<div> <div>%</div> <div>91%</div> <div>7%</div> </div>
2	B	510	<div> <div>6%</div> <div>67%</div> <div>27%</div> <div>.</div> </div>
2	b	510	<div> <div>7%</div> <div>93%</div> <div>.</div> </div>

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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	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	BCT	d	401	-	-	-	X
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	X	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	X
23	CLA	B	601	X	-	-	X
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	X
23	CLA	B	604	X	-	-	X
23	CLA	B	605	X	-	-	X
23	CLA	B	606	X	-	-	X
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	X
23	CLA	B	609	X	-	-	X
23	CLA	B	610	X	-	-	X
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	X
23	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	X
23	CLA	B	616	X	-	-	X
23	CLA	C	501	X	-	-	X
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	X
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	X
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	X
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	X
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	X
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	X
23	CLA	b	605	X	-	-	X
23	CLA	b	606	X	-	-	X
23	CLA	b	607	X	-	-	X
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	X
23	CLA	b	610	X	-	-	X
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	X
23	CLA	b	613	X	-	-	X
23	CLA	b	614	X	-	-	X
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	X
23	CLA	b	620	X	-	-	X
23	CLA	c	501	X	-	-	X
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	X
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	X
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	X
23	CLA	c	510	X	-	-	X
23	CLA	c	511	X	-	-	X
23	CLA	c	512	X	-	-	X
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	X
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	a	410	-	-	-	X
25	PL9	j	101	-	-	-	X
26	OEC	A	409	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	514	-	-	-	X
27	BCR	C	515	-	-	-	X
27	BCR	C	516	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	622	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	h	101	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	y	101	-	-	-	X
27	BCR	z	101	-	-	-	X
28	DGD	B	627	-	-	-	X
28	DGD	C	519	-	-	-	X
28	DGD	D	409	-	-	-	X
28	DGD	b	602	-	-	-	X
28	DGD	d	409	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	414	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	D	408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	b	601	-	-	-	X
30	SQD	d	408	-	-	-	X
30	SQD	f	102	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	521	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	519	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	101	-	-	-	X
31	LMG	k	103	-	-	-	X
32	CL	A	416	-	-	-	X
32	CL	a	418	-	-	-	X
33	LMT	B	625	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	B	629	-	-	-	X
33	LMT	D	410	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	M	102	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	604	-	-	-	X
33	LMT	b	627	-	-	-	X
33	LMT	d	410	-	-	-	X
33	LMT	i	102	-	-	-	X
33	LMT	m	101	-	-	-	X
34	HEM	F	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	f	101	-	-	-	X
34	HEM	v	201	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	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 Z.

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

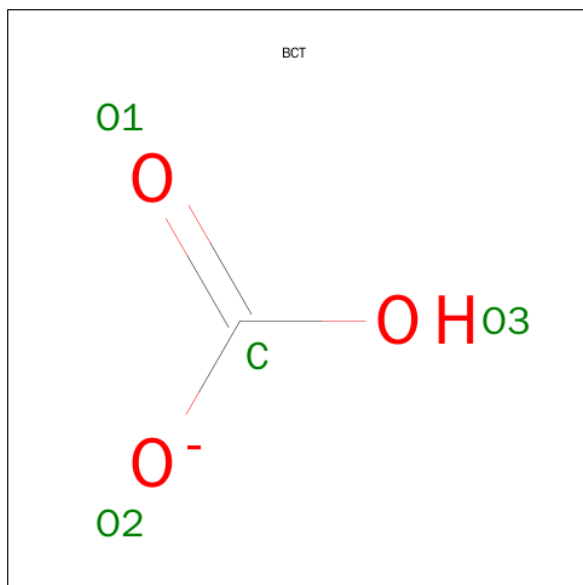
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

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

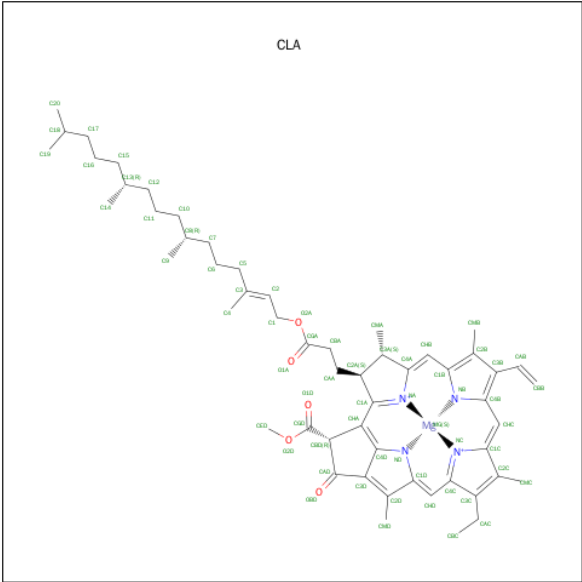
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

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



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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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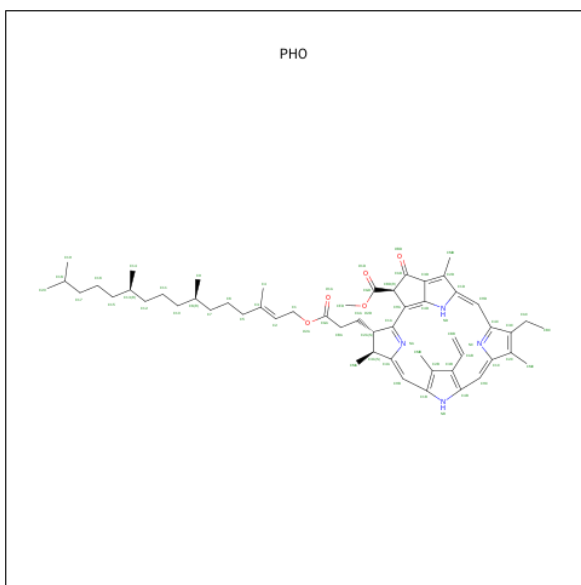
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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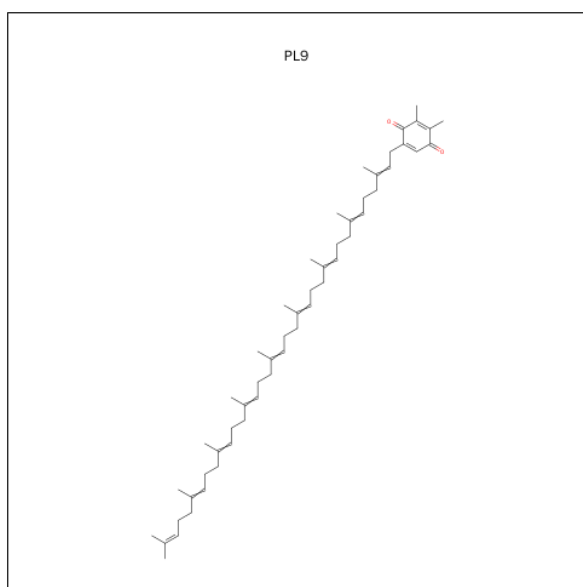
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



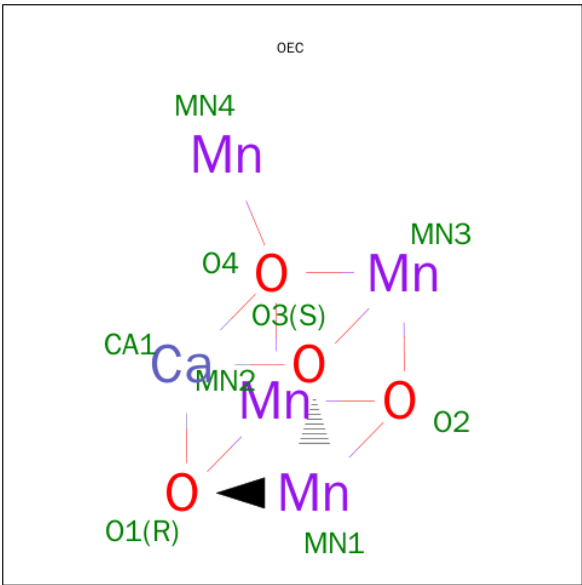
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



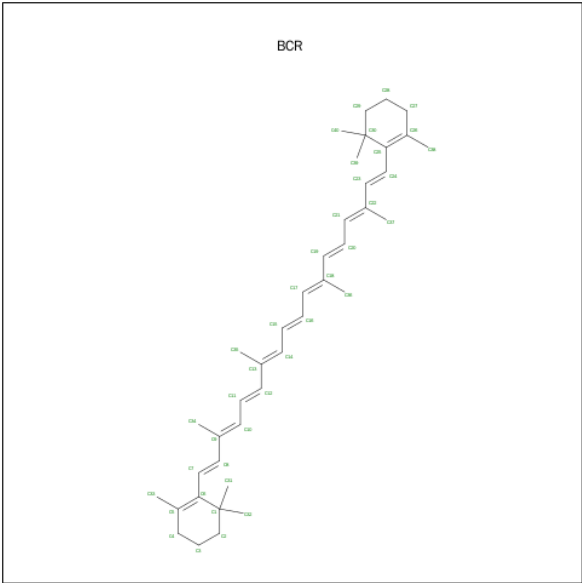
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	J	1	Total	C	O	0	0
			35	33	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			55	53	2		
25	j	1	Total	C	O	0	0
			35	33	2		

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



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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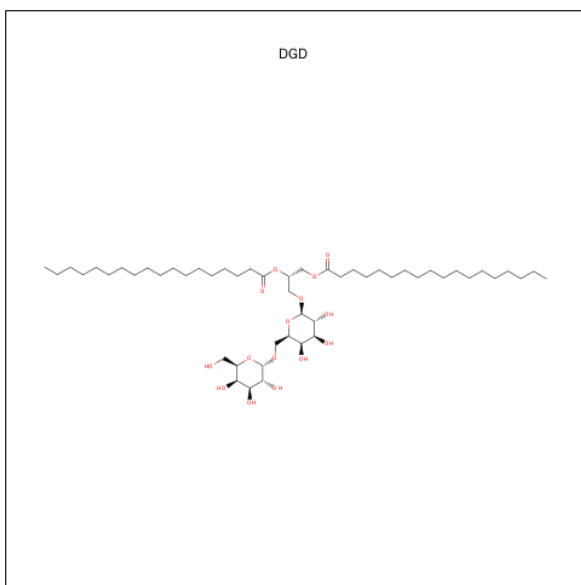
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

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

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



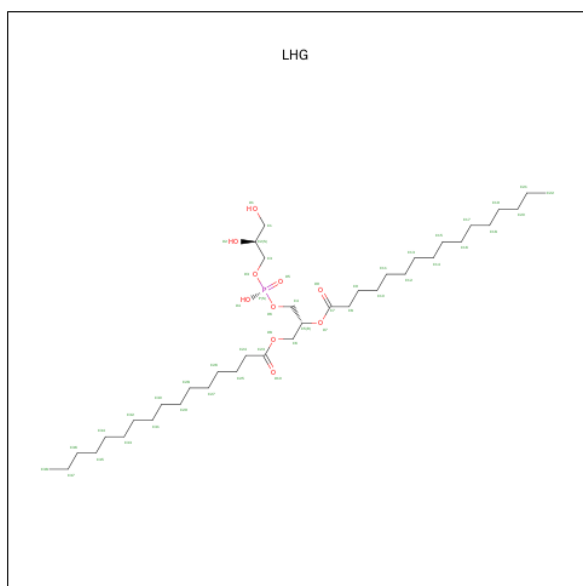
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52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

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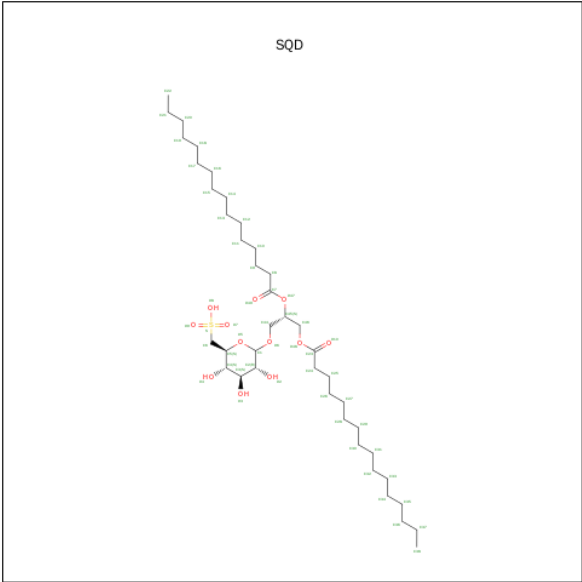
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	0
			53	38	15		
28	c	1	Total	C	O	0	0
			62	47	15		
28	c	1	Total	C	O	0	0
			66	51	15		
28	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



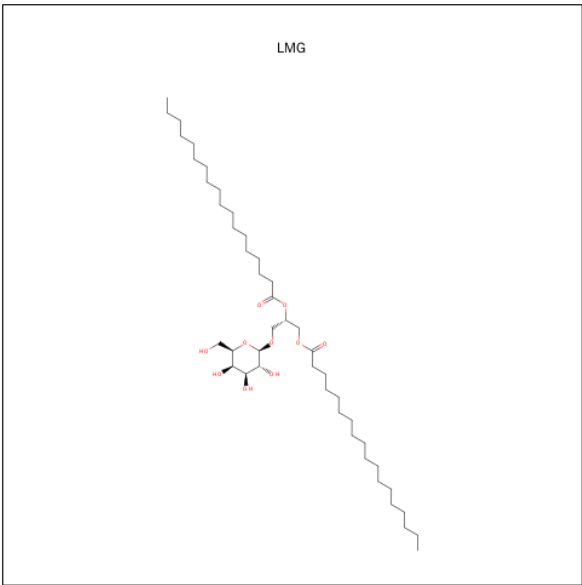
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



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

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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

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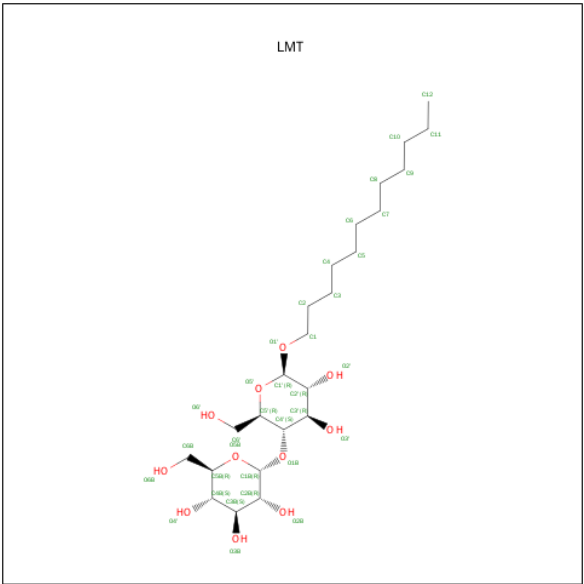
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	b	1	Total	C	O	0	0
			49	39	10		
31	c	1	Total	C	O	0	0
			45	35	10		
31	d	1	Total	C	O	0	0
			46	36	10		
31	d	1	Total	C	O	0	0
			48	38	10		
31	e	1	Total	C	O	0	0
			44	34	10		
31	i	1	Total	C	O	0	0
			43	33	10		
31	k	1	Total	C	O	0	0
			48	38	10		
31	m	1	Total	C	O	0	0
			42	32	10		

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

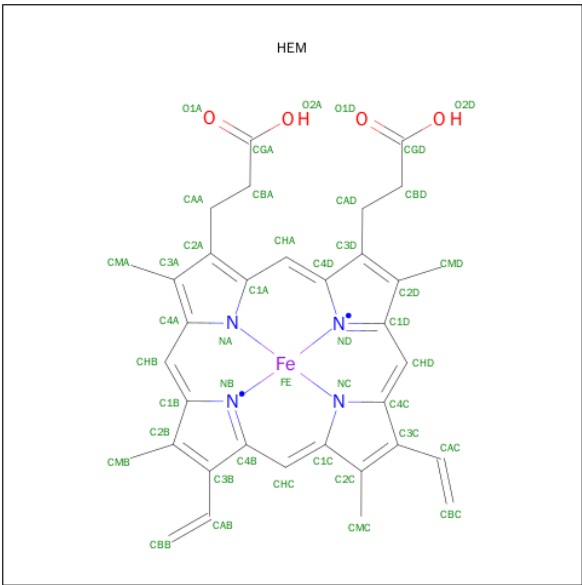
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Cl	0	0
			1	1		
32	a	1	Total	Cl	0	0
			1	1		

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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

- 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	
34	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
34	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	
34	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	

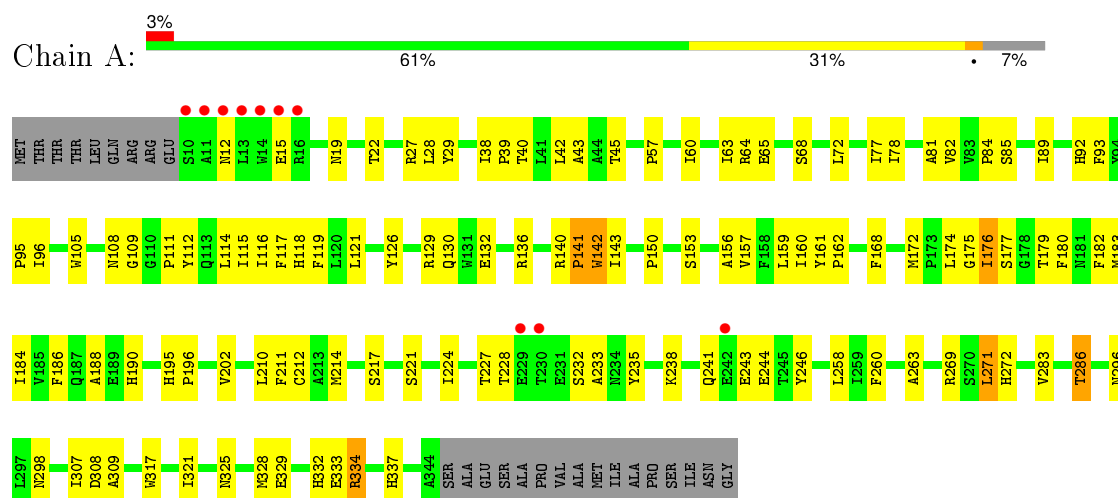
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

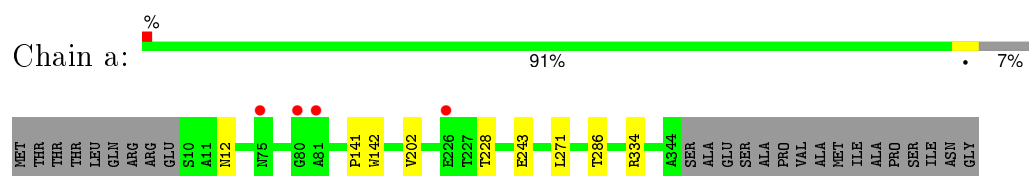
3 Residue-property plots

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

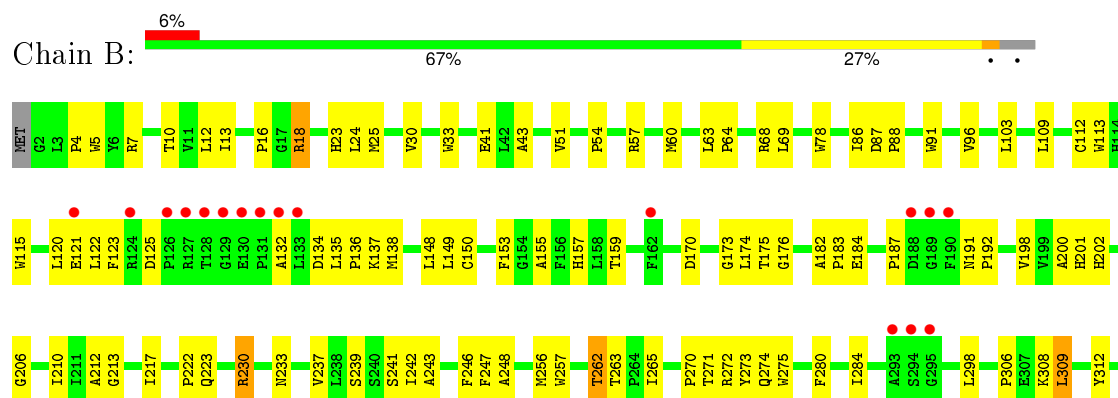
• Molecule 1: Photosystem Q(B) protein 1

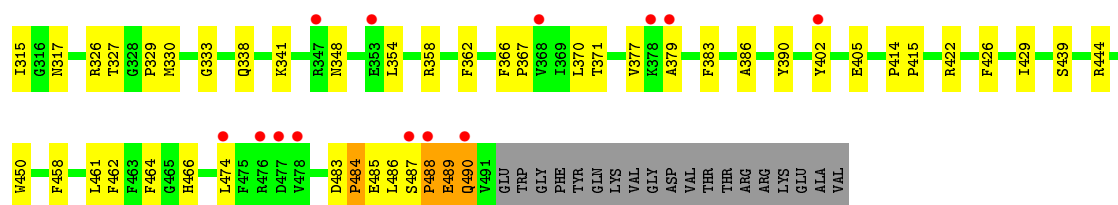


• Molecule 1: Photosystem Q(B) protein 1

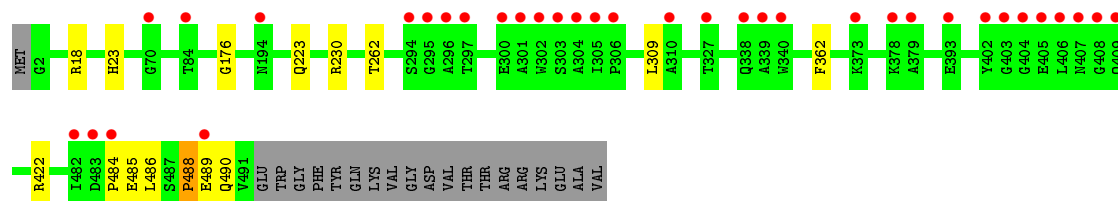
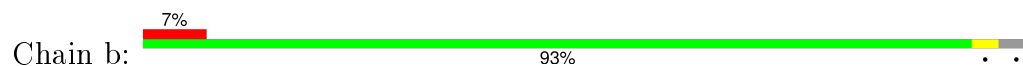


• Molecule 2: Photosystem II core light harvesting protein

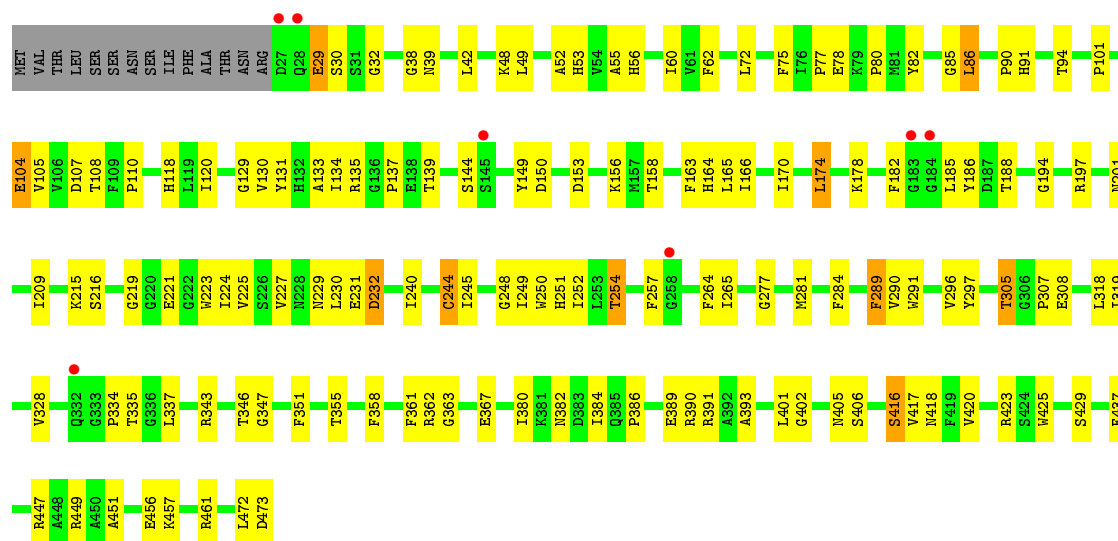




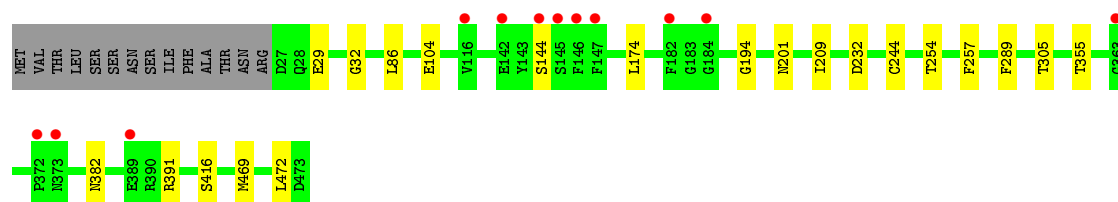
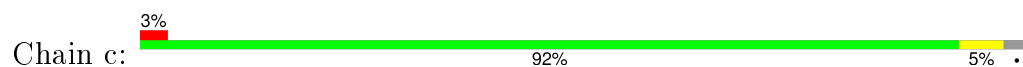
- Molecule 2: Photosystem II core light harvesting protein



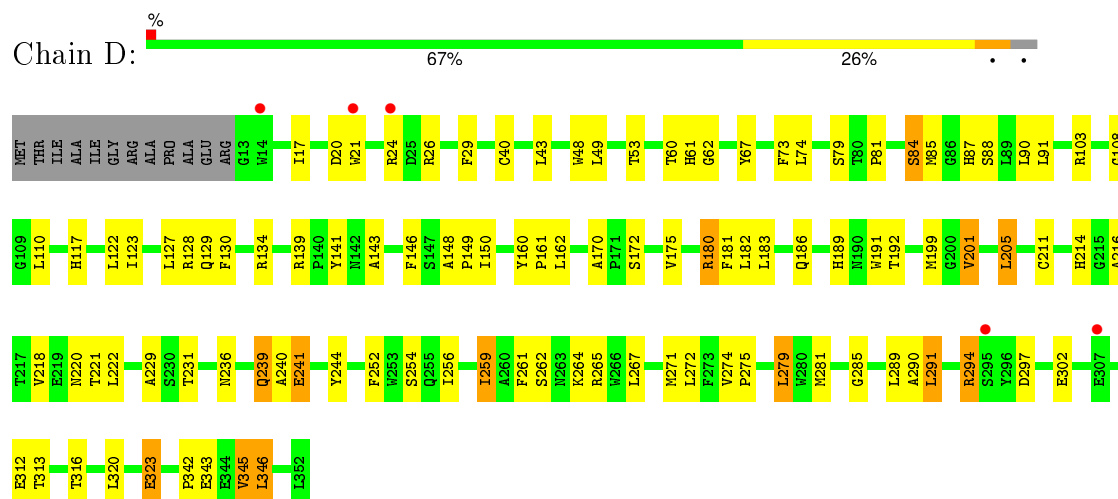
- Molecule 3: Photosystem II CP43 protein



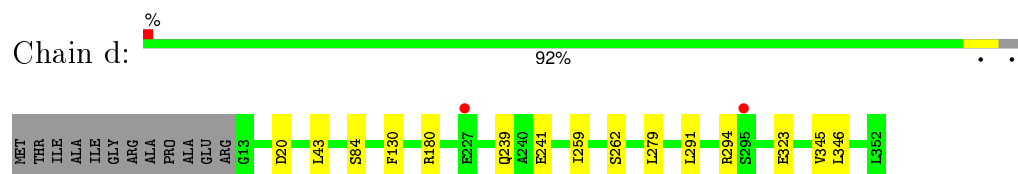
- Molecule 3: Photosystem II CP43 protein



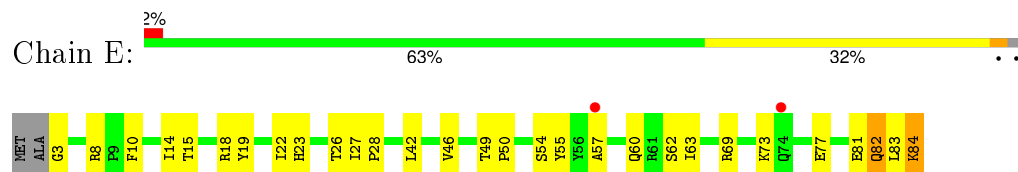
- Molecule 4: Photosystem II D2 protein



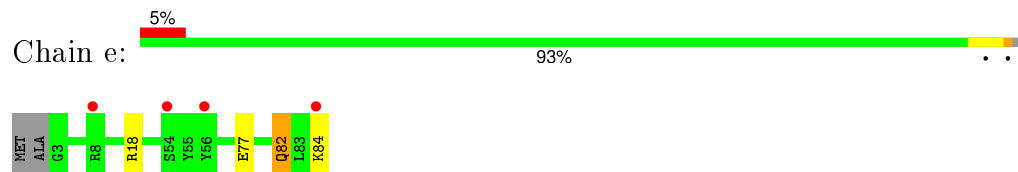
- Molecule 4: Photosystem II D2 protein



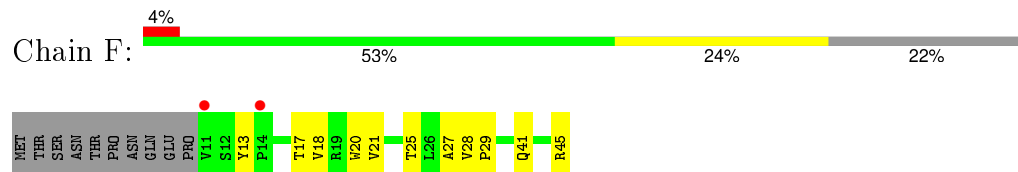
- Molecule 5: Cytochrome b559 subunit alpha



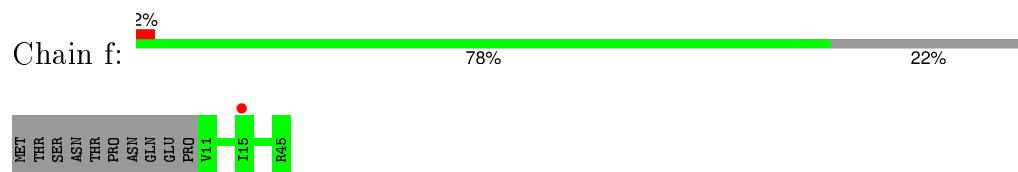
- Molecule 5: Cytochrome b559 subunit alpha



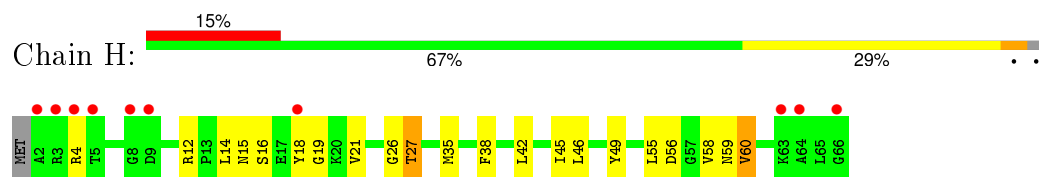
- Molecule 6: Cytochrome b559 subunit beta



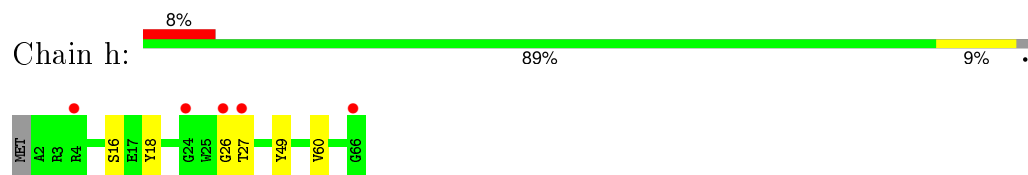
- Molecule 6: Cytochrome b559 subunit beta



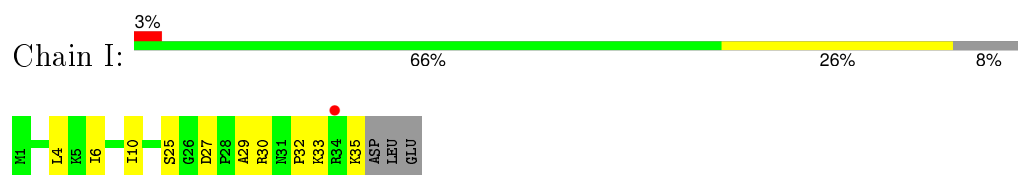
- Molecule 7: Photosystem II reaction center protein H



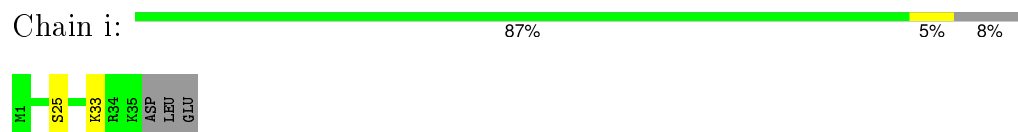
- Molecule 7: Photosystem II reaction center protein H



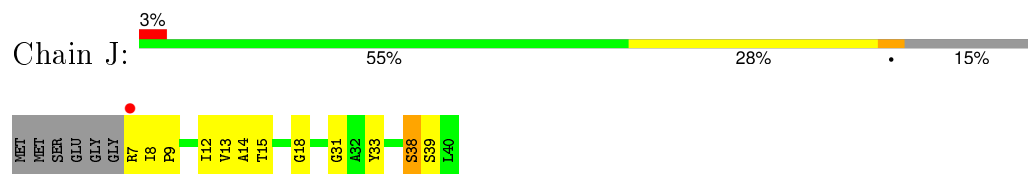
- Molecule 8: Photosystem II reaction center protein I



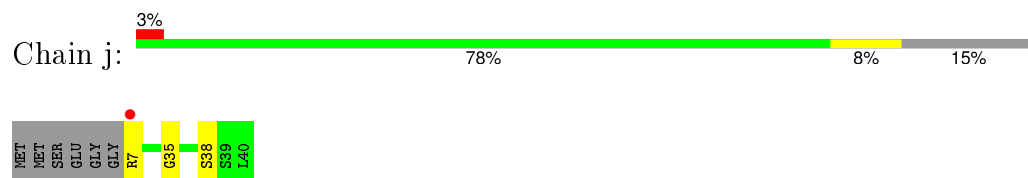
- Molecule 8: Photosystem II reaction center protein I



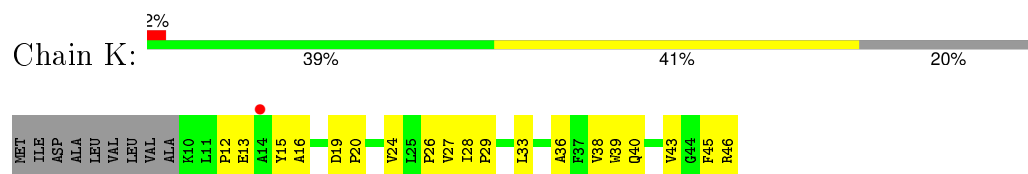
- Molecule 9: Photosystem II reaction center protein J



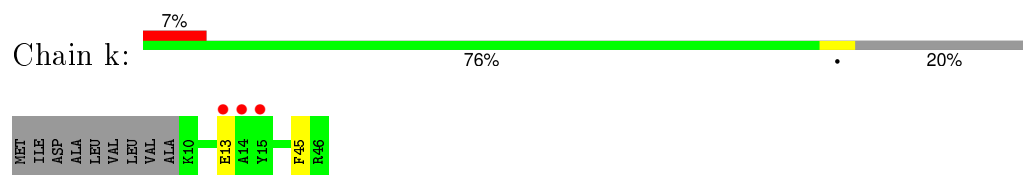
- Molecule 9: Photosystem II reaction center protein J



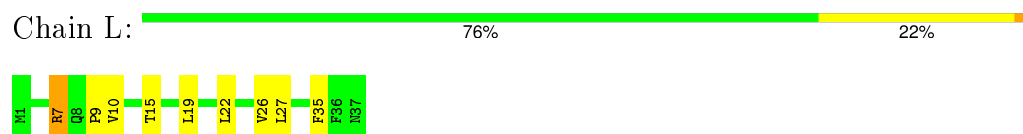
- Molecule 10: Photosystem II reaction center protein K



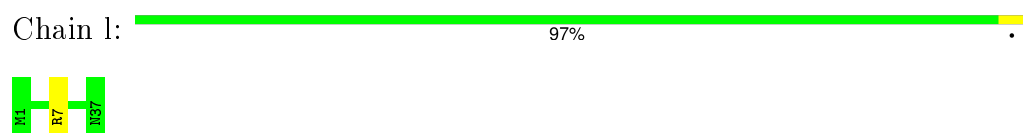
- Molecule 10: Photosystem II reaction center protein K



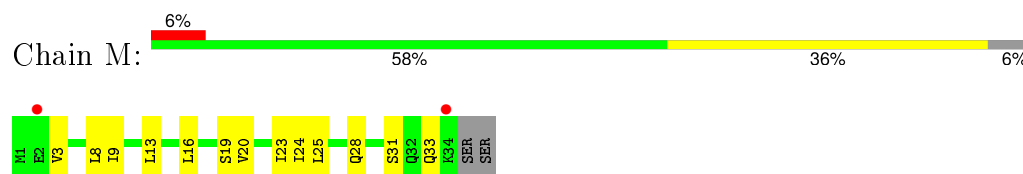
- Molecule 11: Photosystem II reaction center protein L



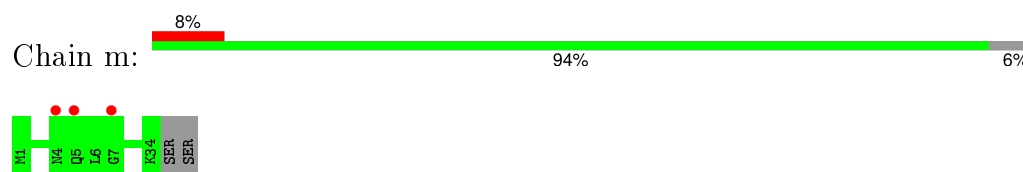
- Molecule 11: Photosystem II reaction center protein L



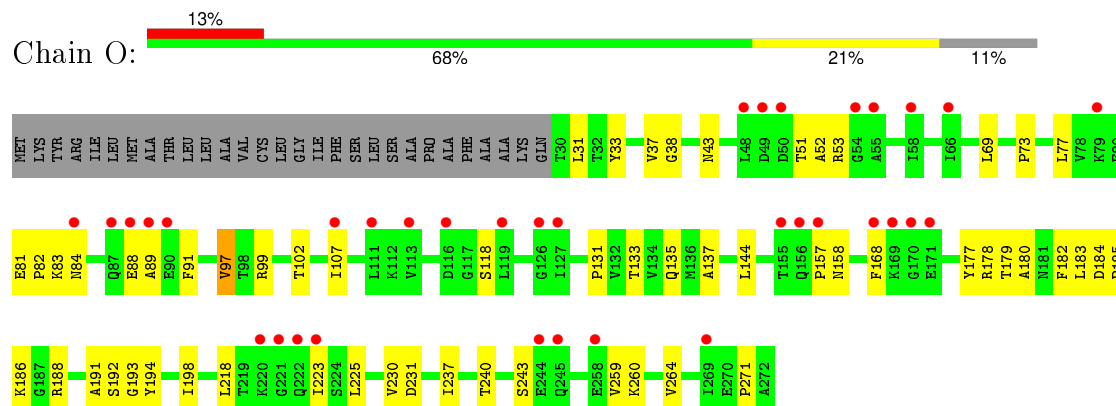
- Molecule 12: Photosystem II reaction center protein M



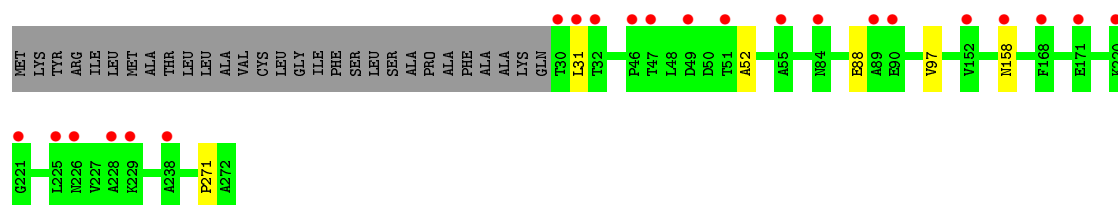
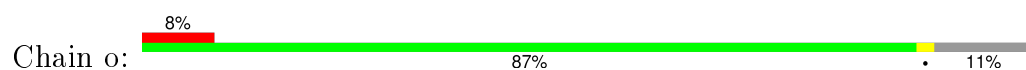
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



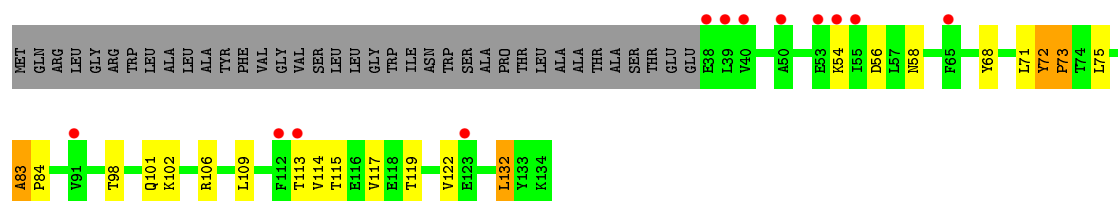
- Molecule 14: Photosystem II reaction center protein T



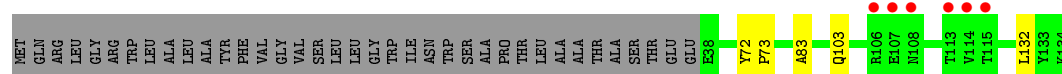
- Molecule 14: Photosystem II reaction center protein T



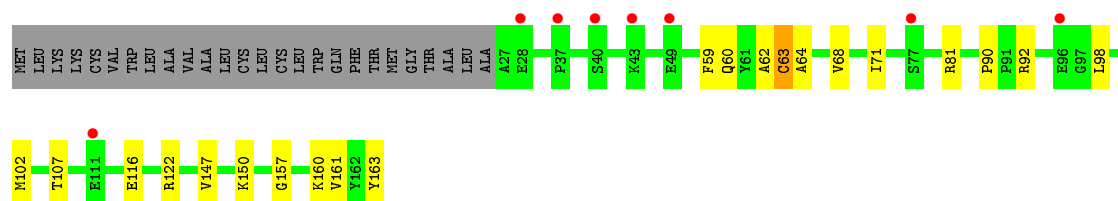
- Molecule 15: Photosystem II 12 kDa extrinsic protein



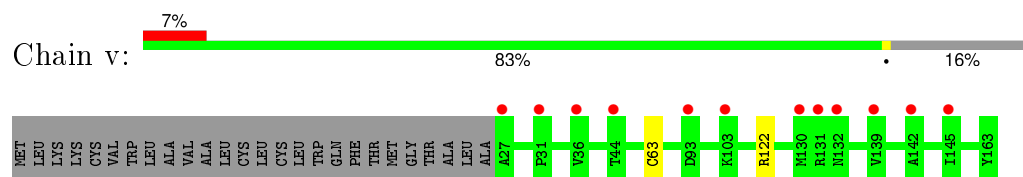
- Molecule 15: Photosystem II 12 kDa extrinsic protein



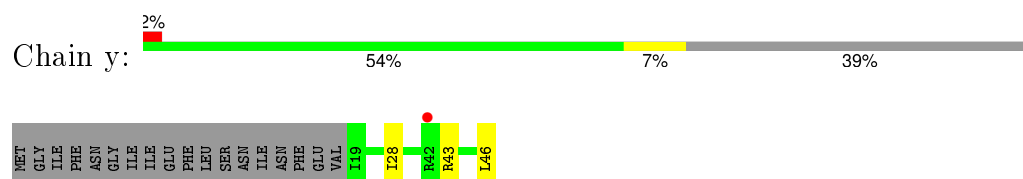
- Molecule 16: Cytochrome c-550



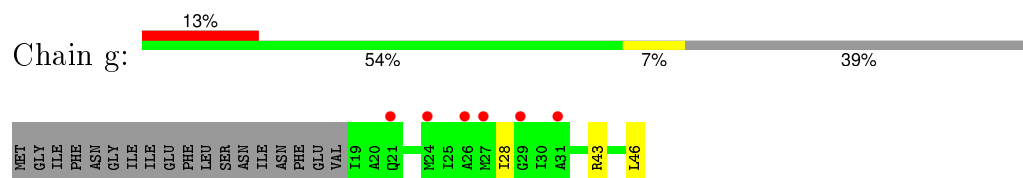
- Molecule 16: Cytochrome c-550



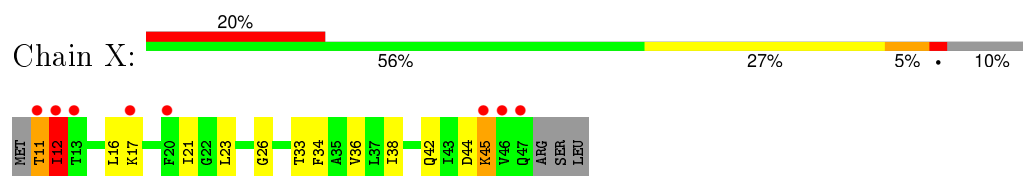
- Molecule 17: Photosystem II reaction center protein ycf12



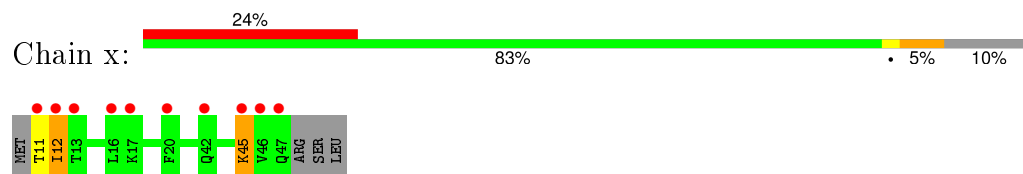
- Molecule 17: Photosystem II reaction center protein ycf12



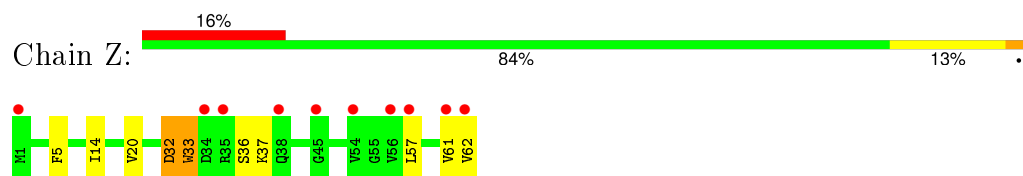
- Molecule 18: Photosystem II reaction center X protein



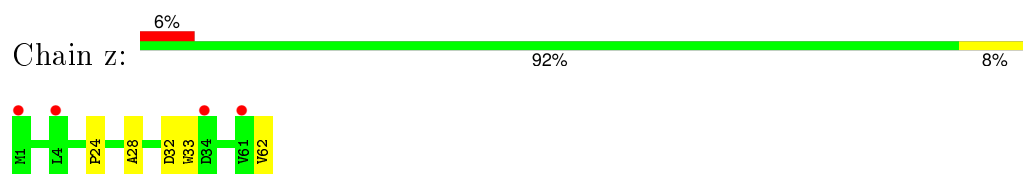
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z

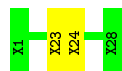


- Molecule 19: Photosystem II reaction center protein Z



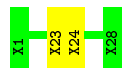
- Molecule 20: Photosystem II reaction center protein Y

Chain G:  93% 7%



- Molecule 20: Photosystem II reaction center protein Y

Chain Y:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.98Å 227.57Å 306.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 5.90 82.97 – 5.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.97-5.90) 98.5 (82.97-5.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.285 , 0.313 0.308 , 0.316	Depositor DCC
R_{free} test set	1200 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	1.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 24671 reflections	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.28	0/3986	0.46	0/5433
3	C	0.28	0/3556	0.46	0/4842
3	c	0.27	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.29	0/685	0.48	0/933
5	e	0.28	0/685	0.48	0/933
6	F	0.28	0/291	0.45	0/397
6	f	0.26	0/291	0.45	0/397
7	H	0.26	0/520	0.49	0/709
7	h	0.27	0/520	0.50	0/709
8	I	0.28	0/293	0.48	0/395
8	i	0.32	0/293	0.49	0/395
9	J	0.29	0/255	0.46	0/346
9	j	0.28	0/255	0.44	0/346
10	K	0.29	0/303	0.52	0/416
10	k	0.28	0/303	0.53	0/416
11	L	0.25	0/311	0.43	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.65	0/367
12	m	0.41	0/270	0.65	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.36	0/284	0.49	0/381
14	t	0.35	0/284	0.47	0/381
15	U	0.27	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.30	0/1081	0.52	0/1468
16	v	0.26	0/1081	0.46	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.24	0/202	0.51	0/272
17	y	0.25	0/202	0.52	0/272
18	X	0.30	0/273	0.52	0/370
18	x	0.32	0/273	0.50	0/370
19	Z	0.30	0/490	0.50	0/669
19	z	0.28	0/490	0.48	0/669
All	All	0.29	0/41948	0.48	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2524	105	0
1	a	2627	0	2524	0	0
2	B	3850	0	3718	137	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	116	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	95	0
4	d	2706	0	2608	0	0
5	E	666	0	651	24	0
5	e	666	0	651	0	0
6	F	282	0	291	11	0
6	f	282	0	291	0	0
7	H	507	0	521	20	0
7	h	507	0	521	0	0
8	I	286	0	308	5	0
8	i	286	0	308	0	0
9	J	249	0	262	8	0
9	j	249	0	262	0	0
10	K	293	0	305	16	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	10	0
11	l	304	0	316	0	0
12	M	267	0	289	13	0
12	m	267	0	289	0	0
13	O	1845	0	1801	39	0
13	o	1845	0	1801	0	0
14	T	275	0	288	17	0
14	t	275	0	288	0	0
15	U	774	0	773	13	0
15	u	774	0	773	0	0
16	V	1060	0	1068	13	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	12	0
18	x	270	0	299	0	0
19	Z	479	0	516	9	0
19	z	479	0	516	0	0
20	G	140	0	32	1	0
20	Y	140	0	32	1	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	1	0	0
22	d	4	0	1	0	0
23	A	260	0	288	48	0
23	B	1040	0	1152	131	0
23	C	845	0	936	66	0
23	D	130	0	144	10	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	5	0
24	D	64	0	74	6	0
24	a	128	0	148	0	0
25	A	45	0	61	2	0
25	D	55	0	80	12	0
25	J	35	0	45	1	0
25	a	45	0	61	0	0
25	d	55	0	80	0	0
25	j	35	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	5	0	0	0	0
26	a	5	0	0	0	0
27	A	40	0	56	7	0
27	B	160	0	224	21	0
27	C	120	0	168	22	0
27	D	40	0	56	3	0
27	H	40	0	56	7	0
27	J	40	0	56	4	0
27	T	80	0	112	11	0
27	a	40	0	56	0	0
27	b	80	0	112	0	0
27	c	80	0	112	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	j	40	0	56	0	0
27	k	40	0	56	0	0
27	y	40	0	56	0	0
27	z	40	0	56	0	0
28	A	56	0	70	1	0
28	B	110	0	136	2	0
28	C	181	0	245	21	0
28	D	63	0	87	2	0
28	a	56	0	70	0	0
28	b	110	0	136	0	0
28	c	181	0	244	0	0
28	d	63	0	87	0	0
29	A	76	0	95	7	0
29	a	76	0	95	0	0
30	A	105	0	147	12	0
30	B	47	0	61	2	0
30	D	43	0	50	5	0
30	F	45	0	54	2	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	A	93	0	125	5	0
31	B	98	0	135	8	0
31	C	93	0	126	5	0
31	D	94	0	126	8	0
31	E	44	0	58	1	0
31	I	43	0	55	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	M	42	0	53	2	0
31	a	93	0	124	0	0
31	b	98	0	135	0	0
31	c	45	0	59	0	0
31	d	94	0	126	0	0
31	e	44	0	58	0	0
31	i	43	0	55	0	0
31	k	48	0	66	0	0
31	m	42	0	53	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	B	140	0	184	5	0
33	D	31	0	35	1	0
33	I	35	0	46	2	0
33	M	35	0	46	1	0
33	b	140	0	184	0	0
33	d	31	0	35	0	0
33	i	35	0	46	0	0
33	m	35	0	46	0	0
34	F	43	0	30	5	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	50232	0	51361	801	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (801) 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)
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.58	0.88
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.57	0.86
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.86
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.59	0.83
27:B:617:BCR:H383	30:B:626:SQD:H92	1.62	0.82
2:B:187:PRO:HB3	23:B:601:CLA:HMB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D:408:SQD:H301	30:D:408:SQD:H171	1.66	0.77
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.66	0.77
23:C:507:CLA:H112	27:C:516:BCR:H362	1.66	0.77
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.77
3:C:297:TYR:O	3:C:423:ARG:NH2	2.31	0.77
3:C:250:TRP:O	3:C:254:THR:OG1	2.03	0.76
3:C:362:ARG:H	28:C:517:DGD:HE4	1.52	0.75
4:D:199:MET:HG2	25:D:404:PL9:H322	1.68	0.75
4:D:29:PHE:O	4:D:128:ARG:NH2	2.23	0.74
23:B:608:CLA:HBA2	30:D:408:SQD:H101	1.70	0.74
24:A:406:PHO:HBC3	4:D:279:LEU:HG	1.70	0.74
23:A:404:CLA:HED1	25:D:404:PL9:H372	1.69	0.73
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.73	0.73
34:V:201:HEM:HBC2	34:V:201:HEM:HHH	1.70	0.73
3:C:291:TRP:O	3:C:305:THR:OG1	2.05	0.73
23:C:508:CLA:HBC3	23:C:510:CLA:H92	1.69	0.73
12:M:25:LEU:O	12:M:28:GLN:HG3	1.93	0.73
23:B:612:CLA:H42	4:D:127:LEU:HD11	30.04	0.73
27:B:618:BCR:H10C	14:T:18:PHE:HB2	43.71	0.73
1:A:183:MET:HB3	23:A:404:CLA:HBC2	5.97	0.72
4:D:259:ILE:HG12	31:D:407:LMG:H292	1.87	0.72
23:B:608:CLA:H42	4:D:127:LEU:HD11	1.72	0.71
2:B:262:THR:HG22	2:B:263:THR:HG23	1.77	0.71
23:B:609:CLA:HBB1	23:B:610:CLA:H51	9.02	0.71
1:A:63:ILE:HB	3:C:335:THR:HG21	1.70	0.71
14:T:18:PHE:HB2	27:T:102:BCR:H10C	1.72	0.71
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.60	0.71
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.24	0.71
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.77	0.71
23:A:405:CLA:HED1	25:D:404:PL9:H372	28.53	0.70
2:B:187:PRO:HB3	23:B:605:CLA:HMB2	31.39	0.70
23:A:403:CLA:H71	23:A:404:CLA:HAB	1.75	0.69
7:H:38:PHE:HB2	27:H:101:BCR:H10C	1.73	0.69
11:L:9:PRO:HB3	31:M:101:LMG:HC61	14.40	0.69
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.96	0.69
23:B:606:CLA:H72	27:B:620:BCR:H311	1.74	0.69
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.74	0.69
4:D:236:ASN:ND2	4:D:239:GLN:O	2.25	0.69
3:C:48:LYS:NZ	3:C:133:ALA:O	2.25	0.69
23:D:403:CLA:H42	18:X:26:GLY:HA3	1.76	0.68
1:A:15:GLU:O	1:A:19:ASN:ND2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:415:LHG:H271	29:A:415:LHG:H101	1.76	0.67
12:M:20:VAL:O	12:M:24:ILE:HG13	1.94	0.67
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	1.77	0.67
3:C:449:ARG:HE	23:C:505:CLA:HED1	1.59	0.67
1:A:29:TYR:O	1:A:129:ARG:NH1	2.29	0.67
4:D:21:TRP:O	4:D:26:ARG:NH2	2.25	0.67
1:A:183:MET:HA	23:A:403:CLA:HMD2	1.77	0.67
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.83	0.67
2:B:149:LEU:HG	23:B:607:CLA:HBC1	27.84	0.66
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.66
3:C:405:ASN:HB2	28:C:518:DGD:HG31	10.27	0.66
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.85	0.66
27:B:618:BCR:H19C	27:B:619:BCR:H363	1.75	0.66
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.66
2:B:149:LEU:HG	23:B:603:CLA:HBC1	1.76	0.65
23:B:607:CLA:H193	7:H:42:LEU:HD12	33.83	0.65
23:B:605:CLA:HBB1	23:B:606:CLA:H51	1.77	0.65
4:D:186:GLN:HB2	23:D:401:CLA:HBC1	1.76	0.65
4:D:24:ARG:NH2	18:X:44:ASP:O	2.29	0.65
1:A:329:GLU:O	1:A:332:HIS:ND1	2.43	0.65
23:C:511:CLA:H171	19:Z:20:VAL:HA	1.78	0.65
2:B:103:LEU:HD21	23:B:609:CLA:HMC3	26.64	0.65
31:A:418:LMG:H112	2:B:43:ALA:HA	42.32	0.64
2:B:150:CYS:HB2	23:B:603:CLA:HMC3	1.80	0.64
2:B:103:LEU:HD21	23:B:605:CLA:HMC3	1.79	0.64
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.32	0.64
3:C:118:HIS:CE1	31:C:521:LMG:H192	2.33	0.64
16:V:62:ALA:O	34:V:201:HEM:HAB	1.98	0.64
6:F:17:THR:HG23	6:F:20:TRP:H	1.63	0.63
23:B:603:CLA:H193	7:H:42:LEU:HD12	1.80	0.63
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.83	0.63
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.26	0.63
23:C:503:CLA:H172	23:C:510:CLA:HBB2	1.80	0.63
23:C:507:CLA:H112	27:C:515:BCR:H362	29.07	0.63
3:C:405:ASN:HB2	28:C:519:DGD:HG31	1.80	0.63
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.81	0.63
31:A:414:LMG:H231	25:D:404:PL9:H352	1.81	0.63
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.83	0.63
1:A:140:ARG:HH22	29:A:412:LHG:P	2.22	0.63
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.63
31:D:407:LMG:HO4	31:D:407:LMG:HO5	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:HB3	23:A:403:CLA:HBC2	1.80	0.62
30:A:413:SQD:H241	29:A:415:LHG:HC81	1.82	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.62
31:D:407:LMG:H111	11:L:19:LEU:HD21	1.81	0.62
2:B:5:TRP:HZ3	23:B:611:CLA:H51	1.64	0.61
23:D:403:CLA:H43	18:X:23:LEU:HA	1.83	0.61
3:C:406:SER:O	3:C:418:ASN:ND2	2.39	0.61
23:C:509:CLA:HBD	23:C:509:CLA:H121	1.84	0.61
4:D:192:THR:HG23	23:D:401:CLA:HBC2	1.82	0.61
1:A:183:MET:HA	23:A:404:CLA:HMD2	8.46	0.60
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.30	0.60
23:A:405:CLA:H42	25:D:404:PL9:H162	18.91	0.60
2:B:458:PHE:HB3	23:B:608:CLA:HBC2	12.78	0.60
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.69	0.60
1:A:72:LEU:HD13	31:A:418:LMG:H111	1.84	0.60
2:B:327:THR:HG21	31:B:623:LMG:H111	1.85	0.59
1:A:28:LEU:HB2	30:A:417:SQD:H91	1.83	0.59
3:C:164:HIS:ND1	23:C:507:CLA:OBD	2.42	0.59
23:B:612:CLA:H151	23:B:613:CLA:H203	19.91	0.59
1:A:64:ARG:O	13:O:178:ARG:NH2	2.36	0.59
3:C:49:LEU:O	3:C:53:HIS:ND1	2.34	0.59
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.87	0.59
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.68	0.58
1:A:217:SER:HA	4:D:272:LEU:HD12	1.94	0.58
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.47	0.58
16:V:59:PHE:HA	16:V:63:CYS:SG	2.48	0.58
23:C:501:CLA:HMB3	27:C:516:BCR:H403	1.86	0.58
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.88	0.58
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.84	0.58
23:B:606:CLA:HBD	23:B:606:CLA:H2	8.35	0.58
3:C:165:LEU:HD21	23:C:506:CLA:HAB	1.85	0.58
23:A:405:CLA:H142	23:D:401:CLA:H151	1.85	0.58
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.58
14:T:21:ILE:HD12	27:T:102:BCR:H332	1.85	0.58
30:A:413:SQD:H223	28:C:519:DGD:HAE1	1.86	0.57
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.85	0.57
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	2.39	0.57
23:B:613:CLA:HMC2	27:H:101:BCR:H343	25.62	0.57
1:A:334:ARG:NH1	13:O:183:LEU:O	2.46	0.57
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.93	0.57
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:601:CLA:HMB3	27:H:101:BCR:H281	1.86	0.57
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.87	0.57
13:O:73:PRO:HG2	13:O:102:THR:HB	1.89	0.57
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.43	0.56
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.43	0.56
23:B:603:CLA:C2D	23:B:605:CLA:H2	2.35	0.56
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.76	0.56
30:D:408:SQD:H241	30:D:408:SQD:H111	1.85	0.56
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.88	0.56
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.45	0.56
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.05	0.56
1:A:153:SER:HB3	23:A:404:CLA:HED1	17.23	0.56
2:B:150:CYS:HA	23:B:607:CLA:HBC2	29.73	0.56
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.80	0.56
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.56
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.01	0.56
2:B:212:ALA:HB2	23:B:609:CLA:HMC3	1.87	0.56
23:C:505:CLA:H11	27:C:515:BCR:H312	50.03	0.56
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.86	0.56
2:B:150:CYS:HA	23:B:603:CLA:HBC2	1.87	0.56
23:C:511:CLA:HMB2	27:C:514:BCR:H382	1.88	0.56
2:B:150:CYS:HB2	23:B:607:CLA:HMC3	24.82	0.55
1:A:190:HIS:O	1:A:298:ASN:HB3	2.12	0.55
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.40	0.55
23:B:609:CLA:H202	23:B:613:CLA:HBB2	21.83	0.55
23:B:612:CLA:HBA2	30:D:408:SQD:H101	22.81	0.55
2:B:121:GLU:O	7:H:12:ARG:NH2	2.41	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.55
30:A:413:SQD:H311	23:C:508:CLA:H71	1.89	0.55
23:C:513:CLA:HAB	27:C:515:BCR:H24C	1.89	0.55
2:B:239:SER:O	2:B:466:HIS:ND1	2.39	0.55
2:B:212:ALA:HB2	23:B:613:CLA:HMC3	27.33	0.55
23:B:608:CLA:H151	23:B:609:CLA:H203	1.89	0.55
3:C:284:PHE:HB3	28:C:517:DGD:HA51	1.89	0.55
24:A:406:PHO:H151	23:D:401:CLA:H172	1.88	0.55
23:C:501:CLA:C2D	23:C:503:CLA:H2	2.37	0.55
27:C:514:BCR:H391	10:K:36:ALA:HB2	2.00	0.55
13:O:83:LYS:HG2	13:O:84:ASN:H	1.75	0.54
2:B:78:TRP:HB3	13:O:137:ALA:HB1	59.82	0.54
1:A:84:PRO:HA	1:A:112:TYR:CG	2.42	0.54
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.99	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.90	0.54
23:A:405:CLA:HAA1	25:D:404:PL9:H362	24.29	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.88	0.54
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.07	0.54
23:C:505:CLA:HBA1	23:C:505:CLA:HBD	2.00	0.54
23:B:608:CLA:HBD	23:B:609:CLA:H43	4.18	0.54
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.54
2:B:201:HIS:HD2	2:B:202:HIS:CE1	2.50	0.54
23:B:615:CLA:H172	23:B:615:CLA:H111	1.90	0.54
28:C:518:DGD:HA41	31:C:520:LMG:H391	1.89	0.54
31:C:520:LMG:HC62	27:J:102:BCR:H271	1.90	0.54
12:M:31:SER:HA	31:M:101:LMG:HC1	1.90	0.54
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.43	0.54
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.89	0.54
2:B:96:VAL:HG22	23:B:610:CLA:HBA1	23.24	0.53
2:B:41:GLU:HB3	2:B:60:MET:SD	2.48	0.53
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.57	0.53
1:A:111:PRO:O	1:A:115:ILE:HG13	2.08	0.53
15:U:98:THR:O	15:U:102:LYS:HG3	2.88	0.53
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.94	0.53
1:A:211:PHE:HA	1:A:214:MET:HB2	1.89	0.53
33:B:628:LMT:H122	14:T:7:VAL:HG12	34.77	0.53
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.00	0.53
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.89	0.53
23:A:404:CLA:HHC	23:A:404:CLA:HBB1	2.46	0.53
2:B:271:THR:HB	2:B:274:GLN:HG3	1.90	0.53
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.46	0.53
5:E:15:THR:HG23	9:J:8:ILE:O	2.10	0.53
23:B:603:CLA:C3D	23:B:605:CLA:H2	2.39	0.53
23:B:604:CLA:HBB1	23:B:607:CLA:CBB	2.38	0.53
4:D:214:HIS:ND1	25:D:404:PL9:O2	2.27	0.53
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.90	0.53
1:A:210:LEU:HG	24:A:406:PHO:NC	2.24	0.53
2:B:198:VAL:O	2:B:202:HIS:ND1	2.35	0.53
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.91	0.53
4:D:49:LEU:O	4:D:53:THR:HG23	2.09	0.53
1:A:244:GLU:HG3	1:A:246:TYR:H	1.73	0.53
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.98	0.53
28:B:627:DGD:HB22	33:B:629:LMT:H72	1.91	0.53
2:B:125:ASP:HB2	2:B:132:ALA:HB3	1.91	0.53
1:A:78:ILE:O	1:A:176:ILE:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:NH2	29:A:412:LHG:O5	2.36	0.52
23:B:602:CLA:H42	7:H:45:ILE:HD11	1.90	0.52
1:A:141:PRO:O	1:A:143:ILE:N	2.47	0.52
23:A:403:CLA:H122	24:D:402:PHO:H3A	1.91	0.52
3:C:437:PHE:HZ	23:C:510:CLA:HMB3	1.75	0.52
23:C:501:CLA:H171	23:C:507:CLA:HMB3	1.91	0.52
23:A:404:CLA:H203	24:D:402:PHO:H71	1.92	0.52
23:B:605:CLA:HMB3	27:H:101:BCR:H281	36.59	0.52
1:A:153:SER:HB2	23:A:404:CLA:H43	14.47	0.52
27:A:410:BCR:H311	30:A:417:SQD:H351	1.92	0.52
2:B:241:SER:HB3	23:B:612:CLA:HED3	1.91	0.52
23:A:405:CLA:H93	23:D:401:CLA:H152	1.92	0.52
31:D:407:LMG:O6	11:L:15:THR:HG21	2.10	0.52
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.52
19:Z:33:TRP:HA	19:Z:36:SER:HB3	1.95	0.52
3:C:334:PRO:HA	13:O:179:THR:OG1	2.22	0.52
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.80	0.52
19:Z:32:ASP:CG	19:Z:33:TRP:H	2.18	0.52
2:B:112:CYS:HG	14:T:18:PHE:HZ	45.61	0.51
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.44	0.51
27:A:410:BCR:H342	30:A:417:SQD:H342	1.92	0.51
2:B:222:PRO:HG3	7:H:27:THR:H	1.75	0.51
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	1.99	0.51
23:C:512:CLA:H143	23:C:513:CLA:H162	2.03	0.51
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.46	0.51
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.75	0.51
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.06	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
3:C:158:THR:O	3:C:251:HIS:HB3	2.09	0.51
23:A:404:CLA:H71	23:A:405:CLA:HAB	27.58	0.51
30:A:417:SQD:H332	23:B:610:CLA:H203	66.31	0.51
23:B:603:CLA:CBB	23:B:605:CLA:H152	2.41	0.51
2:B:462:PHE:CZ	23:B:613:CLA:HMB3	2.46	0.51
23:A:404:CLA:HAA1	25:D:404:PL9:H362	1.91	0.51
13:O:230:VAL:HG12	13:O:231:ASP:H	1.74	0.51
2:B:474:LEU:O	4:D:134:ARG:NH1	2.47	0.51
3:C:380:ILE:HA	3:C:384:ILE:HD11	2.03	0.51
23:B:609:CLA:HMD1	7:H:27:THR:HB	1.92	0.51
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.48	0.51
3:C:85:GLY:N	28:C:518:DGD:HE4	2.25	0.51
23:B:606:CLA:H42	7:H:45:ILE:HD11	29.61	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLY:O	2:B:217:ILE:HG13	2.10	0.51
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.51
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.51
33:D:410:LMT:H72	18:X:26:GLY:HA2	1.92	0.51
3:C:130:VAL:O	3:C:134:ILE:HG12	2.14	0.51
1:A:238:LYS:HD2	14:T:32:LYS:HB3	1.93	0.51
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.93	0.50
2:B:241:SER:HB3	23:B:616:CLA:HED3	28.40	0.50
23:B:602:CLA:HBD	23:B:602:CLA:H2	1.92	0.50
3:C:425:TRP:CE2	23:C:504:CLA:HBA1	2.57	0.50
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.76	0.50
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.93	0.50
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.92	0.50
23:B:611:CLA:H171	23:B:613:CLA:ND	2.26	0.50
3:C:60:ILE:HG23	23:C:510:CLA:HMC2	2.02	0.50
4:D:49:LEU:HD13	27:D:405:BCR:C15	2.45	0.50
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.41	0.50
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.94	0.50
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.50
11:L:10:VAL:O	12:M:28:GLN:NE2	2.34	0.50
2:B:25:MET:HG2	27:T:101:BCR:H23C	37.32	0.50
27:B:618:BCR:H332	14:T:21:ILE:HD12	49.29	0.50
27:C:514:BCR:H311	27:C:514:BCR:H343	1.98	0.50
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.01	0.50
2:B:184:GLU:H	2:B:200:ALA:HB2	1.77	0.50
1:A:119:PHE:HZ	23:A:403:CLA:H8	1.76	0.50
2:B:155:ALA:O	2:B:159:THR:OG1	2.26	0.50
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.46	0.50
23:B:607:CLA:C3D	23:B:609:CLA:H2	40.36	0.50
27:B:617:BCR:H341	27:B:618:BCR:H24C	1.93	0.50
5:E:55:TYR:O	5:E:84:LYS:HE3	2.29	0.50
9:J:14:ALA:O	9:J:18:GLY:N	2.42	0.50
2:B:12:LEU:HB2	23:B:616:CLA:HMC2	13.50	0.50
3:C:429:SER:HB3	28:C:517:DGD:HA81	17.09	0.50
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.82	0.50
3:C:361:PHE:HA	28:C:517:DGD:HE62	1.92	0.49
30:F:102:SQD:H162	18:X:33:THR:HA	1.93	0.49
13:O:118:SER:HB3	13:O:157:PRO:HA	1.95	0.49
23:B:604:CLA:HBB1	23:B:607:CLA:HBB2	1.93	0.49
2:B:329:PRO:HB3	23:B:607:CLA:HED1	1.94	0.49
23:B:612:CLA:H51	23:B:613:CLA:H101	18.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:HH21	31:B:622:LMG:HC3	1.76	0.49
23:C:501:CLA:HMB3	27:C:515:BCR:H403	24.91	0.49
29:A:412:LHG:HC32	4:D:229:ALA:O	2.12	0.49
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.93	0.49
18:X:34:PHE:O	18:X:38:ILE:HG12	2.12	0.49
23:B:613:CLA:HMB1	23:B:613:CLA:HBB1	1.95	0.49
23:A:404:CLA:CHA	23:A:404:CLA:HBA1	2.42	0.49
3:C:56:HIS:HE1	3:C:60:ILE:HD11	1.78	0.49
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.94	0.49
23:B:607:CLA:C2D	23:B:609:CLA:H2	40.11	0.49
13:O:77:LEU:HB2	13:O:260:LYS:HB3	1.95	0.49
3:C:248:GLY:O	3:C:252:ILE:HG12	2.24	0.49
3:C:319:ILE:HG21	3:C:389:GLU:HG3	1.98	0.49
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.49	0.49
1:A:283:VAL:O	1:A:286:THR:HG22	2.14	0.49
3:C:405:ASN:CB	28:C:518:DGD:HG31	10.72	0.49
12:M:28:GLN:O	12:M:31:SER:OG	3.44	0.49
2:B:25:MET:HG2	27:T:101:BCR:C23	36.57	0.49
1:A:116:ILE:HG13	1:A:117:PHE:N	2.27	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	2.09	0.49
3:C:405:ASN:CB	28:C:519:DGD:HG31	2.43	0.49
3:C:62:PHE:HZ	10:K:28:ILE:HD12	1.77	0.49
23:C:508:CLA:H172	28:C:518:DGD:HBW2	1.95	0.48
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.58	0.48
23:B:611:CLA:H41	23:B:614:CLA:HBC3	1.95	0.48
27:B:618:BCR:H352	27:B:619:BCR:H382	1.95	0.48
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.48
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.13	0.48
1:A:232:SER:OG	31:A:414:LMG:O3	2.21	0.48
23:B:606:CLA:HAA2	7:H:45:ILE:HD12	27.42	0.48
12:M:19:SER:O	12:M:23:ILE:HG13	2.14	0.48
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	1.95	0.48
23:B:607:CLA:H2	23:B:609:CLA:H93	34.05	0.48
3:C:53:HIS:HB3	23:C:512:CLA:OBD	2.29	0.48
3:C:343:ARG:NH1	3:C:347:GLY:O	2.46	0.48
23:A:405:CLA:HAB	23:D:401:CLA:H72	1.96	0.48
2:B:327:THR:HG22	23:B:607:CLA:H12	1.94	0.48
3:C:429:SER:HB3	28:C:518:DGD:HA81	1.95	0.48
23:A:405:CLA:HBA1	23:A:405:CLA:CHA	3.90	0.48
23:A:403:CLA:H51	24:D:402:PHO:C3B	2.43	0.48
4:D:73:PHE:CZ	31:D:406:LMG:H172	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:403:CLA:HBB1	23:A:403:CLA:HHC	1.95	0.48
23:B:616:CLA:H72	23:B:616:CLA:H12	1.96	0.48
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.95	0.48
14:T:4:ILE:HD13	27:T:102:BCR:H381	1.94	0.48
3:C:42:LEU:HD13	23:C:511:CLA:HMA3	1.95	0.48
2:B:488:PRO:O	2:B:490:GLN:N	2.47	0.48
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.00	0.48
23:A:404:CLA:H122	23:A:404:CLA:HMA1	1.95	0.48
3:C:91:HIS:O	3:C:94:THR:OG1	2.42	0.48
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.48
27:A:410:BCR:H342	30:A:417:SQD:H311	1.95	0.48
4:D:146:PHE:O	4:D:149:PRO:HD2	2.13	0.48
1:A:57:PRO:HG3	1:A:68:SER:CB	2.51	0.48
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.08	0.48
23:B:606:CLA:H162	23:B:606:CLA:H122	4.25	0.47
23:B:607:CLA:H41	23:B:607:CLA:H61	3.01	0.47
23:A:404:CLA:H42	25:D:404:PL9:H162	1.96	0.47
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.04	0.47
3:C:363:GLY:O	3:C:367:GLU:HG2	2.13	0.47
27:B:620:BCR:H351	27:B:620:BCR:H15C	1.75	0.47
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.96	0.47
1:A:157:VAL:HG13	1:A:172:MET:HB3	1.95	0.47
23:A:405:CLA:H122	23:A:405:CLA:HMA1	8.91	0.47
1:A:43:ALA:HB1	27:A:410:BCR:H362	1.96	0.47
23:B:602:CLA:H162	23:B:602:CLA:H122	1.54	0.47
23:B:611:CLA:H193	11:L:27:LEU:HD11	15.90	0.47
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.54	0.47
2:B:25:MET:HG2	27:B:617:BCR:C23	2.45	0.47
23:C:501:CLA:H193	23:C:507:CLA:H111	2.03	0.47
27:B:618:BCR:HC32	31:D:407:LMG:H392	57.86	0.47
1:A:269:ARG:NH1	4:D:231:THR:HB	2.36	0.47
1:A:174:LEU:HD22	24:D:402:PHO:H151	1.97	0.47
27:A:410:BCR:H341	27:A:410:BCR:H11C	1.79	0.47
23:B:609:CLA:HMA1	23:B:610:CLA:HBA2	10.53	0.47
3:C:425:TRP:CZ2	23:C:504:CLA:HBA1	2.61	0.47
2:B:487:SER:N	2:B:488:PRO:HD2	2.30	0.47
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.50	0.47
2:B:33:TRP:CD1	27:B:618:BCR:H391	2.50	0.47
3:C:240:ILE:O	3:C:244:CYS:HB2	2.22	0.47
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.96	0.47
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:90:PRO:O	16:V:92:ARG:HD3	2.15	0.47
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.04	0.47
1:A:114:LEU:O	1:A:118:HIS:ND1	2.53	0.47
23:A:404:CLA:H3A	23:A:404:CLA:HBA1	3.88	0.47
1:A:221:SER:HB2	4:D:139:ARG:O	2.15	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.96	0.47
10:K:16:ALA:O	10:K:19:ASP:HB2	2.15	0.47
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.01	0.47
23:B:602:CLA:H62	23:B:602:CLA:H41	1.50	0.47
23:B:608:CLA:HBA1	23:B:608:CLA:CHA	2.45	0.47
27:C:514:BCR:HC7	27:C:514:BCR:H331	1.60	0.47
2:B:135:LEU:HA	2:B:138:MET:HE3	2.03	0.47
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.97	0.47
23:B:612:CLA:HBA1	23:B:612:CLA:CHA	3.80	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.46
2:B:317:ASN:HA	2:B:330:MET:HE1	2.06	0.46
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.15	0.46
2:B:120:LEU:HD13	23:B:616:CLA:HMD2	1.97	0.46
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.97	0.46
4:D:312:GLU:HB2	13:O:185:PRO:CG	2.45	0.46
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.04	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
23:A:404:CLA:HBD	23:A:405:CLA:HAC2	15.21	0.46
2:B:25:MET:HG2	27:B:617:BCR:H23C	1.97	0.46
23:C:502:CLA:HBB2	23:C:510:CLA:H152	1.97	0.46
27:C:516:BCR:H351	27:C:516:BCR:H15C	1.78	0.46
23:C:505:CLA:H11	27:C:516:BCR:H312	1.96	0.46
23:C:511:CLA:H151	19:Z:20:VAL:O	2.15	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.97	0.46
2:B:256:MET:HA	2:B:263:THR:HG21	1.97	0.46
23:C:509:CLA:H11	23:C:509:CLA:H51	1.71	0.46
33:B:629:LMT:H62	8:I:4:LEU:HD22	81.59	0.46
1:A:156:ALA:HA	1:A:160:ILE:HB	1.98	0.46
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.05	0.46
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.34	0.46
23:A:404:CLA:H191	31:D:407:LMG:H352	7.96	0.46
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.51	0.46
23:B:608:CLA:HBB1	23:B:611:CLA:CBB	17.30	0.46
27:B:620:BCR:H11C	27:B:620:BCR:H341	1.82	0.46
2:B:18:ARG:NH2	30:B:626:SQD:O9	2.49	0.46
23:C:506:CLA:H202	23:C:506:CLA:H161	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:GLU:C	5:E:83:LEU:H	2.19	0.46
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.51	0.46
3:C:85:GLY:N	28:C:517:DGD:HE4	23.32	0.46
5:E:19:TYR:O	5:E:23:HIS:ND1	2.40	0.46
1:A:180:PHE:HA	1:A:183:MET:HE2	2.11	0.46
2:B:464:PHE:HD2	23:B:615:CLA:HAC2	28.72	0.46
23:B:612:CLA:H171	23:B:613:CLA:HBB2	1.98	0.46
3:C:245:ILE:O	3:C:249:ILE:HG12	2.15	0.46
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.98	0.46
18:X:12:ILE:HA	18:X:16:LEU:HD12	2.12	0.46
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.98	0.46
23:B:613:CLA:H191	27:B:619:BCR:H333	1.98	0.46
24:D:402:PHO:H62	24:D:402:PHO:H41	1.38	0.46
23:C:511:CLA:H93	27:C:514:BCR:H272	1.99	0.46
31:I:101:LMG:H221	33:I:102:LMT:H81	2.01	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.98	0.46
2:B:137:LYS:HD2	7:H:14:LEU:O	2.16	0.46
24:A:406:PHO:HMA2	25:A:408:PL9:H222	1.98	0.45
3:C:56:HIS:CE1	3:C:60:ILE:HD11	2.51	0.45
4:D:252:PHE:O	4:D:256:ILE:HG22	2.19	0.45
2:B:201:HIS:HD2	2:B:202:HIS:ND1	2.35	0.45
1:A:153:SER:HB3	23:A:403:CLA:HED1	1.98	0.45
2:B:247:PHE:HB2	23:B:608:CLA:HBC1	1.98	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.16	0.45
23:C:504:CLA:H2	28:C:517:DGD:HA22	25.68	0.45
5:E:26:THR:HB	34:F:101:HEM:CAB	2.51	0.45
3:C:224:ILE:O	3:C:227:VAL:HG23	2.16	0.45
27:C:514:BCR:H351	27:C:514:BCR:H15C	1.74	0.45
13:O:240:THR:HA	13:O:264:VAL:HA	1.98	0.45
12:M:8:LEU:HG	12:M:9:ILE:HD12	7.09	0.45
23:C:507:CLA:H62	23:C:507:CLA:H92	1.72	0.45
4:D:146:PHE:C	4:D:149:PRO:HD2	2.36	0.45
23:A:407:CLA:H162	23:A:407:CLA:H141	1.63	0.45
2:B:464:PHE:HD2	23:B:611:CLA:HAC2	1.80	0.45
23:B:603:CLA:H192	23:B:603:CLA:H162	1.78	0.45
23:B:613:CLA:HMD1	7:H:27:THR:HB	39.53	0.45
5:E:50:PRO:HB3	5:E:54:SER:O	2.16	0.45
23:A:403:CLA:H172	24:D:402:PHO:H43	1.97	0.45
23:B:603:CLA:H2	23:B:605:CLA:H93	1.97	0.45
2:B:329:PRO:HB3	23:B:611:CLA:HED1	41.27	0.45
23:C:506:CLA:HMC2	23:C:507:CLA:H102	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:274:VAL:HG13	25:D:404:PL9:C23	2.57	0.45
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.99	0.45
13:O:177:TYR:HD2	13:O:178:ARG:HG2	1.81	0.45
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.73	0.45
13:O:192:SER:OG	13:O:193:GLY:N	2.55	0.45
3:C:229:ASN:ND2	3:C:231:GLU:HB2	2.39	0.45
1:A:244:GLU:CD	4:D:264:LYS:HZ3	2.20	0.45
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.00	0.45
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.32	0.45
3:C:166:ILE:O	3:C:170:ILE:HG13	2.20	0.45
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.72	0.45
23:A:403:CLA:HBA1	23:A:403:CLA:H3A	1.61	0.45
5:E:10:PHE:N	31:E:101:LMG:O3	2.52	0.45
23:B:612:CLA:HMA1	4:D:130:PHE:CE1	22.72	0.45
6:F:27:ALA:HB1	34:F:101:HEM:CAC	2.47	0.45
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.45
4:D:85:MET:HA	5:E:69:ARG:HB3	2.15	0.45
15:U:106:ARG:HA	15:U:109:LEU:HG	1.98	0.45
33:B:628:LMT:H1B	33:B:628:LMT:H3'	1.56	0.45
28:A:411:DGD:HAT2	3:C:281:MET:HG3	1.98	0.45
30:A:413:SQD:H162	25:J:101:PL9:H533	1.99	0.45
27:T:101:BCR:H341	27:T:102:BCR:H24C	1.98	0.45
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.57	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.88	0.45
3:C:29:GLU:HB2	3:C:30:SER:H	1.66	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
23:A:404:CLA:H202	23:A:404:CLA:H162	1.75	0.45
23:A:405:CLA:H162	23:A:405:CLA:H202	4.13	0.45
23:B:603:CLA:H41	23:B:603:CLA:H61	1.80	0.45
31:C:521:LMG:H111	31:C:521:LMG:H292	1.99	0.45
27:H:101:BCR:H15C	27:H:101:BCR:H351	1.85	0.45
31:I:101:LMG:H181	33:I:102:LMT:H42	2.01	0.45
23:D:401:CLA:H61	23:D:401:CLA:H41	1.65	0.44
30:D:408:SQD:H3	30:D:408:SQD:H441	2.01	0.44
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.89	0.44
23:C:511:CLA:H141	19:Z:20:VAL:HG13	2.02	0.44
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.05	0.44
23:B:614:CLA:H112	23:B:614:CLA:H91	1.76	0.44
2:B:96:VAL:HG22	23:B:606:CLA:HBA1	1.98	0.44
4:D:261:PHE:HB2	25:D:404:PL9:H522	1.99	0.44
27:D:405:BCR:H351	27:D:405:BCR:H15C	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:294:ARG:HG2	4:D:294:ARG:H	1.65	0.44
4:D:216:ALA:O	4:D:220:ASN:ND2	2.52	0.44
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.99	0.44
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.68	0.44
2:B:247:PHE:HE1	23:B:602:CLA:H101	1.82	0.44
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.76	0.44
4:D:40:CYS:HB3	4:D:117:HIS:O	2.18	0.44
23:C:511:CLA:H93	23:C:511:CLA:H61	1.81	0.44
2:B:327:THR:HG22	23:B:611:CLA:H12	26.94	0.44
3:C:456:GLU:HG2	3:C:457:LYS:HG3	1.99	0.44
23:C:501:CLA:C1D	23:C:503:CLA:H2	2.47	0.44
3:C:240:ILE:HD11	27:C:516:BCR:H372	1.99	0.44
1:A:298:ASN:ND2	3:C:402:GLY:O	2.50	0.44
23:B:608:CLA:H161	23:B:608:CLA:H202	4.72	0.44
2:B:68:ARG:HH22	23:B:604:CLA:HED1	1.82	0.44
3:C:361:PHE:HD1	28:C:517:DGD:HE61	1.83	0.44
23:C:504:CLA:H121	28:C:518:DGD:HBE2	1.99	0.44
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.08	0.44
23:A:403:CLA:H202	23:A:404:CLA:H93	2.00	0.44
27:B:619:BCR:H341	27:B:619:BCR:H11C	1.84	0.44
23:C:510:CLA:H61	23:C:510:CLA:H2	1.73	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.81	0.44
1:A:29:TYR:O	1:A:129:ARG:HD2	2.18	0.44
1:A:57:PRO:HA	1:A:68:SER:HA	2.00	0.44
2:B:338:GLN:HB3	13:O:84:ASN:HB3	38.65	0.44
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.00	0.44
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.18	0.44
2:B:148:LEU:HA	2:B:210:ILE:HD11	2.00	0.44
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.44
27:A:410:BCR:H15C	27:A:410:BCR:H351	1.80	0.44
23:B:606:CLA:H3A	23:B:606:CLA:HBA2	1.30	0.44
23:B:610:CLA:H3A	23:B:610:CLA:HBA2	2.62	0.44
2:B:462:PHE:CE1	23:B:613:CLA:HMB3	2.53	0.44
3:C:163:PHE:CG	23:C:512:CLA:HAB	2.54	0.44
23:D:403:CLA:H61	23:D:403:CLA:H41	1.89	0.44
1:A:141:PRO:HB2	1:A:142:TRP:H	1.62	0.44
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.53	0.44
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.99	0.44
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.46	0.44
27:H:101:BCR:H371	27:H:101:BCR:H24C	1.81	0.44
3:C:52:ALA:HA	23:C:511:CLA:HMB3	2.03	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:GLY:O	2:B:439:SER:HB3	2.23	0.44
4:D:320:LEU:HD23	4:D:323:GLU:OE1	2.18	0.44
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
2:B:174:LEU:HD23	2:B:308:LYS:HG2	1.99	0.43
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.09	0.43
2:B:134:ASP:OD2	2:B:137:LYS:HE3	2.18	0.43
8:I:6:ILE:O	8:I:10:ILE:HG12	2.30	0.43
1:A:150:PRO:HB2	23:A:404:CLA:H61	9.28	0.43
23:B:604:CLA:HBD	23:B:605:CLA:H43	2.00	0.43
3:C:265:ILE:HG12	23:C:505:CLA:HED1	2.00	0.43
24:A:406:PHO:H161	4:D:48:TRP:CE2	2.53	0.43
9:J:33:TYR:HB3	27:J:102:BCR:H383	2.05	0.43
27:T:102:BCR:H341	27:T:102:BCR:H11C	1.79	0.43
27:C:514:BCR:H11C	27:C:514:BCR:H341	1.79	0.43
4:D:285:GLY:O	4:D:289:LEU:HG	2.18	0.43
3:C:386:PRO:O	3:C:390:ARG:HG2	2.26	0.43
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.90	0.43
23:B:607:CLA:H202	4:D:281:MET:SD	2.57	0.43
3:C:38:GLY:HA3	23:C:511:CLA:HMD3	2.02	0.43
10:K:43:VAL:CG2	10:K:46:ARG:HE	2.32	0.43
1:A:238:LYS:O	1:A:241:GLN:HG3	2.18	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
5:E:81:GLU:O	5:E:83:LEU:N	2.46	0.43
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.87	0.43
19:Z:5:PHE:CG	19:Z:61:VAL:HG21	2.53	0.43
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.07	0.43
2:B:458:PHE:CG	23:B:604:CLA:HMC3	2.54	0.43
23:B:606:CLA:H41	23:B:606:CLA:H62	1.80	0.43
23:B:608:CLA:HAB	4:D:123:ILE:HG23	2.01	0.43
4:D:148:ALA:HB1	4:D:279:LEU:HB2	2.00	0.43
23:B:614:CLA:OBD	11:L:10:VAL:HG21	2.18	0.43
31:A:414:LMG:H211	11:L:26:VAL:HG21	2.00	0.43
27:B:618:BCR:H381	14:T:4:ILE:HD13	25.19	0.43
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.53	0.43
23:B:602:CLA:H72	7:H:46:LEU:HD13	2.01	0.43
4:D:275:PRO:O	4:D:279:LEU:HD23	2.17	0.43
7:H:12:ARG:HD3	7:H:12:ARG:O	2.21	0.43
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.27	0.43
13:O:218:LEU:HD22	15:U:119:THR:HG21	2.01	0.43
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.53	0.43
23:A:405:CLA:H11	23:A:405:CLA:H51	4.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:417:SQD:HO8	2:B:113:TRP:HE1	62.90	0.43
2:B:247:PHE:HB2	23:B:612:CLA:HBC1	19.75	0.43
4:D:313:THR:OG1	4:D:316:THR:HG23	2.18	0.43
23:A:403:CLA:H62	23:A:403:CLA:H102	1.80	0.43
23:A:407:CLA:HMC3	27:A:410:BCR:H12C	1.99	0.43
23:B:607:CLA:HBA2	23:B:607:CLA:C4A	2.48	0.43
27:J:102:BCR:H351	27:J:102:BCR:H15C	1.60	0.43
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.52	0.43
1:A:308:ASP:O	6:F:45:ARG:NE	2.66	0.43
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.43
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.54	0.43
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.01	0.43
1:A:153:SER:CB	23:A:404:CLA:H11	11.39	0.43
23:B:607:CLA:H192	31:B:622:LMG:H342	2.01	0.43
3:C:137:PRO:HG3	23:C:513:CLA:HED2	2.00	0.43
3:C:277:GLY:C	23:C:505:CLA:HBC2	2.53	0.43
23:B:612:CLA:HAB	4:D:123:ILE:HG23	27.95	0.43
27:J:102:BCR:H24C	27:J:102:BCR:H371	1.87	0.43
27:B:618:BCR:C10	14:T:18:PHE:HB2	44.35	0.43
2:B:191:ASN:HD21	7:H:59:ASN:C	2.36	0.43
2:B:69:LEU:HD21	23:B:603:CLA:HED3	2.01	0.43
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.43
23:B:604:CLA:H11	23:B:605:CLA:H11	2.00	0.43
2:B:248:ALA:HA	23:B:607:CLA:H42	25.07	0.43
23:B:609:CLA:HMC2	27:H:101:BCR:H343	2.00	0.43
23:B:612:CLA:H18	23:B:613:CLA:H192	22.11	0.43
23:C:504:CLA:H202	28:C:519:DGD:HAF2	2.01	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.55	0.43
2:B:354:LEU:HB3	2:B:370:LEU:HB3	2.00	0.43
4:D:79:SER:HA	4:D:172:SER:HB3	2.01	0.43
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.01	0.42
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.88	0.42
2:B:461:LEU:HA	2:B:461:LEU:HD23	1.90	0.42
5:E:22:ILE:O	5:E:26:THR:HG23	2.19	0.42
23:C:509:CLA:H112	23:C:509:CLA:H142	1.88	0.42
2:B:206:GLY:O	2:B:210:ILE:HG13	2.19	0.42
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.49	0.42
2:B:170:ASP:OD1	2:B:175:THR:N	2.53	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.53	0.42
23:B:608:CLA:H51	23:B:609:CLA:H101	2.01	0.42
27:T:101:BCR:H351	27:T:101:BCR:H15C	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16:LEU:O	12:M:20:VAL:HG23	2.20	0.42
28:B:627:DGD:O1B	28:B:627:DGD:O2D	2.37	0.42
2:B:230:ARG:O	2:B:233:ASN:HB3	2.19	0.42
13:O:144:LEU:HD13	13:O:259:VAL:HG11	2.01	0.42
13:O:51:THR:O	13:O:53:ARG:N	2.53	0.42
2:B:450:TRP:NE1	23:B:611:CLA:HBA1	29.68	0.42
23:B:612:CLA:H8	23:B:612:CLA:H122	1.87	0.42
13:O:168:PHE:HB2	13:O:225:LEU:HB2	2.02	0.42
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.71	0.42
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.04	0.42
1:A:119:PHE:HZ	23:A:404:CLA:H8	8.98	0.42
4:D:239:GLN:HB3	4:D:240:ALA:H	1.57	0.42
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.55	0.42
4:D:342:PRO:O	4:D:345:VAL:HG12	2.30	0.42
1:A:224:ILE:O	4:D:265:ARG:NH2	2.54	0.42
27:B:618:BCR:H341	27:B:618:BCR:H11C	1.69	0.42
4:D:274:VAL:HA	25:D:404:PL9:H253	2.17	0.42
31:C:520:LMG:H322	10:K:27:VAL:HG23	2.02	0.42
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.73	0.42
2:B:386:ALA:HB3	15:U:132:LEU:HD11	2.01	0.42
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.05	0.42
1:A:81:ALA:HB2	1:A:175:GLY:HA3	2.07	0.42
2:B:18:ARG:NH1	2:B:115:TRP:O	2.43	0.42
23:B:605:CLA:H41	23:B:605:CLA:H62	1.75	0.42
3:C:174:LEU:HG	23:C:512:CLA:H92	2.02	0.42
27:C:514:BCR:H371	27:C:514:BCR:H24C	1.88	0.42
2:B:483:ASP:OD2	2:B:484:PRO:HD2	2.20	0.42
1:A:40:THR:HG21	1:A:121:LEU:HD23	2.01	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.19	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.20	0.42
3:C:72:LEU:HD11	3:C:108:THR:HB	2.10	0.42
1:A:176:ILE:HD12	23:A:405:CLA:HED3	27.29	0.42
3:C:418:ASN:HB2	28:C:519:DGD:O4E	2.20	0.42
23:C:503:CLA:H161	23:C:503:CLA:H193	1.80	0.42
23:C:503:CLA:HMD2	23:C:503:CLA:H201	2.09	0.42
23:C:512:CLA:H61	23:C:512:CLA:H13	2.02	0.42
27:C:515:BCR:H20C	27:C:515:BCR:H361	1.93	0.42
4:D:180:ARG:HG3	4:D:181:PHE:N	2.34	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.64	0.42
4:D:201:VAL:O	4:D:205:LEU:HB2	2.20	0.42
2:B:489:GLU:HB2	5:E:3:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:504:CLA:H2	28:C:518:DGD:HA22	2.01	0.42
10:K:24:VAL:O	10:K:27:VAL:HG12	2.20	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.01	0.42
1:A:172:MET:SD	1:A:179:THR:HG23	2.81	0.42
18:X:11:THR:HG23	18:X:12:ILE:HG22	2.01	0.42
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.05	0.42
23:A:404:CLA:HHC	23:A:404:CLA:CBB	2.73	0.42
23:B:614:CLA:H51	23:B:614:CLA:H12	4.49	0.42
4:D:67:TYR:CD1	31:D:406:LMG:HC72	2.67	0.42
4:D:81:PRO:HG3	4:D:108:GLY:O	2.19	0.42
28:D:409:DGD:O5E	28:D:409:DGD:O4E	2.31	0.42
4:D:346:LEU:HD12	4:D:346:LEU:HA	1.85	0.42
2:B:7:ARG:NH2	31:B:622:LMG:HC3	2.35	0.41
3:C:457:LYS:HG2	4:D:229:ALA:HA	2.05	0.41
1:A:176:ILE:HD12	23:A:404:CLA:HED3	2.02	0.41
23:B:603:CLA:HBB2	23:B:603:CLA:H92	2.02	0.41
23:B:610:CLA:H12	23:B:610:CLA:H51	1.78	0.41
27:B:619:BCR:H351	27:B:619:BCR:H15C	1.81	0.41
23:C:504:CLA:H141	23:C:504:CLA:H161	1.90	0.41
3:C:86:LEU:HB3	3:C:90:PRO:HD3	2.10	0.41
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.63	0.41
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.50	0.41
13:O:33:TYR:O	13:O:37:VAL:HG23	2.26	0.41
1:A:321:ILE:HG22	1:A:325:ASN:ND2	2.35	0.41
3:C:264:PHE:HE1	23:C:507:CLA:HAB	1.86	0.41
23:C:506:CLA:HBB2	23:C:507:CLA:H52	2.08	0.41
23:C:513:CLA:HBA2	23:C:513:CLA:H3A	1.80	0.41
14:T:8:PHE:CD1	27:T:102:BCR:H373	2.55	0.41
14:T:3:THR:O	14:T:7:VAL:HG23	2.21	0.41
3:C:215:LYS:HG2	3:C:221:GLU:HB3	2.12	0.41
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.02	0.41
28:D:409:DGD:O2D	28:D:409:DGD:HG32	2.23	0.41
23:B:614:CLA:H41	23:B:614:CLA:H62	3.58	0.41
23:B:616:CLA:H143	23:B:616:CLA:H111	1.83	0.41
31:B:623:LMG:H142	11:L:35:PHE:CE1	2.56	0.41
23:B:606:CLA:C3D	33:B:624:LMT:H11	2.50	0.41
12:M:13:LEU:HD12	27:T:101:BCR:H333	12.28	0.41
16:V:147:VAL:O	16:V:150:LYS:HB2	2.22	0.41
5:E:14:ILE:HG22	9:J:13:VAL:HG11	2.06	0.41
2:B:86:ILE:HG13	2:B:86:ILE:H	1.81	0.41
2:B:247:PHE:HE1	23:B:606:CLA:H101	33.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:451:ALA:HA	3:C:456:GLU:CD	2.40	0.41
27:T:101:BCR:H11C	27:T:101:BCR:H341	1.86	0.41
5:E:49:THR:HA	5:E:50:PRO:HD3	1.93	0.41
7:H:35:MET:HB2	7:H:35:MET:HE3	1.89	0.41
6:F:21:VAL:O	6:F:25:THR:HG23	2.20	0.41
23:A:405:CLA:HMD3	4:D:182:LEU:HD11	2.02	0.41
29:A:412:LHG:H382	23:C:510:CLA:H93	2.02	0.41
11:L:22:LEU:O	11:L:26:VAL:HG22	2.20	0.41
5:E:10:PHE:CE1	34:F:101:HEM:HBD2	2.64	0.41
12:M:20:VAL:HG13	12:M:20:VAL:HG13	0.00	0.41
2:B:272:ARG:HG3	2:B:273:TYR:N	2.41	0.41
2:B:242:ILE:HG22	2:B:466:HIS:HB2	2.04	0.41
16:V:81:ARG:NE	16:V:157:GLY:HA3	2.47	0.41
2:B:298:LEU:HA	2:B:298:LEU:HD12	1.90	0.41
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.41
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.94	0.41
30:A:413:SQD:H172	29:A:415:LHG:H172	2.03	0.41
3:C:290:VAL:O	3:C:423:ARG:NH1	2.53	0.41
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.59	0.41
1:A:307:ILE:HD11	6:F:45:ARG:NH2	2.51	0.41
13:O:194:TYR:CE1	13:O:198:ILE:HD13	2.56	0.41
2:B:153:PHE:O	2:B:157:HIS:HB3	2.20	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
1:A:22:THR:HG21	8:I:30:ARG:HD3	2.11	0.41
4:D:267:LEU:O	4:D:271:MET:HG3	2.20	0.41
30:A:417:SQD:H311	30:A:417:SQD:H342	1.86	0.41
2:B:30:VAL:HG12	23:B:609:CLA:HHD	31.13	0.41
23:B:603:CLA:HBB2	23:B:605:CLA:H152	2.03	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.52	0.41
3:C:318:LEU:HG	3:C:328:VAL:HG11	2.03	0.41
19:Z:5:PHE:HB2	19:Z:57:LEU:HG	2.12	0.41
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.41
2:B:182:ALA:HA	2:B:183:PRO:HD3	1.93	0.41
23:B:604:CLA:H41	23:B:604:CLA:H61	1.91	0.41
1:A:180:PHE:O	1:A:184:ILE:HG13	2.23	0.41
23:B:616:CLA:H8	23:B:616:CLA:H122	3.34	0.41
27:B:619:BCR:H24C	27:B:619:BCR:H371	1.89	0.41
31:B:623:LMG:HC3	33:M:102:LMT:O2'	2.21	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.36	0.41
3:C:120:ILE:HD11	27:C:514:BCR:HC8	2.08	0.41
2:B:257:TRP:CD2	4:D:291:LEU:HD12	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.67	0.41
14:T:29:ILE:O	14:T:31:LYS:N	2.54	0.41
20:Y:23:UNK:O	20:Y:24:UNK:C	2.68	0.41
2:B:10:THR:O	2:B:13:ILE:HG13	2.29	0.41
3:C:447:ARG:HH11	3:C:447:ARG:HG2	1.88	0.41
4:D:74:LEU:O	4:D:175:VAL:HB	2.20	0.41
5:E:8:ARG:HB2	6:F:13:TYR:HB3	2.02	0.41
2:B:87:ASP:HA	2:B:88:PRO:HD2	1.97	0.41
5:E:42:LEU:O	5:E:46:VAL:HG23	2.28	0.41
2:B:91:TRP:CH2	23:B:606:CLA:H12	2.56	0.41
3:C:174:LEU:HD13	23:C:502:CLA:H111	2.07	0.41
27:C:515:BCR:H11C	27:C:515:BCR:H341	1.87	0.41
27:D:405:BCR:H11C	27:D:405:BCR:H341	1.75	0.41
18:X:12:ILE:O	18:X:12:ILE:HG23	2.23	0.41
4:D:84:SER:HB2	4:D:85:MET:HE2	2.04	0.41
2:B:192:PRO:HD2	7:H:60:VAL:HG12	2.09	0.41
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.03	0.41
3:C:101:PRO:O	3:C:104:GLU:HB2	2.33	0.41
1:A:271:LEU:HD11	25:A:408:PL9:C4	2.51	0.40
23:A:405:CLA:H62	23:A:405:CLA:H41	3.14	0.40
2:B:109:LEU:O	27:B:620:BCR:H21C	2.21	0.40
23:B:603:CLA:H3A	23:B:603:CLA:CGA	2.51	0.40
3:C:406:SER:HA	3:C:420:VAL:HG23	2.02	0.40
23:C:510:CLA:OBD	10:K:33:LEU:HD23	2.39	0.40
1:A:258:LEU:O	4:D:128:ARG:NH1	2.55	0.40
20:G:23:UNK:O	20:G:24:UNK:C	2.68	0.40
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.02	0.40
23:B:604:CLA:H161	23:B:604:CLA:H202	1.79	0.40
23:B:605:CLA:H202	23:B:605:CLA:H162	1.96	0.40
23:C:501:CLA:H52	23:C:503:CLA:H92	2.05	0.40
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.79	0.40
10:K:19:ASP:N	10:K:20:PRO:HD2	2.36	0.40
13:O:97:VAL:HG12	13:O:133:THR:O	2.21	0.40
3:C:107:ASP:O	3:C:110:PRO:HD2	2.27	0.40
3:C:77:PRO:HG2	3:C:78:GLU:OE2	2.27	0.40
1:A:177:SER:HA	1:A:180:PHE:CD2	2.56	0.40
23:B:607:CLA:H122	31:B:623:LMG:H412	2.03	0.40
23:B:608:CLA:H18	23:B:609:CLA:H192	2.03	0.40
28:C:517:DGD:HAW2	28:C:517:DGD:HA91	4.31	0.40
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.04	0.40
10:K:43:VAL:HG22	10:K:46:ARG:HE	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:68:VAL:O	16:V:71:ILE:HG12	2.20	0.40
14:T:9:ILE:O	14:T:13:ILE:HG13	2.27	0.40
23:B:607:CLA:HBB1	31:B:623:LMG:H341	2.03	0.40
3:C:416:SER:OG	3:C:417:VAL:N	2.54	0.40
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.56	0.40
1:A:182:PHE:O	1:A:186:PHE:HB2	2.22	0.40
16:V:60:GLN:HA	16:V:64:ALA:HB2	2.02	0.40
23:B:607:CLA:H92	23:B:607:CLA:HBB2	11.47	0.40
23:B:609:CLA:H161	23:B:609:CLA:H141	4.20	0.40
23:C:511:CLA:H42	10:K:39:TRP:CD1	2.56	0.40
15:U:73:PRO:HG2	16:V:107:THR:HB	2.07	0.40
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.88	0.40
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.04	0.40
1:A:42:LEU:HA	1:A:45:THR:HG22	2.03	0.40
11:L:7:ARG:HG3	11:L:7:ARG:H	1.73	0.40
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	311 (93%)	17 (5%)	5 (2%)	13	57
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	16	61
2	B	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	19	65
2	b	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	19	65
3	C	445/461 (96%)	406 (91%)	33 (7%)	6 (1%)	15	60
3	c	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	15	60
4	D	338/352 (96%)	316 (94%)	20 (6%)	2 (1%)	30	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	30	74
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	60
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	60
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	31
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	31
8	I	33/38 (87%)	27 (82%)	4 (12%)	2 (6%)	2	25
8	i	33/38 (87%)	28 (85%)	4 (12%)	1 (3%)	5	42
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	42
9	j	32/40 (80%)	28 (88%)	2 (6%)	2 (6%)	2	25
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	27
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	27
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	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%)	206 (86%)	31 (13%)	4 (2%)	11	55
13	o	241/272 (89%)	208 (86%)	29 (12%)	4 (2%)	11	55
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	40
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	40
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	41
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	41
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	37
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4	37
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	27
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	27
19	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	55
19	z	60/62 (97%)	54 (90%)	3 (5%)	3 (5%)	3	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5138/5650 (91%)	4681 (91%)	378 (7%)	79 (2%)	13 57

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA
14	T	30	THR
18	X	45	LYS
1	a	12	ASN
1	a	142	TRP
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
14	t	30	THR
18	x	45	LYS
1	A	141	PRO
2	B	489	GLU
3	C	32	GLY
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
7	H	26	GLY
17	y	43	ARG
19	Z	32	ASP
1	a	141	PRO
2	b	489	GLU
3	c	32	GLY
3	c	144	SER
3	c	257	PHE
3	c	416	SER
4	d	239	GLN
5	e	82	GLN
7	h	26	GLY
9	j	38	SER
17	g	43	ARG
19	z	32	ASP

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Mol	Chain	Res	Type
1	A	142	TRP
3	C	194	GLY
5	E	82	GLN
9	J	38	SER
13	O	88	GLU
15	U	83	ALA
1	a	334	ARG
3	c	194	GLY
13	o	88	GLU
13	o	271	PRO
15	u	72	TYR
1	A	334	ARG
4	D	262	SER
13	O	271	PRO
15	U	72	TYR
4	d	262	SER
7	h	16	SER
8	i	25	SER
10	k	45	PHE
13	o	158	ASN
15	u	83	ALA
2	B	176	GLY
2	B	230	ARG
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
15	U	73	PRO
2	b	176	GLY
10	k	13	GLU
18	x	12	ILE
8	I	25	SER
13	O	158	ASN
18	X	12	ILE
2	b	230	ARG
19	z	28	ALA
15	u	73	PRO
8	I	32	PRO
3	C	209	ILE
1	A	176	ILE
3	c	209	ILE
19	z	24	PRO
9	j	35	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	271/291 (93%)	266 (98%)	5 (2%)	66	87
1	a	271/291 (93%)	266 (98%)	5 (2%)	66	87
2	B	390/407 (96%)	380 (97%)	10 (3%)	54	80
2	b	390/407 (96%)	379 (97%)	11 (3%)	51	78
3	C	347/362 (96%)	333 (96%)	14 (4%)	38	71
3	c	347/362 (96%)	332 (96%)	15 (4%)	35	70
4	D	275/283 (97%)	260 (94%)	15 (6%)	27	64
4	d	275/283 (97%)	262 (95%)	13 (5%)	32	68
5	E	72/73 (99%)	68 (94%)	4 (6%)	26	63
5	e	72/73 (99%)	68 (94%)	4 (6%)	26	63
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	17	54
7	h	53/55 (96%)	50 (94%)	3 (6%)	25	62
8	I	32/35 (91%)	31 (97%)	1 (3%)	47	77
8	i	32/35 (91%)	31 (97%)	1 (3%)	47	77
9	J	24/28 (86%)	23 (96%)	1 (4%)	36	70
9	j	24/28 (86%)	23 (96%)	1 (4%)	36	70
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	50	78
11	l	35/35 (100%)	34 (97%)	1 (3%)	50	78
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	82	92
13	o	202/228 (89%)	200 (99%)	2 (1%)	82	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	29/29 (100%)	28 (97%)	1 (3%)	44	75
14	t	29/29 (100%)	28 (97%)	1 (3%)	44	75
15	U	84/112 (75%)	83 (99%)	1 (1%)	78	90
15	u	84/112 (75%)	82 (98%)	2 (2%)	57	82
16	V	116/138 (84%)	114 (98%)	2 (2%)	68	87
16	v	116/138 (84%)	114 (98%)	2 (2%)	68	87
17	g	20/37 (54%)	18 (90%)	2 (10%)	9	38
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	38
18	X	30/34 (88%)	27 (90%)	3 (10%)	9	38
18	x	30/34 (88%)	27 (90%)	3 (10%)	9	38
19	Z	52/52 (100%)	49 (94%)	3 (6%)	25	61
19	z	52/52 (100%)	50 (96%)	2 (4%)	40	73
All	All	4244/4616 (92%)	4107 (97%)	137 (3%)	46	76

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	VAL
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	223	GLN
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	232	ASP

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Mol	Chain	Res	Type
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	84	SER
4	D	91	LEU
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU
16	V	63	CYS
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU

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Mol	Chain	Res	Type
18	X	11	THR
18	X	12	ILE
18	X	45	LYS
19	Z	14	ILE
19	Z	33	TRP
19	Z	62	VAL
1	a	202	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	223	GLN
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	488	PRO
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	232	ASP
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	305	THR
3	c	355	THR
3	c	382	ASN
3	c	391	ARG
3	c	469	MET
3	c	472	LEU
4	d	20	ASP
4	d	43	LEU
4	d	84	SER
4	d	130	PHE
4	d	180	ARG

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Mol	Chain	Res	Type
4	d	241	GLU
4	d	259	ILE
4	d	279	LEU
4	d	291	LEU
4	d	294	ARG
4	d	323	GLU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	77	GLU
5	e	82	GLN
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
7	h	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	103	GLN
15	u	132	LEU
16	v	63	CYS
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	11	THR
18	x	12	ILE
18	x	45	LYS
19	z	33	TRP
19	z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	303	ASN
4	D	117	HIS
17	y	45	ASN
1	a	241	GLN
2	b	201	HIS

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Mol	Chain	Res	Type
15	u	93	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	BCT	A	402	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	403	-	55,73,73	0.95	4 (7%)	61,113,113	1.19	9 (14%)
23	CLA	A	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.22	8 (13%)
23	CLA	A	405	-	55,73,73	0.93	3 (5%)	61,113,113	1.27	8 (13%)
24	PHO	A	406	-	67,69,69	1.25	12 (17%)	84,99,99	1.09	6 (7%)
23	CLA	A	407	-	55,73,73	0.94	4 (7%)	61,113,113	1.18	6 (9%)
25	PL9	A	408	-	45,45,55	1.46	7 (15%)	56,57,69	1.74	14 (25%)
26	OEC	A	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	A	410	-	41,41,41	0.70	0	56,56,56	1.92	11 (19%)
28	DGD	A	411	-	57,57,67	1.20	7 (12%)	71,71,81	1.56	12 (16%)
29	LHG	A	412	-	38,38,48	1.01	2 (5%)	39,44,54	1.01	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	A	413	-	50,51,54	0.97	3 (6%)	58,62,65	1.65	10 (17%)
31	LMG	A	414	-	51,51,55	1.12	6 (11%)	59,59,63	1.35	4 (6%)
29	LHG	A	415	-	36,36,48	1.04	2 (5%)	37,42,54	1.10	3 (8%)
30	SQD	A	417	-	53,54,54	1.00	4 (7%)	61,65,65	1.71	11 (18%)
31	LMG	A	418	-	42,42,55	1.20	6 (14%)	50,50,63	1.52	9 (18%)
23	CLA	B	601	-	55,73,73	0.98	4 (7%)	61,113,113	1.20	8 (13%)
23	CLA	B	602	-	55,73,73	0.95	3 (5%)	61,113,113	1.16	6 (9%)
23	CLA	B	603	-	55,73,73	0.96	3 (5%)	61,113,113	1.22	7 (11%)
23	CLA	B	604	-	55,73,73	0.97	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	B	605	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	9 (14%)
23	CLA	B	606	-	55,73,73	0.95	4 (7%)	61,113,113	1.23	7 (11%)
23	CLA	B	607	-	55,73,73	0.93	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	B	608	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	B	609	-	55,73,73	0.96	4 (7%)	61,113,113	1.20	7 (11%)
23	CLA	B	610	-	55,73,73	0.97	3 (5%)	61,113,113	1.23	7 (11%)
23	CLA	B	611	-	55,73,73	0.95	4 (7%)	61,113,113	1.22	7 (11%)
23	CLA	B	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	8 (13%)
23	CLA	B	613	-	55,73,73	0.93	4 (7%)	61,113,113	1.13	5 (8%)
23	CLA	B	614	-	55,73,73	0.96	3 (5%)	61,113,113	1.16	6 (9%)
23	CLA	B	615	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	5 (8%)
23	CLA	B	616	-	55,73,73	0.95	4 (7%)	61,113,113	1.21	8 (13%)
27	BCR	B	617	-	41,41,41	0.67	0	56,56,56	1.86	14 (25%)
27	BCR	B	618	-	41,41,41	0.64	0	56,56,56	2.31	18 (32%)
27	BCR	B	619	-	41,41,41	0.64	0	56,56,56	1.88	17 (30%)
27	BCR	B	620	-	41,41,41	0.70	0	56,56,56	2.18	15 (26%)
28	DGD	B	621	-	59,59,67	1.20	8 (13%)	73,73,81	1.12	4 (5%)
31	LMG	B	622	-	49,49,55	1.11	7 (14%)	57,57,63	1.33	6 (10%)
31	LMG	B	623	-	49,49,55	1.16	8 (16%)	57,57,63	1.42	8 (14%)
33	LMT	B	624	-	36,36,36	0.41	0	47,47,47	0.72	0
33	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.71	0
30	SQD	B	626	-	46,47,54	1.01	4 (8%)	54,58,65	1.72	9 (16%)
28	DGD	B	627	-	53,53,67	1.19	6 (11%)	67,67,81	1.48	10 (14%)
33	LMT	B	628	-	36,36,36	0.44	0	47,47,47	0.81	1 (2%)
33	LMT	B	629	-	36,36,36	0.44	0	47,47,47	0.66	0
23	CLA	C	501	-	55,73,73	0.94	3 (5%)	61,113,113	1.16	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	502	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	7 (11%)
23	CLA	C	503	-	55,73,73	0.92	3 (5%)	61,113,113	1.22	8 (13%)
23	CLA	C	504	-	55,73,73	0.97	3 (5%)	61,113,113	1.21	7 (11%)
23	CLA	C	505	-	55,73,73	0.97	4 (7%)	61,113,113	1.21	8 (13%)
23	CLA	C	506	-	55,73,73	0.96	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	C	507	-	55,73,73	0.94	3 (5%)	61,113,113	1.26	7 (11%)
23	CLA	C	508	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	7 (11%)
23	CLA	C	509	-	55,73,73	0.96	4 (7%)	61,113,113	1.14	6 (9%)
23	CLA	C	510	-	55,73,73	0.97	3 (5%)	61,113,113	1.18	8 (13%)
23	CLA	C	511	3	55,73,73	0.97	4 (7%)	61,113,113	1.23	9 (14%)
23	CLA	C	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.25	9 (14%)
23	CLA	C	513	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
27	BCR	C	514	-	41,41,41	0.70	0	56,56,56	2.36	18 (32%)
27	BCR	C	515	-	41,41,41	0.64	0	56,56,56	1.92	15 (26%)
27	BCR	C	516	-	41,41,41	0.66	0	56,56,56	1.98	16 (28%)
28	DGD	C	517	-	54,54,67	1.18	6 (11%)	68,68,81	1.31	7 (10%)
28	DGD	C	518	-	63,63,67	1.19	10 (15%)	77,77,81	1.31	7 (9%)
28	DGD	C	519	-	67,67,67	1.10	6 (8%)	81,81,81	1.45	10 (12%)
31	LMG	C	520	-	48,48,55	1.10	6 (12%)	56,56,63	1.32	7 (12%)
31	LMG	C	521	-	45,45,55	1.16	6 (13%)	53,53,63	1.40	9 (16%)
23	CLA	D	401	-	55,73,73	0.92	3 (5%)	61,113,113	1.26	8 (13%)
24	PHO	D	402	-	67,69,69	1.21	12 (17%)	84,99,99	1.07	7 (8%)
23	CLA	D	403	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
25	PL9	D	404	-	55,55,55	1.46	8 (14%)	68,69,69	1.82	20 (29%)
27	BCR	D	405	-	41,41,41	0.64	0	56,56,56	2.22	16 (28%)
31	LMG	D	406	-	46,46,55	1.15	5 (10%)	54,54,63	1.39	7 (12%)
31	LMG	D	407	-	48,48,55	1.16	8 (16%)	56,56,63	1.48	7 (12%)
30	SQD	D	408	-	42,43,54	1.09	4 (9%)	50,54,65	2.19	9 (18%)
28	DGD	D	409	-	64,64,67	1.12	6 (9%)	78,78,81	1.52	8 (10%)
33	LMT	D	410	-	32,32,36	0.49	0	43,43,47	0.72	2 (4%)
31	LMG	E	101	-	44,44,55	1.16	7 (15%)	52,52,63	1.35	7 (13%)
34	HEM	F	101	5,6	30,50,50	2.04	8 (26%)	24,82,82	2.38	10 (41%)
30	SQD	F	102	-	44,45,54	1.03	4 (9%)	52,56,65	1.82	10 (19%)
27	BCR	H	101	-	41,41,41	0.68	0	56,56,56	1.77	14 (25%)
31	LMG	I	101	-	43,43,55	1.23	8 (18%)	51,51,63	1.33	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMT	I	102	-	36,36,36	0.41	0	47,47,47	0.70	2 (4%)
25	PL9	J	101	-	35,35,55	1.36	5 (14%)	44,45,69	1.66	8 (18%)
27	BCR	J	102	-	41,41,41	0.70	0	56,56,56	3.42	26 (46%)
31	LMG	M	101	-	42,42,55	1.25	7 (16%)	50,50,63	1.54	9 (18%)
33	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.69	0
27	BCR	T	101	-	41,41,41	0.66	0	56,56,56	1.79	12 (21%)
27	BCR	T	102	-	41,41,41	0.66	0	56,56,56	2.29	18 (32%)
34	HEM	V	201	16	30,50,50	2.29	8 (26%)	24,82,82	2.12	6 (25%)
30	SQD	a	401	-	53,54,54	0.98	4 (7%)	61,65,65	1.76	10 (16%)
31	LMG	a	402	-	42,42,55	1.20	6 (14%)	50,50,63	1.53	8 (16%)
23	CLA	a	404	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	CLA	a	405	-	55,73,73	0.95	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	a	406	-	55,73,73	0.93	3 (5%)	61,113,113	1.27	8 (13%)
24	PHO	a	407	-	67,69,69	1.22	11 (16%)	84,99,99	1.06	8 (9%)
24	PHO	a	408	-	67,69,69	1.23	9 (13%)	84,99,99	1.05	5 (5%)
23	CLA	a	409	-	55,73,73	0.94	4 (7%)	61,113,113	1.19	8 (13%)
25	PL9	a	410	-	45,45,55	1.42	7 (15%)	56,57,69	1.82	16 (28%)
26	OEC	a	411	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	a	412	-	41,41,41	0.71	0	56,56,56	1.95	13 (23%)
28	DGD	a	413	-	57,57,67	1.17	7 (12%)	71,71,81	1.50	12 (16%)
29	LHG	a	414	-	38,38,48	1.03	2 (5%)	39,44,54	1.03	4 (10%)
30	SQD	a	415	-	50,51,54	0.96	4 (8%)	58,62,65	1.69	9 (15%)
31	LMG	a	416	-	51,51,55	1.09	6 (11%)	59,59,63	1.38	5 (8%)
29	LHG	a	417	-	36,36,48	1.05	2 (5%)	37,42,54	1.04	2 (5%)
30	SQD	b	601	-	46,47,54	1.00	4 (8%)	54,58,65	1.82	10 (18%)
28	DGD	b	602	-	53,53,67	1.20	5 (9%)	67,67,81	1.41	10 (14%)
33	LMT	b	603	-	36,36,36	0.43	0	47,47,47	0.78	1 (2%)
33	LMT	b	604	-	36,36,36	0.39	0	47,47,47	0.64	0
23	CLA	b	605	-	55,73,73	0.96	4 (7%)	61,113,113	1.25	8 (13%)
23	CLA	b	606	-	55,73,73	0.97	3 (5%)	61,113,113	1.23	7 (11%)
23	CLA	b	607	-	55,73,73	0.93	3 (5%)	61,113,113	1.25	8 (13%)
23	CLA	b	608	-	55,73,73	0.95	3 (5%)	61,113,113	1.16	6 (9%)
23	CLA	b	609	-	55,73,73	0.96	4 (7%)	61,113,113	1.16	8 (13%)
23	CLA	b	610	-	55,73,73	0.97	3 (5%)	61,113,113	1.23	8 (13%)
23	CLA	b	611	-	55,73,73	0.96	3 (5%)	61,113,113	1.14	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	b	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.18	8 (13%)
23	CLA	b	614	-	55,73,73	0.94	3 (5%)	61,113,113	1.24	6 (9%)
23	CLA	b	615	-	55,73,73	0.96	4 (7%)	61,113,113	1.22	7 (11%)
23	CLA	b	616	-	55,73,73	0.93	4 (7%)	61,113,113	1.24	7 (11%)
23	CLA	b	617	-	55,73,73	0.95	3 (5%)	61,113,113	1.27	8 (13%)
23	CLA	b	618	-	55,73,73	0.97	3 (5%)	61,113,113	1.17	6 (9%)
23	CLA	b	619	-	55,73,73	0.94	4 (7%)	61,113,113	1.21	8 (13%)
23	CLA	b	620	-	55,73,73	0.98	5 (9%)	61,113,113	1.15	7 (11%)
27	BCR	b	621	-	41,41,41	0.62	0	56,56,56	1.99	18 (32%)
27	BCR	b	622	-	41,41,41	0.69	0	56,56,56	2.25	15 (26%)
28	DGD	b	623	-	59,59,67	1.17	7 (11%)	73,73,81	1.16	5 (6%)
31	LMG	b	624	-	49,49,55	1.14	7 (14%)	57,57,63	1.31	8 (14%)
31	LMG	b	625	-	49,49,55	1.15	8 (16%)	57,57,63	1.45	10 (17%)
33	LMT	b	626	-	36,36,36	0.38	0	47,47,47	0.75	1 (2%)
33	LMT	b	627	-	36,36,36	0.42	0	47,47,47	0.66	0
23	CLA	c	501	-	55,73,73	0.94	3 (5%)	61,113,113	1.24	9 (14%)
23	CLA	c	502	-	55,73,73	0.97	4 (7%)	61,113,113	1.22	8 (13%)
23	CLA	c	503	-	55,73,73	0.93	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	c	504	-	55,73,73	0.92	3 (5%)	61,113,113	1.25	7 (11%)
23	CLA	c	505	-	55,73,73	0.96	4 (7%)	61,113,113	1.23	8 (13%)
23	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.29	7 (11%)
23	CLA	c	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	8 (13%)
23	CLA	c	508	-	55,73,73	0.94	3 (5%)	61,113,113	1.27	8 (13%)
23	CLA	c	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.12	6 (9%)
23	CLA	c	510	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	8 (13%)
23	CLA	c	511	-	55,73,73	0.97	4 (7%)	61,113,113	1.16	7 (11%)
23	CLA	c	512	-	55,73,73	0.93	3 (5%)	61,113,113	1.26	9 (14%)
23	CLA	c	513	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
27	BCR	c	514	-	41,41,41	0.67	0	56,56,56	2.39	18 (32%)
27	BCR	c	515	-	41,41,41	0.66	0	56,56,56	2.02	16 (28%)
28	DGD	c	516	-	54,54,67	1.21	6 (11%)	68,68,81	1.31	8 (11%)
28	DGD	c	517	-	63,63,67	1.18	10 (15%)	77,77,81	1.36	7 (9%)
28	DGD	c	518	-	67,67,67	1.09	6 (8%)	81,81,81	1.49	12 (14%)
31	LMG	c	519	-	45,45,55	1.19	6 (13%)	53,53,63	1.36	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCT	d	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	402	-	55,73,73	0.93	3 (5%)	61,113,113	1.28	8 (13%)
23	CLA	d	403	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	6 (9%)
25	PL9	d	404	-	55,55,55	1.46	8 (14%)	68,69,69	1.91	20 (29%)
27	BCR	d	405	-	41,41,41	0.64	0	56,56,56	2.19	16 (28%)
31	LMG	d	406	-	46,46,55	1.16	7 (15%)	54,54,63	1.33	6 (11%)
31	LMG	d	407	-	48,48,55	1.14	8 (16%)	56,56,63	1.55	6 (10%)
30	SQD	d	408	-	42,43,54	1.10	4 (9%)	50,54,65	2.17	9 (18%)
28	DGD	d	409	-	64,64,67	1.11	5 (7%)	78,78,81	1.53	10 (12%)
33	LMT	d	410	-	32,32,36	0.47	0	43,43,47	0.71	1 (2%)
31	LMG	e	101	-	44,44,55	1.19	8 (18%)	52,52,63	1.37	9 (17%)
34	HEM	f	101	5,6	30,50,50	2.04	9 (30%)	24,82,82	2.42	11 (45%)
30	SQD	f	102	-	44,45,54	1.02	3 (6%)	52,56,65	1.80	10 (19%)
27	BCR	h	101	-	41,41,41	0.70	0	56,56,56	1.77	14 (25%)
31	LMG	i	101	-	43,43,55	1.24	8 (18%)	51,51,63	1.32	7 (13%)
33	LMT	i	102	-	36,36,36	0.46	1 (2%)	47,47,47	0.72	1 (2%)
25	PL9	j	101	-	35,35,55	1.35	5 (14%)	44,45,69	1.67	8 (18%)
27	BCR	j	102	-	41,41,41	0.68	0	56,56,56	3.41	25 (44%)
27	BCR	k	102	-	41,41,41	0.70	0	56,56,56	1.99	15 (26%)
31	LMG	k	103	-	48,48,55	1.11	6 (12%)	56,56,63	1.29	7 (12%)
33	LMT	m	101	-	36,36,36	0.41	0	47,47,47	0.68	0
31	LMG	m	102	-	42,42,55	1.30	7 (16%)	50,50,63	1.60	10 (20%)
34	HEM	v	201	16	30,50,50	2.21	7 (23%)	24,82,82	2.17	6 (25%)
27	BCR	y	101	-	41,41,41	0.69	0	56,56,56	1.97	16 (28%)
27	BCR	z	101	-	41,41,41	0.62	0	56,56,56	1.85	13 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCT	A	402	21	-	0/0/0/0	0/0/0/0
23	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	406	-	-	0/53/103/103	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	407	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	A	408	-	-	0/41/61/73	0/1/1/1
26	OEC	A	409	1,3	-	0/0/0/54	0/0/0/5
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
28	DGD	A	411	-	-	0/45/85/95	0/2/2/2
29	LHG	A	412	-	-	0/43/43/53	0/0/0/0
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
31	LMG	A	414	-	-	0/46/66/70	0/1/1/1
29	LHG	A	415	-	-	0/41/41/53	0/0/0/0
30	SQD	A	417	-	-	0/49/69/69	0/1/1/1
31	LMG	A	418	-	-	0/37/57/70	0/1/1/1
23	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	DGD	B	621	-	-	0/47/87/95	0/2/2/2
31	LMG	B	622	-	-	0/44/64/70	0/1/1/1
31	LMG	B	623	-	-	0/44/64/70	0/1/1/1
33	LMT	B	624	-	-	0/21/61/61	0/2/2/2
33	LMT	B	625	-	-	0/21/61/61	0/2/2/2
30	SQD	B	626	-	-	0/42/62/69	0/1/1/1
28	DGD	B	627	-	-	0/41/81/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	B	628	-	-	0/21/61/61	0/2/2/2
33	LMT	B	629	-	-	0/21/61/61	0/2/2/2
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	BCR	C	516	-	-	0/29/63/63	0/2/2/2
28	DGD	C	517	-	-	0/42/82/95	0/2/2/2
28	DGD	C	518	-	-	2/51/91/95	0/2/2/2
28	DGD	C	519	-	-	0/55/95/95	0/2/2/2
31	LMG	C	520	-	-	0/43/63/70	0/1/1/1
31	LMG	C	521	-	-	0/40/60/70	0/1/1/1
23	CLA	D	401	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	D	404	-	-	0/53/73/73	0/1/1/1
27	BCR	D	405	-	-	0/29/63/63	0/2/2/2
31	LMG	D	406	-	-	0/41/61/70	0/1/1/1
31	LMG	D	407	-	-	0/43/63/70	0/1/1/1
30	SQD	D	408	-	-	2/38/58/69	0/1/1/1
28	DGD	D	409	-	-	1/52/92/95	0/2/2/2
33	LMT	D	410	-	-	0/17/57/61	0/2/2/2
31	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
30	SQD	F	102	-	-	0/40/60/69	0/1/1/1
27	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	LMG	I	101	-	-	0/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	I	102	-	-	0/21/61/61	0/2/2/2
25	PL9	J	101	-	-	0/29/49/73	0/1/1/1
27	BCR	J	102	-	-	0/29/63/63	0/2/2/2
31	LMG	M	101	-	-	1/37/57/70	0/1/1/1
33	LMT	M	102	-	-	0/21/61/61	0/2/2/2
27	BCR	T	101	-	-	0/29/63/63	0/2/2/2
27	BCR	T	102	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/10/54/54	0/0/8/8
30	SQD	a	401	-	-	0/49/69/69	0/1/1/1
31	LMG	a	402	-	-	0/37/57/70	0/1/1/1
23	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6
23	CLA	a	409	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	a	410	-	-	0/41/61/73	0/1/1/1
26	OEC	a	411	1,3	-	0/0/0/54	0/0/0/5
27	BCR	a	412	-	-	0/29/63/63	0/2/2/2
28	DGD	a	413	-	-	0/45/85/95	0/2/2/2
29	LHG	a	414	-	-	0/43/43/53	0/0/0/0
30	SQD	a	415	-	-	0/46/66/69	0/1/1/1
31	LMG	a	416	-	-	0/46/66/70	0/1/1/1
29	LHG	a	417	-	-	0/41/41/53	0/0/0/0
30	SQD	b	601	-	-	0/42/62/69	0/1/1/1
28	DGD	b	602	-	-	0/41/81/95	0/2/2/2
33	LMT	b	603	-	-	0/21/61/61	0/2/2/2
33	LMT	b	604	-	-	0/21/61/61	0/2/2/2
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	BCR	b	622	-	-	0/29/63/63	0/2/2/2
28	DGD	b	623	-	-	0/47/87/95	0/2/2/2
31	LMG	b	624	-	-	0/44/64/70	0/1/1/1
31	LMG	b	625	-	-	0/44/64/70	0/1/1/1
33	LMT	b	626	-	-	0/21/61/61	0/2/2/2
33	LMT	b	627	-	-	0/21/61/61	0/2/2/2
23	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
28	DGD	c	516	-	-	0/42/82/95	0/2/2/2
28	DGD	c	517	-	-	2/51/91/95	0/2/2/2
28	DGD	c	518	-	-	0/55/95/95	0/2/2/2
31	LMG	c	519	-	-	0/40/60/70	0/1/1/1
22	BCT	d	401	21	-	0/0/0/0	0/0/0/0
23	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	d	404	-	-	0/53/73/73	0/1/1/1
27	BCR	d	405	-	-	0/29/63/63	0/2/2/2
31	LMG	d	406	-	-	0/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	d	407	-	-	0/43/63/70	0/1/1/1
30	SQD	d	408	-	-	2/38/58/69	0/1/1/1
28	DGD	d	409	-	-	1/52/92/95	0/2/2/2
33	LMT	d	410	-	-	0/17/57/61	0/2/2/2
31	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
30	SQD	f	102	-	-	0/40/60/69	0/1/1/1
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
31	LMG	i	101	-	-	0/38/58/70	0/1/1/1
33	LMT	i	102	-	-	0/21/61/61	0/2/2/2
25	PL9	j	101	-	-	0/29/49/73	0/1/1/1
27	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
31	LMG	k	103	-	-	0/43/63/70	0/1/1/1
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
31	LMG	m	102	-	-	1/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/10/54/54	0/0/8/8
27	BCR	y	101	-	-	0/29/63/63	0/2/2/2
27	BCR	z	101	-	-	0/29/63/63	0/2/2/2

All (643) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-8.34	1.44	1.51
34	v	201	HEM	C3B-C4B	-7.51	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.01	1.46	1.51
34	f	101	HEM	C3B-C4B	-5.99	1.46	1.51
34	F	101	HEM	C3D-C4D	-5.17	1.44	1.51
34	f	101	HEM	C3D-C4D	-4.85	1.45	1.51
34	V	201	HEM	C3D-C4D	-4.71	1.45	1.51
34	v	201	HEM	C3D-C4D	-4.66	1.45	1.51
34	V	201	HEM	C2C-C1C	-4.15	1.44	1.52
34	v	201	HEM	C2C-C1C	-3.80	1.45	1.52
34	f	101	HEM	C2C-C1C	-3.49	1.46	1.52
34	F	101	HEM	C2C-C1C	-3.48	1.46	1.52
31	D	406	LMG	O7-C8	-3.12	1.38	1.46
28	C	517	DGD	O2G-C2G	-3.12	1.38	1.46
28	B	621	DGD	O2G-C2G	-3.09	1.38	1.46
31	i	101	LMG	O7-C8	-3.05	1.38	1.46
31	d	406	LMG	O7-C8	-3.04	1.38	1.46
31	D	407	LMG	O7-C8	-3.04	1.38	1.46
31	B	622	LMG	O7-C8	-3.00	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	m	102	LMG	O1-C7	-2.99	1.38	1.43
28	b	623	DGD	O2G-C2G	-2.96	1.39	1.46
31	C	520	LMG	O7-C8	-2.95	1.39	1.46
31	I	101	LMG	O7-C8	-2.93	1.39	1.46
28	c	516	DGD	O2G-C2G	-2.91	1.39	1.46
31	k	103	LMG	O7-C8	-2.91	1.39	1.46
31	D	407	LMG	O3-C3	-2.90	1.36	1.43
31	m	102	LMG	O7-C8	-2.88	1.39	1.46
31	A	418	LMG	O7-C8	-2.87	1.39	1.46
31	b	625	LMG	O7-C8	-2.87	1.39	1.46
23	b	615	CLA	CMB-C2B	-2.86	1.45	1.51
31	b	624	LMG	O7-C8	-2.84	1.39	1.46
28	a	413	DGD	O2G-C2G	-2.84	1.39	1.46
31	d	407	LMG	O7-C8	-2.83	1.39	1.46
31	a	416	LMG	O7-C8	-2.83	1.39	1.46
31	a	402	LMG	O7-C8	-2.81	1.39	1.46
28	c	517	DGD	O2G-C2G	-2.81	1.39	1.46
31	A	414	LMG	O3-C3	-2.78	1.36	1.43
28	C	518	DGD	O2G-C2G	-2.78	1.39	1.46
31	B	623	LMG	O7-C8	-2.78	1.39	1.46
28	D	409	DGD	O2G-C2G	-2.77	1.39	1.46
31	b	625	LMG	O3-C3	-2.77	1.36	1.43
23	B	611	CLA	CMB-C2B	-2.75	1.46	1.51
31	B	623	LMG	O3-C3	-2.74	1.36	1.43
31	M	101	LMG	O1-C7	-2.73	1.38	1.43
31	M	101	LMG	O7-C8	-2.73	1.39	1.46
31	A	414	LMG	O7-C8	-2.73	1.39	1.46
31	e	101	LMG	O7-C8	-2.71	1.39	1.46
31	d	407	LMG	O3-C3	-2.71	1.36	1.43
31	a	416	LMG	O3-C3	-2.69	1.36	1.43
31	A	418	LMG	O8-C9	-2.69	1.39	1.45
23	C	510	CLA	CMB-C2B	-2.69	1.46	1.51
28	d	409	DGD	O2G-C2G	-2.68	1.39	1.46
31	m	102	LMG	O8-C9	-2.67	1.39	1.45
28	B	627	DGD	O2G-C2G	-2.66	1.39	1.46
31	c	519	LMG	O7-C8	-2.65	1.39	1.46
31	i	101	LMG	O8-C9	-2.64	1.39	1.45
23	b	612	CLA	CMB-C2B	-2.63	1.46	1.51
31	m	102	LMG	O3-C3	-2.62	1.36	1.43
23	b	605	CLA	CMB-C2B	-2.62	1.46	1.51
28	B	621	DGD	O3G-C3G	-2.61	1.38	1.43
31	D	406	LMG	O3-C3	-2.61	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	101	LMG	O8-C9	-2.60	1.39	1.45
31	i	101	LMG	O3-C3	-2.60	1.36	1.43
23	b	610	CLA	CMB-C2B	-2.60	1.46	1.51
31	c	519	LMG	O3-C3	-2.60	1.36	1.43
31	d	406	LMG	O3-C3	-2.59	1.36	1.43
23	B	601	CLA	CMB-C2B	-2.59	1.46	1.51
23	c	510	CLA	CMD-C2D	-2.59	1.46	1.51
28	b	602	DGD	O2G-C2G	-2.59	1.40	1.46
31	M	101	LMG	O3-C3	-2.58	1.36	1.43
23	b	620	CLA	CMB-C2B	-2.58	1.46	1.51
31	e	101	LMG	O8-C9	-2.58	1.39	1.45
31	a	402	LMG	O3-C3	-2.58	1.36	1.43
31	I	101	LMG	O3-C3	-2.58	1.36	1.43
23	B	604	CLA	CMB-C2B	-2.57	1.46	1.51
23	c	508	CLA	CMB-C2B	-2.57	1.46	1.51
28	C	519	DGD	O2G-C2G	-2.57	1.40	1.46
28	A	411	DGD	O2G-C2G	-2.56	1.40	1.46
23	C	508	CLA	CMB-C2B	-2.56	1.46	1.51
28	c	518	DGD	O4D-C4D	-2.56	1.36	1.43
23	B	610	CLA	CMB-C2B	-2.56	1.46	1.51
23	b	617	CLA	CMB-C2B	-2.55	1.46	1.51
23	B	616	CLA	CMB-C2B	-2.55	1.46	1.51
23	B	603	CLA	CMB-C2B	-2.55	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.55	1.46	1.51
23	B	606	CLA	CMB-C2B	-2.55	1.46	1.51
31	E	101	LMG	O8-C9	-2.55	1.39	1.45
31	C	521	LMG	O7-C8	-2.54	1.40	1.46
31	E	101	LMG	O7-C8	-2.54	1.40	1.46
28	C	519	DGD	O4D-C4D	-2.54	1.36	1.43
23	C	507	CLA	CMB-C2B	-2.53	1.46	1.51
23	A	404	CLA	CMB-C2B	-2.53	1.46	1.51
23	b	618	CLA	CMB-C2B	-2.53	1.46	1.51
28	B	627	DGD	O6E-C5E	-2.53	1.38	1.44
23	c	502	CLA	CMB-C2B	-2.52	1.46	1.51
23	B	608	CLA	CMB-C2B	-2.52	1.46	1.51
31	c	519	LMG	O8-C9	-2.52	1.39	1.45
31	C	520	LMG	O3-C3	-2.52	1.36	1.43
31	b	624	LMG	O3-C3	-2.52	1.36	1.43
23	b	606	CLA	CMB-C2B	-2.52	1.46	1.51
31	e	101	LMG	O3-C3	-2.51	1.36	1.43
28	A	411	DGD	O4D-C4D	-2.51	1.36	1.43
31	B	623	LMG	O8-C9	-2.51	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	CMB-C2B	-2.51	1.46	1.51
23	B	612	CLA	CMD-C2D	-2.51	1.46	1.51
28	c	518	DGD	O2G-C2G	-2.51	1.40	1.46
31	I	101	LMG	O8-C9	-2.51	1.39	1.45
23	a	405	CLA	CMB-C2B	-2.51	1.46	1.51
31	b	625	LMG	O8-C9	-2.50	1.39	1.45
23	c	505	CLA	CMB-C2B	-2.50	1.46	1.51
31	C	521	LMG	O3-C3	-2.50	1.37	1.43
31	a	416	LMG	O8-C9	-2.50	1.39	1.45
23	C	505	CLA	CMB-C2B	-2.50	1.46	1.51
23	b	614	CLA	CMB-C2B	-2.49	1.46	1.51
31	A	418	LMG	O3-C3	-2.49	1.37	1.43
23	c	510	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	615	CLA	CMB-C2B	-2.49	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.48	1.46	1.51
31	d	406	LMG	O8-C9	-2.48	1.39	1.45
31	k	103	LMG	O3-C3	-2.48	1.37	1.43
23	C	513	CLA	CMB-C2B	-2.48	1.46	1.51
23	b	607	CLA	CMB-C2B	-2.48	1.46	1.51
23	c	504	CLA	CMB-C2B	-2.48	1.46	1.51
23	A	403	CLA	CMD-C2D	-2.48	1.46	1.51
23	B	613	CLA	CMB-C2B	-2.47	1.46	1.51
23	b	611	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	501	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	405	CLA	CMB-C2B	-2.47	1.46	1.51
31	E	101	LMG	O3-C3	-2.47	1.37	1.43
23	B	607	CLA	CMB-C2B	-2.47	1.46	1.51
23	B	605	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	407	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	511	CLA	CMB-C2B	-2.46	1.46	1.51
23	c	513	CLA	CMB-C2B	-2.46	1.46	1.51
23	A	403	CLA	CMB-C2B	-2.46	1.46	1.51
31	B	622	LMG	O8-C9	-2.46	1.39	1.45
23	C	509	CLA	CMB-C2B	-2.46	1.46	1.51
31	B	622	LMG	O3-C3	-2.46	1.37	1.43
23	a	404	CLA	CMD-C2D	-2.46	1.46	1.51
23	a	404	CLA	CMB-C2B	-2.46	1.46	1.51
28	b	602	DGD	O6E-C5E	-2.45	1.38	1.44
31	b	624	LMG	O6-C5	-2.45	1.38	1.44
23	C	505	CLA	CMD-C2D	-2.45	1.46	1.51
23	C	502	CLA	CMB-C2B	-2.45	1.46	1.51
23	c	506	CLA	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CMB-C2B	-2.45	1.46	1.51
23	d	402	CLA	CMD-C2D	-2.45	1.46	1.51
23	c	501	CLA	CMB-C2B	-2.44	1.46	1.51
23	B	608	CLA	CMD-C2D	-2.44	1.46	1.51
23	C	506	CLA	CMB-C2B	-2.44	1.46	1.51
23	D	403	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	616	CLA	CMD-C2D	-2.44	1.46	1.51
28	b	623	DGD	O3G-C3G	-2.44	1.39	1.43
23	c	512	CLA	CMB-C2B	-2.44	1.46	1.51
31	A	414	LMG	O8-C9	-2.44	1.39	1.45
23	B	614	CLA	CMB-C2B	-2.43	1.46	1.51
23	b	609	CLA	CMB-C2B	-2.43	1.46	1.51
28	C	518	DGD	O4D-C4D	-2.43	1.37	1.43
31	D	407	LMG	O8-C9	-2.43	1.39	1.45
28	c	517	DGD	O5D-C6D	-2.43	1.39	1.43
23	B	602	CLA	CMB-C2B	-2.43	1.46	1.51
28	C	519	DGD	O3G-C3G	-2.43	1.39	1.43
23	B	614	CLA	CMD-C2D	-2.42	1.46	1.51
28	c	517	DGD	O4D-C4D	-2.42	1.37	1.43
23	C	503	CLA	CMB-C2B	-2.42	1.46	1.51
31	b	624	LMG	O8-C9	-2.42	1.39	1.45
23	B	604	CLA	CMD-C2D	-2.42	1.46	1.51
23	B	609	CLA	CMB-C2B	-2.41	1.46	1.51
23	c	511	CLA	CMB-C2B	-2.41	1.46	1.51
23	b	619	CLA	CMB-C2B	-2.41	1.46	1.51
23	c	505	CLA	CMD-C2D	-2.41	1.46	1.51
31	d	407	LMG	O8-C9	-2.41	1.39	1.45
31	D	406	LMG	O8-C9	-2.40	1.39	1.45
23	C	510	CLA	CMD-C2D	-2.40	1.46	1.51
23	b	613	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	618	CLA	CMD-C2D	-2.40	1.46	1.51
23	d	403	CLA	CMB-C2B	-2.40	1.46	1.51
23	d	402	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	406	CLA	CMD-C2D	-2.40	1.46	1.51
23	c	503	CLA	CMB-C2B	-2.40	1.46	1.51
23	a	406	CLA	CMB-C2B	-2.39	1.46	1.51
23	b	608	CLA	CMD-C2D	-2.39	1.46	1.51
23	c	509	CLA	CMB-C2B	-2.39	1.46	1.51
31	C	521	LMG	O8-C9	-2.39	1.39	1.45
31	A	418	LMG	O1-C7	-2.39	1.39	1.43
28	a	413	DGD	O4D-C4D	-2.38	1.37	1.43
31	C	520	LMG	O8-C9	-2.38	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	CMB-C2B	-2.38	1.46	1.51
23	B	603	CLA	CMD-C2D	-2.38	1.46	1.51
23	c	502	CLA	CMD-C2D	-2.38	1.46	1.51
28	c	516	DGD	O4D-C4D	-2.37	1.37	1.43
23	b	612	CLA	CMD-C2D	-2.37	1.46	1.51
31	i	101	LMG	O1-C7	-2.37	1.39	1.43
23	C	508	CLA	CMD-C2D	-2.37	1.46	1.51
23	D	401	CLA	CMD-C2D	-2.37	1.46	1.51
30	A	417	SQD	O2-C2	-2.36	1.37	1.43
23	b	609	CLA	CMD-C2D	-2.36	1.46	1.51
23	d	403	CLA	CMD-C2D	-2.36	1.46	1.51
28	A	411	DGD	O3G-C3G	-2.36	1.39	1.43
23	B	612	CLA	CMB-C2B	-2.35	1.46	1.51
28	C	517	DGD	O6E-C5E	-2.35	1.38	1.44
23	B	611	CLA	CMD-C2D	-2.35	1.46	1.51
23	C	502	CLA	CMD-C2D	-2.34	1.46	1.51
23	D	401	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	616	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	611	CLA	CMD-C2D	-2.34	1.46	1.51
28	b	602	DGD	O4D-C4D	-2.34	1.37	1.43
28	c	516	DGD	O6E-C5E	-2.33	1.38	1.44
28	a	413	DGD	O3G-C3G	-2.33	1.39	1.43
23	D	403	CLA	CMD-C2D	-2.33	1.46	1.51
28	c	517	DGD	O6E-C5E	-2.33	1.38	1.44
23	b	617	CLA	CMD-C2D	-2.32	1.46	1.51
31	A	414	LMG	O1-C7	-2.32	1.39	1.43
28	C	518	DGD	O5D-C6D	-2.32	1.39	1.43
23	c	507	CLA	CMD-C2D	-2.32	1.46	1.51
23	B	605	CLA	CMD-C2D	-2.31	1.46	1.51
23	b	615	CLA	CMD-C2D	-2.31	1.46	1.51
24	A	406	PHO	C1C-NC	-2.31	1.33	1.38
23	c	501	CLA	CMD-C2D	-2.31	1.46	1.51
31	I	101	LMG	O1-C7	-2.31	1.39	1.43
24	D	402	PHO	C1C-NC	-2.31	1.33	1.38
31	B	622	LMG	O6-C5	-2.30	1.38	1.44
28	C	518	DGD	O6E-C5E	-2.30	1.38	1.44
31	a	402	LMG	O8-C9	-2.30	1.40	1.45
31	b	624	LMG	O1-C7	-2.30	1.39	1.43
23	B	606	CLA	CMD-C2D	-2.30	1.46	1.51
28	B	621	DGD	O4D-C4D	-2.30	1.37	1.43
28	A	411	DGD	O1G-C1G	-2.29	1.40	1.45
23	b	610	CLA	CMD-C2D	-2.29	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	623	LMG	O1-C7	-2.29	1.39	1.43
30	A	417	SQD	C4-C5	-2.29	1.48	1.53
23	b	605	CLA	CMD-C2D	-2.29	1.46	1.51
28	B	627	DGD	O4D-C4D	-2.28	1.37	1.43
23	A	407	CLA	CMD-C2D	-2.28	1.46	1.51
31	d	406	LMG	O1-C7	-2.28	1.39	1.43
23	B	601	CLA	CMD-C2D	-2.28	1.46	1.51
28	C	518	DGD	C4D-C5D	-2.28	1.48	1.53
23	a	405	CLA	CMD-C2D	-2.27	1.46	1.51
23	b	620	CLA	CMD-C2D	-2.27	1.46	1.51
23	C	506	CLA	CMD-C2D	-2.27	1.46	1.51
23	C	504	CLA	CMD-C2D	-2.27	1.46	1.51
23	B	609	CLA	CMD-C2D	-2.26	1.46	1.51
24	a	408	PHO	C1C-NC	-2.26	1.33	1.38
23	B	602	CLA	CMD-C2D	-2.26	1.46	1.51
23	B	607	CLA	CMD-C2D	-2.26	1.46	1.51
23	c	513	CLA	CMD-C2D	-2.26	1.46	1.51
31	k	103	LMG	O8-C9	-2.25	1.40	1.45
23	B	615	CLA	CMD-C2D	-2.25	1.46	1.51
23	a	409	CLA	CMD-C2D	-2.24	1.46	1.51
30	a	401	SQD	O2-C2	-2.24	1.37	1.43
23	B	610	CLA	CMD-C2D	-2.24	1.46	1.51
23	b	606	CLA	CMD-C2D	-2.24	1.46	1.51
23	C	512	CLA	CMD-C2D	-2.24	1.46	1.51
23	c	506	CLA	CMD-C2D	-2.24	1.46	1.51
23	A	404	CLA	CMD-C2D	-2.24	1.46	1.51
23	A	405	CLA	CMD-C2D	-2.24	1.46	1.51
23	c	511	CLA	CMD-C2D	-2.23	1.46	1.51
23	b	613	CLA	CMD-C2D	-2.22	1.46	1.51
31	a	402	LMG	O1-C7	-2.22	1.39	1.43
31	k	103	LMG	O1-C7	-2.22	1.39	1.43
23	c	504	CLA	CMD-C2D	-2.22	1.46	1.51
23	c	512	CLA	CMD-C2D	-2.21	1.46	1.51
23	c	503	CLA	CMD-C2D	-2.21	1.46	1.51
23	C	513	CLA	CMD-C2D	-2.21	1.46	1.51
31	a	416	LMG	O1-C7	-2.21	1.39	1.43
23	b	607	CLA	CMD-C2D	-2.20	1.46	1.51
31	i	101	LMG	O6-C5	-2.20	1.38	1.44
28	c	517	DGD	O1G-C1G	-2.20	1.40	1.45
23	C	503	CLA	CMD-C2D	-2.20	1.46	1.51
23	B	616	CLA	CMD-C2D	-2.20	1.46	1.51
30	B	626	SQD	O2-C2	-2.20	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	407	LMG	O2-C2	-2.19	1.37	1.43
23	C	511	CLA	CMD-C2D	-2.19	1.46	1.51
23	b	619	CLA	CMD-C2D	-2.19	1.46	1.51
23	C	501	CLA	CMD-C2D	-2.19	1.46	1.51
28	C	517	DGD	O4D-C4D	-2.18	1.37	1.43
31	I	101	LMG	O6-C5	-2.18	1.38	1.44
23	c	509	CLA	CMD-C2D	-2.18	1.46	1.51
23	c	508	CLA	CMD-C2D	-2.18	1.46	1.51
28	c	518	DGD	O3G-C3G	-2.18	1.39	1.43
31	d	407	LMG	O2-C2	-2.17	1.37	1.43
23	C	509	CLA	CMD-C2D	-2.17	1.46	1.51
31	m	102	LMG	O6-C5	-2.17	1.38	1.44
23	C	507	CLA	CMD-C2D	-2.16	1.46	1.51
31	D	407	LMG	O6-C5	-2.16	1.38	1.44
28	B	621	DGD	O6D-C5D	-2.16	1.38	1.44
28	a	413	DGD	O1G-C1G	-2.15	1.40	1.45
28	b	623	DGD	O6E-C5E	-2.15	1.39	1.44
24	a	407	PHO	C1C-NC	-2.15	1.33	1.38
31	B	623	LMG	O6-C5	-2.14	1.39	1.44
28	c	517	DGD	O6D-C5D	-2.14	1.39	1.44
31	d	407	LMG	O1-C7	-2.14	1.39	1.43
28	d	409	DGD	O4D-C4D	-2.13	1.37	1.43
31	c	519	LMG	O6-C5	-2.13	1.39	1.44
30	b	601	SQD	O2-C2	-2.13	1.37	1.43
34	f	101	HEM	C2B-C1B	-2.13	1.44	1.51
34	F	101	HEM	C2B-C1B	-2.12	1.44	1.51
24	a	407	PHO	CMB-C2B	-2.12	1.46	1.50
28	C	518	DGD	O5D-C1E	-2.12	1.36	1.40
23	b	616	CLA	CMC-C2C	-2.12	1.46	1.50
30	A	413	SQD	O2-C2	-2.12	1.37	1.43
24	D	402	PHO	CMD-C2D	-2.11	1.46	1.50
30	a	401	SQD	C4-C5	-2.11	1.48	1.53
28	D	409	DGD	O4D-C4D	-2.11	1.37	1.43
23	B	616	CLA	CMC-C2C	-2.11	1.46	1.50
23	B	613	CLA	CMD-C2D	-2.11	1.47	1.51
31	E	101	LMG	O6-C5	-2.10	1.39	1.44
31	d	407	LMG	O6-C5	-2.10	1.39	1.44
23	C	502	CLA	CMC-C2C	-2.10	1.46	1.50
31	b	625	LMG	O6-C5	-2.10	1.39	1.44
23	b	614	CLA	CMD-C2D	-2.10	1.47	1.51
28	b	623	DGD	O4D-C4D	-2.10	1.37	1.43
23	b	605	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	CMD-C2D	-2.09	1.46	1.50
31	e	101	LMG	O6-C5	-2.09	1.39	1.44
28	B	627	DGD	C4E-C5E	-2.08	1.48	1.53
28	C	517	DGD	C4E-C5E	-2.08	1.48	1.53
28	D	409	DGD	O6E-C5E	-2.08	1.39	1.44
23	a	409	CLA	CMC-C2C	-2.08	1.46	1.50
31	I	101	LMG	C4-C5	-2.08	1.48	1.53
23	C	508	CLA	CMC-C2C	-2.08	1.46	1.50
30	D	408	SQD	O3-C3	-2.08	1.38	1.43
23	b	620	CLA	CMC-C2C	-2.08	1.46	1.50
28	C	518	DGD	C4E-C5E	-2.07	1.48	1.53
28	C	519	DGD	O1G-C1G	-2.07	1.40	1.45
23	C	511	CLA	C3B-C2B	-2.07	1.37	1.40
28	B	621	DGD	O1G-C1G	-2.07	1.40	1.45
30	d	408	SQD	O3-C3	-2.07	1.38	1.43
28	D	409	DGD	O5D-C6D	-2.07	1.39	1.43
30	F	102	SQD	O2-C2	-2.07	1.38	1.43
23	C	509	CLA	C3B-C2B	-2.07	1.37	1.40
28	c	517	DGD	C4D-C5D	-2.07	1.48	1.53
23	b	620	CLA	C3B-C2B	-2.07	1.37	1.40
31	e	101	LMG	C4-C5	-2.07	1.48	1.53
23	B	606	CLA	CMC-C2C	-2.07	1.46	1.50
31	C	520	LMG	O1-C7	-2.07	1.39	1.43
23	c	502	CLA	CMC-C2C	-2.06	1.46	1.50
31	b	625	LMG	O2-C2	-2.06	1.38	1.43
23	A	407	CLA	CMC-C2C	-2.06	1.46	1.50
31	C	521	LMG	O6-C5	-2.06	1.39	1.44
28	a	413	DGD	O6E-C5E	-2.06	1.39	1.44
34	F	101	HEM	C2D-C1D	-2.05	1.45	1.51
28	B	621	DGD	O6E-C5E	-2.05	1.39	1.44
30	D	408	SQD	O4-C4	-2.05	1.38	1.43
30	f	102	SQD	O2-C2	-2.04	1.38	1.43
24	D	402	PHO	CMC-C2C	-2.04	1.46	1.50
30	B	626	SQD	O3-C3	-2.04	1.38	1.43
23	B	601	CLA	CMC-C2C	-2.04	1.46	1.50
31	E	101	LMG	O2-C2	-2.04	1.38	1.43
28	C	518	DGD	O6D-C5D	-2.04	1.39	1.44
31	b	625	LMG	O1-C7	-2.04	1.40	1.43
28	c	517	DGD	O5D-C1E	-2.04	1.36	1.40
24	A	406	PHO	CMC-C2C	-2.04	1.46	1.50
31	B	623	LMG	O2-C2	-2.04	1.38	1.43
23	C	505	CLA	C3B-C2B	-2.04	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	407	LMG	O1-C7	-2.03	1.40	1.43
31	M	101	LMG	O6-C5	-2.03	1.39	1.44
23	c	505	CLA	CMC-C2C	-2.03	1.46	1.50
23	b	615	CLA	CMC-C2C	-2.03	1.46	1.50
28	d	409	DGD	O6E-C5E	-2.03	1.39	1.44
28	b	623	DGD	O6D-C5D	-2.03	1.39	1.44
30	d	408	SQD	O4-C4	-2.03	1.38	1.43
24	A	406	PHO	CMD-C2D	-2.03	1.46	1.50
30	b	601	SQD	O3-C3	-2.03	1.38	1.43
23	B	611	CLA	CMC-C2C	-2.03	1.46	1.50
30	F	102	SQD	O3-C3	-2.02	1.38	1.43
28	c	518	DGD	O6E-C5E	-2.02	1.39	1.44
31	e	101	LMG	O2-C2	-2.02	1.38	1.43
23	b	609	CLA	CMC-C2C	-2.02	1.46	1.50
24	A	406	PHO	CMB-C2B	-2.01	1.46	1.50
28	c	516	DGD	C4E-C5E	-2.01	1.48	1.53
24	a	408	PHO	CMD-C2D	-2.01	1.46	1.50
28	A	411	DGD	O6E-C5E	-2.01	1.39	1.44
31	B	622	LMG	O1-C7	-2.01	1.40	1.43
23	A	403	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	609	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	613	CLA	CMC-C2C	-2.01	1.46	1.50
31	i	101	LMG	C4-C5	-2.01	1.48	1.53
31	d	406	LMG	O6-C5	-2.01	1.39	1.44
30	a	415	SQD	O2-C2	-2.01	1.38	1.43
23	c	511	CLA	CMC-C2C	-2.00	1.46	1.50
30	a	415	SQD	O3-C3	-2.00	1.38	1.43
23	b	619	CLA	CMC-C2C	-2.00	1.46	1.50
24	a	408	PHO	C4B-NB	2.00	1.41	1.37
33	i	102	LMT	O1'-C1'	2.01	1.43	1.40
34	f	101	HEM	FE-NC	2.01	2.03	1.95
24	D	402	PHO	CHB-C4A	2.02	1.44	1.40
24	a	407	PHO	CHD-C1D	2.04	1.42	1.38
24	A	406	PHO	C4B-NB	2.06	1.41	1.37
34	V	201	HEM	C1C-NC	2.06	1.38	1.36
24	D	402	PHO	C4B-NB	2.07	1.41	1.37
34	V	201	HEM	C3C-CAC	2.11	1.55	1.51
34	v	201	HEM	C1C-NC	2.11	1.38	1.36
34	f	101	HEM	C3B-CAB	2.12	1.55	1.51
34	f	101	HEM	C1C-NC	2.12	1.38	1.36
34	V	201	HEM	CAA-C2A	2.13	1.55	1.52
24	a	407	PHO	C4C-C3C	2.13	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	C1B-C2B	2.16	1.50	1.45
23	d	402	CLA	CHC-C1C	2.17	1.42	1.35
24	a	407	PHO	C1B-C2B	2.17	1.50	1.45
34	v	201	HEM	C3C-CAC	2.17	1.55	1.51
24	A	406	PHO	C4C-C3C	2.18	1.49	1.45
34	F	101	HEM	C3B-CAB	2.18	1.55	1.51
24	A	406	PHO	C1C-C2C	2.18	1.50	1.45
25	j	101	PL9	C28-C29	2.18	1.38	1.32
25	J	101	PL9	C28-C29	2.19	1.39	1.32
24	D	402	PHO	CHD-C1D	2.19	1.43	1.38
24	D	402	PHO	C1A-NA	2.20	1.42	1.37
24	a	408	PHO	C1A-NA	2.21	1.42	1.37
24	A	406	PHO	C1A-NA	2.21	1.42	1.37
34	f	101	HEM	C3C-CAC	2.24	1.55	1.51
23	C	502	CLA	CHC-C1C	2.25	1.42	1.35
23	b	605	CLA	CHC-C1C	2.26	1.42	1.35
23	c	507	CLA	CHC-C1C	2.26	1.42	1.35
24	D	402	PHO	C4C-C3C	2.27	1.49	1.45
23	b	616	CLA	CHC-C1C	2.28	1.42	1.35
23	b	608	CLA	CHC-C1C	2.28	1.42	1.35
34	F	101	HEM	C3C-CAC	2.29	1.55	1.51
24	a	407	PHO	CHB-C4A	2.30	1.44	1.40
34	V	201	HEM	C4C-NC	2.30	1.38	1.36
23	B	606	CLA	CHC-C1C	2.31	1.42	1.35
34	v	201	HEM	C4C-NC	2.31	1.38	1.36
23	b	615	CLA	CHC-C1C	2.31	1.42	1.35
34	F	101	HEM	FE-NC	2.31	2.04	1.95
28	B	621	DGD	O2G-C1B	2.33	1.41	1.34
23	b	620	CLA	CHC-C1C	2.34	1.42	1.35
23	c	513	CLA	CHC-C1C	2.34	1.42	1.35
23	B	616	CLA	CHC-C1C	2.35	1.42	1.35
23	b	612	CLA	CHC-C1C	2.35	1.42	1.35
31	A	418	LMG	O8-C28	2.35	1.40	1.33
28	D	409	DGD	O2G-C1B	2.36	1.41	1.34
23	a	404	CLA	CHC-C1C	2.36	1.42	1.35
23	A	407	CLA	CHC-C1C	2.37	1.42	1.35
23	b	617	CLA	CHC-C1C	2.37	1.42	1.35
23	c	504	CLA	CHC-C1C	2.38	1.42	1.35
34	V	201	HEM	FE-ND	2.38	2.10	1.97
23	C	510	CLA	CHC-C1C	2.38	1.42	1.35
23	B	615	CLA	CHC-C1C	2.40	1.42	1.35
31	i	101	LMG	O8-C28	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	623	DGD	O2G-C1B	2.40	1.41	1.34
24	D	402	PHO	C4C-NC	2.40	1.42	1.37
23	A	405	CLA	CHC-C1C	2.41	1.42	1.35
23	C	505	CLA	CHC-C1C	2.41	1.42	1.35
23	b	607	CLA	CHC-C1C	2.41	1.42	1.35
24	a	407	PHO	C1A-NA	2.42	1.43	1.37
23	c	505	CLA	CHC-C1C	2.42	1.42	1.35
23	C	501	CLA	CHC-C1C	2.43	1.42	1.35
23	C	503	CLA	CHC-C1C	2.43	1.42	1.35
23	a	405	CLA	CHC-C1C	2.43	1.42	1.35
23	b	611	CLA	CHC-C1C	2.43	1.42	1.35
23	C	507	CLA	CHC-C1C	2.43	1.42	1.35
23	B	611	CLA	CHC-C1C	2.43	1.42	1.35
23	D	401	CLA	CHC-C1C	2.43	1.42	1.35
23	c	503	CLA	CHC-C1C	2.43	1.42	1.35
23	c	512	CLA	CHC-C1C	2.44	1.42	1.35
28	d	409	DGD	O2G-C1B	2.44	1.41	1.34
23	b	610	CLA	CHC-C1C	2.44	1.42	1.35
23	c	501	CLA	CHC-C1C	2.44	1.42	1.35
31	D	407	LMG	O7-C10	2.44	1.41	1.34
23	B	613	CLA	CHC-C1C	2.44	1.42	1.35
23	B	604	CLA	CHC-C1C	2.44	1.42	1.35
31	D	406	LMG	O8-C28	2.44	1.40	1.33
23	b	613	CLA	CHC-C1C	2.44	1.42	1.35
31	D	406	LMG	O7-C10	2.44	1.41	1.34
23	C	511	CLA	CHC-C1C	2.45	1.43	1.35
31	k	103	LMG	O7-C10	2.45	1.41	1.34
24	A	406	PHO	CHD-C1D	2.46	1.43	1.38
23	d	403	CLA	CHC-C1C	2.46	1.43	1.35
23	A	403	CLA	CHC-C1C	2.46	1.43	1.35
23	B	601	CLA	CHC-C1C	2.46	1.43	1.35
23	C	512	CLA	CHC-C1C	2.47	1.43	1.35
31	d	406	LMG	O8-C28	2.47	1.40	1.33
31	C	520	LMG	O7-C10	2.48	1.41	1.34
23	b	614	CLA	CHC-C1C	2.48	1.43	1.35
23	c	502	CLA	CHC-C1C	2.48	1.43	1.35
31	b	625	LMG	O8-C28	2.49	1.40	1.33
23	B	612	CLA	CHC-C1C	2.49	1.43	1.35
23	B	614	CLA	CHC-C1C	2.49	1.43	1.35
24	a	408	PHO	C4C-C3C	2.49	1.49	1.45
31	d	406	LMG	O7-C10	2.50	1.41	1.34
31	i	101	LMG	O7-C10	2.50	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	CHC-C1C	2.51	1.43	1.35
28	a	413	DGD	O2G-C1B	2.51	1.41	1.34
23	B	605	CLA	CHC-C1C	2.51	1.43	1.35
23	D	403	CLA	CHC-C1C	2.51	1.43	1.35
23	C	506	CLA	CHC-C1C	2.51	1.43	1.35
31	B	623	LMG	O8-C28	2.51	1.40	1.33
23	c	508	CLA	CHC-C1C	2.51	1.43	1.35
24	A	406	PHO	C4C-NC	2.51	1.42	1.37
23	C	509	CLA	CHC-C1C	2.51	1.43	1.35
28	C	517	DGD	O2G-C1B	2.52	1.41	1.34
23	C	504	CLA	CHC-C1C	2.52	1.43	1.35
23	b	618	CLA	CHC-C1C	2.53	1.43	1.35
23	c	506	CLA	CHC-C1C	2.53	1.43	1.35
23	C	513	CLA	CHC-C1C	2.53	1.43	1.35
23	B	603	CLA	CHC-C1C	2.54	1.43	1.35
23	B	610	CLA	CHC-C1C	2.54	1.43	1.35
23	a	406	CLA	CHC-C1C	2.54	1.43	1.35
31	B	622	LMG	O7-C10	2.54	1.41	1.34
31	I	101	LMG	O8-C28	2.54	1.41	1.33
24	a	407	PHO	C4C-NC	2.54	1.42	1.37
24	a	408	PHO	C4C-NC	2.54	1.42	1.37
23	b	609	CLA	CHC-C1C	2.55	1.43	1.35
23	B	607	CLA	CHC-C1C	2.55	1.43	1.35
31	B	622	LMG	O8-C28	2.55	1.41	1.33
31	D	407	LMG	O8-C28	2.55	1.41	1.33
31	d	407	LMG	O7-C10	2.56	1.41	1.34
28	C	518	DGD	O2G-C1B	2.56	1.41	1.34
31	A	414	LMG	O8-C28	2.56	1.41	1.33
23	B	602	CLA	CHC-C1C	2.57	1.43	1.35
23	c	509	CLA	CHC-C1C	2.57	1.43	1.35
23	c	510	CLA	CHC-C1C	2.57	1.43	1.35
23	B	608	CLA	CHC-C1C	2.57	1.43	1.35
23	B	609	CLA	CHC-C1C	2.58	1.43	1.35
30	a	415	SQD	O47-C7	2.58	1.42	1.34
24	D	402	PHO	CHC-C1C	2.58	1.43	1.38
31	a	416	LMG	O8-C28	2.58	1.41	1.33
31	d	407	LMG	O8-C28	2.59	1.41	1.33
28	c	517	DGD	O2G-C1B	2.59	1.42	1.34
23	b	619	CLA	CHC-C1C	2.59	1.43	1.35
31	e	101	LMG	O8-C28	2.59	1.41	1.33
31	C	520	LMG	O8-C28	2.60	1.41	1.33
28	c	517	DGD	O1G-C1A	2.60	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	626	SQD	O47-C7	2.60	1.42	1.34
31	b	624	LMG	O7-C10	2.60	1.42	1.34
31	a	402	LMG	O8-C28	2.60	1.41	1.33
31	I	101	LMG	O7-C10	2.61	1.42	1.34
24	a	408	PHO	CHD-C1D	2.61	1.43	1.38
31	e	101	LMG	O7-C10	2.61	1.42	1.34
31	E	101	LMG	O8-C28	2.61	1.41	1.33
30	A	413	SQD	O47-C7	2.62	1.42	1.34
31	b	624	LMG	O8-C28	2.62	1.41	1.33
23	c	511	CLA	CHC-C1C	2.62	1.43	1.35
23	A	404	CLA	CHC-C1C	2.62	1.43	1.35
31	a	402	LMG	O7-C10	2.63	1.42	1.34
31	A	418	LMG	O7-C10	2.63	1.42	1.34
31	M	101	LMG	O8-C28	2.63	1.41	1.33
31	c	519	LMG	O8-C28	2.64	1.41	1.33
23	a	409	CLA	CHC-C1C	2.64	1.43	1.35
31	b	625	LMG	O7-C10	2.64	1.42	1.34
30	f	102	SQD	O47-C7	2.64	1.42	1.34
28	a	413	DGD	O1G-C1A	2.65	1.41	1.33
28	B	621	DGD	O1G-C1A	2.66	1.41	1.33
28	A	411	DGD	O1G-C1A	2.67	1.41	1.33
23	b	606	CLA	CHC-C1C	2.67	1.43	1.35
31	m	102	LMG	O8-C28	2.68	1.41	1.33
30	a	401	SQD	O47-C7	2.68	1.42	1.34
28	c	516	DGD	O2G-C1B	2.69	1.42	1.34
31	E	101	LMG	O7-C10	2.69	1.42	1.34
28	C	519	DGD	O1G-C1A	2.69	1.41	1.33
31	C	521	LMG	O8-C28	2.70	1.41	1.33
31	m	102	LMG	O7-C10	2.70	1.42	1.34
34	v	201	HEM	FE-NC	2.70	2.06	1.95
30	b	601	SQD	O47-C7	2.71	1.42	1.34
31	k	103	LMG	O8-C28	2.71	1.41	1.33
28	b	602	DGD	O2G-C1B	2.73	1.42	1.34
24	a	407	PHO	C3B-C4B	2.73	1.49	1.43
28	c	518	DGD	O1G-C1A	2.74	1.41	1.33
31	a	416	LMG	O7-C10	2.74	1.42	1.34
28	b	623	DGD	O1G-C1A	2.75	1.41	1.33
34	f	101	HEM	FE-ND	2.75	2.12	1.97
30	A	417	SQD	O47-C7	2.76	1.42	1.34
28	B	627	DGD	O2G-C1B	2.77	1.42	1.34
31	A	414	LMG	O7-C10	2.78	1.42	1.34
31	c	519	LMG	O7-C10	2.78	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	PHO	CHC-C1C	2.79	1.44	1.38
30	F	102	SQD	O47-C7	2.79	1.42	1.34
28	A	411	DGD	O2G-C1B	2.80	1.42	1.34
31	M	101	LMG	O7-C10	2.80	1.42	1.34
31	B	623	LMG	O7-C10	2.81	1.42	1.34
28	C	518	DGD	O1G-C1A	2.81	1.41	1.33
30	D	408	SQD	O47-C7	2.82	1.42	1.34
31	C	521	LMG	O7-C10	2.83	1.42	1.34
24	D	402	PHO	C3B-C4B	2.84	1.49	1.43
28	d	409	DGD	O1G-C1A	2.84	1.41	1.33
30	d	408	SQD	O47-C7	2.84	1.42	1.34
28	C	517	DGD	O1G-C1A	2.85	1.41	1.33
25	D	404	PL9	C28-C29	2.85	1.38	1.33
28	B	627	DGD	O1G-C1A	2.87	1.42	1.33
28	D	409	DGD	O1G-C1A	2.89	1.42	1.33
25	a	410	PL9	C28-C29	2.91	1.38	1.33
30	F	102	SQD	O48-C23	2.94	1.42	1.33
28	c	518	DGD	O2G-C1B	2.94	1.43	1.34
24	a	408	PHO	CHC-C1C	2.96	1.44	1.38
25	A	408	PL9	C38-C39	2.96	1.41	1.32
28	C	519	DGD	O2G-C1B	2.96	1.43	1.34
30	f	102	SQD	O48-C23	2.98	1.42	1.33
24	a	408	PHO	C3B-C4B	2.99	1.50	1.43
25	a	410	PL9	C38-C39	2.99	1.41	1.32
28	c	516	DGD	O1G-C1A	3.00	1.42	1.33
30	B	626	SQD	O48-C23	3.01	1.42	1.33
30	A	417	SQD	O48-C23	3.01	1.42	1.33
25	A	408	PL9	C28-C29	3.02	1.38	1.33
30	b	601	SQD	O48-C23	3.06	1.42	1.33
25	D	404	PL9	C13-C14	3.07	1.39	1.33
25	d	404	PL9	C28-C29	3.07	1.39	1.33
28	b	602	DGD	O1G-C1A	3.07	1.42	1.33
25	D	404	PL9	C8-C9	3.09	1.39	1.33
25	a	410	PL9	C18-C19	3.09	1.39	1.33
25	a	410	PL9	C8-C9	3.10	1.39	1.33
30	a	415	SQD	O48-C23	3.11	1.42	1.33
30	A	413	SQD	O48-C23	3.11	1.42	1.33
30	D	408	SQD	O48-C23	3.12	1.42	1.33
30	a	401	SQD	O48-C23	3.16	1.42	1.33
30	d	408	SQD	O48-C23	3.17	1.42	1.33
25	d	404	PL9	C8-C9	3.19	1.39	1.33
24	A	406	PHO	C3B-C4B	3.20	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	PL9	C18-C19	3.21	1.39	1.33
25	d	404	PL9	C13-C14	3.24	1.39	1.33
25	A	408	PL9	C8-C9	3.26	1.39	1.33
25	D	404	PL9	C23-C24	3.26	1.39	1.33
25	a	410	PL9	C23-C24	3.27	1.39	1.33
25	A	408	PL9	C23-C24	3.29	1.39	1.33
25	a	410	PL9	C13-C14	3.30	1.39	1.33
25	A	408	PL9	C13-C14	3.31	1.39	1.33
24	A	406	PHO	CHC-C1C	3.31	1.45	1.38
25	D	404	PL9	C18-C19	3.32	1.39	1.33
25	J	101	PL9	C18-C19	3.33	1.39	1.33
25	d	404	PL9	C23-C24	3.33	1.39	1.33
25	J	101	PL9	C13-C14	3.33	1.39	1.33
25	j	101	PL9	C8-C9	3.34	1.39	1.33
25	A	408	PL9	C18-C19	3.38	1.39	1.33
25	J	101	PL9	C8-C9	3.39	1.39	1.33
25	j	101	PL9	C23-C24	3.39	1.39	1.33
25	j	101	PL9	C18-C19	3.41	1.39	1.33
25	j	101	PL9	C13-C14	3.47	1.39	1.33
25	J	101	PL9	C23-C24	3.63	1.40	1.33
25	d	404	PL9	C43-C44	3.65	1.40	1.33
25	D	404	PL9	C43-C44	3.91	1.40	1.33
29	A	415	LHG	O7-C7	3.91	1.46	1.34
29	A	412	LHG	O7-C7	3.93	1.46	1.34
29	a	414	LHG	O7-C7	3.93	1.46	1.34
25	d	404	PL9	C33-C34	3.95	1.40	1.33
29	a	417	LHG	O7-C7	3.97	1.46	1.34
25	D	404	PL9	C33-C34	4.00	1.40	1.33
25	a	410	PL9	C33-C34	4.01	1.40	1.33
25	d	404	PL9	C38-C39	4.02	1.40	1.33
29	A	412	LHG	O8-C23	4.12	1.45	1.33
25	D	404	PL9	C38-C39	4.14	1.41	1.33
29	A	415	LHG	O8-C23	4.15	1.45	1.33
29	a	417	LHG	O8-C23	4.17	1.45	1.33
29	a	414	LHG	O8-C23	4.23	1.46	1.33
25	A	408	PL9	C33-C34	4.24	1.41	1.33

All (1453) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	j	102	BCR	C32-C1-C6	-14.13	88.14	110.30
27	J	102	BCR	C32-C1-C6	-13.83	88.62	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	102	BCR	C7-C8-C9	-8.70	112.96	126.22
27	B	618	BCR	C7-C8-C9	-8.55	113.18	126.22
27	J	102	BCR	C32-C1-C31	-8.06	82.55	108.37
27	j	102	BCR	C32-C1-C31	-8.03	82.62	108.37
27	d	405	BCR	C7-C8-C9	-6.68	116.04	126.22
27	D	405	BCR	C7-C8-C9	-6.38	116.49	126.22
27	J	102	BCR	C28-C27-C26	-6.07	104.23	113.87
27	J	102	BCR	C15-C14-C13	-6.03	118.48	127.20
27	J	102	BCR	C32-C1-C2	-6.02	87.22	108.79
27	b	622	BCR	C24-C23-C22	-5.97	117.11	126.22
27	j	102	BCR	C32-C1-C2	-5.95	87.49	108.79
27	b	622	BCR	C3-C4-C5	-5.88	104.54	113.87
27	a	412	BCR	C33-C5-C6	-5.83	118.88	124.61
27	j	102	BCR	C28-C27-C26	-5.77	104.72	113.87
27	c	514	BCR	C33-C5-C6	-5.64	119.07	124.61
27	D	405	BCR	C28-C27-C26	-5.59	105.00	113.87
27	C	514	BCR	C33-C5-C6	-5.49	119.21	124.61
25	d	404	PL9	C3-C2-C1	-5.48	119.63	122.97
27	B	618	BCR	C11-C10-C9	-5.46	119.32	127.20
27	d	405	BCR	C28-C27-C26	-5.44	105.24	113.87
27	c	514	BCR	C15-C14-C13	-5.40	119.40	127.20
27	A	410	BCR	C33-C5-C6	-5.37	119.33	124.61
27	B	620	BCR	C24-C23-C22	-5.31	118.12	126.22
27	j	102	BCR	C15-C14-C13	-5.30	119.54	127.20
27	B	618	BCR	C3-C4-C5	-5.30	105.46	113.87
27	B	620	BCR	C3-C4-C5	-5.27	105.51	113.87
27	z	101	BCR	C15-C14-C13	-5.25	119.62	127.20
25	D	404	PL9	C3-C2-C1	-5.23	119.78	122.97
27	T	102	BCR	C28-C27-C26	-5.23	105.58	113.87
27	T	102	BCR	C3-C4-C5	-5.15	105.70	113.87
25	a	410	PL9	C3-C2-C1	-5.08	119.87	122.97
25	d	404	PL9	C7-C3-C2	-5.01	119.26	123.42
27	D	405	BCR	C11-C10-C9	-4.96	120.04	127.20
27	j	102	BCR	C20-C21-C22	-4.93	120.07	127.20
27	k	102	BCR	C38-C26-C25	-4.93	119.77	124.61
27	H	101	BCR	C33-C5-C6	-4.91	119.78	124.61
27	B	620	BCR	C38-C26-C25	-4.89	119.80	124.61
27	C	516	BCR	C7-C8-C9	-4.89	118.76	126.22
27	j	102	BCR	C24-C23-C22	-4.87	118.79	126.22
27	d	405	BCR	C33-C5-C6	-4.84	119.85	124.61
27	D	405	BCR	C33-C5-C6	-4.84	119.86	124.61
27	j	102	BCR	C11-C10-C9	-4.83	120.22	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	J	102	BCR	C20-C21-C22	-4.83	120.23	127.20
27	B	619	BCR	C28-C27-C26	-4.78	106.29	113.87
27	y	101	BCR	C15-C14-C13	-4.76	120.32	127.20
25	A	408	PL9	C3-C2-C1	-4.74	120.08	122.97
25	J	101	PL9	C7-C3-C2	-4.70	119.52	123.42
27	b	621	BCR	C28-C27-C26	-4.68	106.44	113.87
27	a	412	BCR	C38-C26-C25	-4.66	120.03	124.61
27	C	515	BCR	C15-C14-C13	-4.66	120.47	127.20
27	B	618	BCR	C28-C27-C26	-4.65	106.48	113.87
27	b	622	BCR	C38-C26-C25	-4.65	120.04	124.61
27	T	101	BCR	C33-C5-C6	-4.59	120.10	124.61
27	J	102	BCR	C24-C23-C22	-4.58	119.23	126.22
27	c	515	BCR	C7-C8-C9	-4.58	119.24	126.22
27	h	101	BCR	C33-C5-C6	-4.58	120.11	124.61
27	B	620	BCR	C16-C17-C18	-4.57	120.59	127.20
25	j	101	PL9	C3-C2-C1	-4.57	120.18	122.97
25	j	101	PL9	C7-C3-C2	-4.54	119.66	123.42
28	c	517	DGD	O5D-C6D-C5D	-4.53	100.87	109.08
27	C	514	BCR	C3-C4-C5	-4.52	106.70	113.87
27	T	102	BCR	C11-C10-C9	-4.51	120.68	127.20
27	k	102	BCR	C15-C14-C13	-4.50	120.70	127.20
27	c	515	BCR	C28-C27-C26	-4.46	106.80	113.87
27	b	622	BCR	C16-C17-C18	-4.43	120.80	127.20
27	y	101	BCR	C38-C26-C25	-4.42	120.27	124.61
27	J	102	BCR	C11-C10-C9	-4.41	120.82	127.20
27	B	617	BCR	C33-C5-C6	-4.40	120.28	124.61
27	k	102	BCR	C24-C23-C22	-4.38	119.54	126.22
27	C	515	BCR	C33-C5-C6	-4.35	120.33	124.61
27	y	101	BCR	C7-C8-C9	-4.35	119.59	126.22
27	C	514	BCR	C15-C14-C13	-4.34	120.93	127.20
27	y	101	BCR	C3-C4-C5	-4.33	106.99	113.87
27	b	621	BCR	C15-C14-C13	-4.32	120.96	127.20
27	c	515	BCR	C15-C14-C13	-4.30	120.99	127.20
25	J	101	PL9	C3-C2-C1	-4.29	120.36	122.97
27	y	101	BCR	C16-C17-C18	-4.28	121.01	127.20
27	C	516	BCR	C38-C26-C25	-4.28	120.40	124.61
27	J	102	BCR	C16-C17-C18	-4.28	121.02	127.20
27	B	619	BCR	C20-C21-C22	-4.27	121.03	127.20
27	B	617	BCR	C16-C17-C18	-4.27	121.03	127.20
28	C	519	DGD	C1D-O6D-C5D	-4.26	105.49	113.75
27	B	620	BCR	C15-C14-C13	-4.25	121.06	127.20
28	c	518	DGD	C1D-O6D-C5D	-4.25	105.50	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	j	102	BCR	C7-C8-C9	-4.20	119.81	126.22
28	C	518	DGD	O5D-C6D-C5D	-4.20	101.47	109.08
27	C	516	BCR	C28-C27-C26	-4.19	107.21	113.87
25	a	410	PL9	C7-C3-C2	-4.19	119.94	123.42
27	b	621	BCR	C7-C8-C9	-4.16	119.87	126.22
27	C	516	BCR	C15-C14-C13	-4.16	121.19	127.20
27	A	410	BCR	C38-C26-C25	-4.14	120.54	124.61
27	a	412	BCR	C3-C4-C5	-4.14	107.30	113.87
27	b	622	BCR	C7-C8-C9	-4.12	119.94	126.22
27	b	622	BCR	C4-C5-C6	-4.12	117.53	122.78
27	a	412	BCR	C16-C17-C18	-4.08	121.31	127.20
25	A	408	PL9	C7-C3-C2	-4.07	120.04	123.42
27	C	515	BCR	C16-C17-C18	-4.06	121.34	127.20
27	D	405	BCR	C16-C17-C18	-4.05	121.34	127.20
27	A	410	BCR	C3-C4-C5	-4.05	107.44	113.87
27	c	514	BCR	C3-C4-C5	-4.05	107.44	113.87
27	d	405	BCR	C15-C14-C13	-4.04	121.37	127.20
27	d	405	BCR	C11-C10-C9	-4.03	121.37	127.20
27	C	516	BCR	C33-C5-C6	-4.02	120.65	124.61
27	b	621	BCR	C3-C4-C5	-4.01	107.50	113.87
27	T	101	BCR	C24-C23-C22	-4.01	120.10	126.22
27	z	101	BCR	C33-C5-C6	-4.01	120.67	124.61
27	c	515	BCR	C16-C17-C18	-4.01	121.41	127.20
27	A	410	BCR	C15-C14-C13	-4.00	121.42	127.20
27	a	412	BCR	C24-C23-C22	-3.99	120.14	126.22
27	c	515	BCR	C33-C5-C6	-3.99	120.69	124.61
27	B	617	BCR	C7-C8-C9	-3.99	120.14	126.22
27	z	101	BCR	C16-C17-C18	-3.96	121.47	127.20
27	b	621	BCR	C20-C21-C22	-3.96	121.48	127.20
27	B	618	BCR	C38-C26-C25	-3.95	120.73	124.61
27	k	102	BCR	C7-C8-C9	-3.95	120.20	126.22
27	c	515	BCR	C38-C26-C25	-3.94	120.73	124.61
27	B	617	BCR	C24-C23-C22	-3.93	120.22	126.22
28	A	411	DGD	C1D-O6D-C5D	-3.92	106.15	113.75
27	B	617	BCR	C15-C14-C13	-3.91	121.55	127.20
27	B	620	BCR	C4-C5-C6	-3.90	117.81	122.78
27	b	622	BCR	C15-C14-C13	-3.89	121.58	127.20
27	T	102	BCR	C38-C26-C25	-3.89	120.79	124.61
27	D	405	BCR	C15-C14-C13	-3.88	121.59	127.20
27	k	102	BCR	C3-C4-C5	-3.87	107.72	113.87
27	a	412	BCR	C15-C14-C13	-3.87	121.61	127.20
27	z	101	BCR	C3-C4-C5	-3.87	107.73	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	101	BCR	C15-C14-C13	-3.85	121.64	127.20
27	C	515	BCR	C3-C4-C5	-3.85	107.76	113.87
27	C	515	BCR	C24-C23-C22	-3.85	120.35	126.22
23	b	614	CLA	CMB-C2B-C1B	-3.84	122.01	128.36
27	c	514	BCR	C11-C10-C9	-3.84	121.66	127.20
23	B	610	CLA	CMB-C2B-C1B	-3.83	122.02	128.36
27	k	102	BCR	C33-C5-C6	-3.83	120.84	124.61
27	B	620	BCR	C20-C21-C22	-3.83	121.67	127.20
27	T	101	BCR	C20-C21-C22	-3.81	121.69	127.20
27	k	102	BCR	C16-C17-C18	-3.80	121.70	127.20
27	B	619	BCR	C15-C14-C13	-3.80	121.70	127.20
27	J	102	BCR	C7-C8-C9	-3.79	120.44	126.22
27	b	621	BCR	C24-C23-C22	-3.78	120.45	126.22
25	D	404	PL9	C7-C3-C2	-3.78	120.28	123.42
27	h	101	BCR	C16-C17-C18	-3.77	121.75	127.20
27	D	405	BCR	C24-C23-C22	-3.76	120.49	126.22
27	b	622	BCR	C11-C10-C9	-3.75	121.79	127.20
27	d	405	BCR	C16-C17-C18	-3.75	121.79	127.20
31	d	407	LMG	C1-O6-C5	-3.70	106.56	113.75
27	j	102	BCR	C16-C17-C18	-3.69	121.86	127.20
27	z	101	BCR	C24-C23-C22	-3.65	120.65	126.22
27	j	102	BCR	C27-C26-C25	-3.62	118.17	122.78
23	b	616	CLA	CMB-C2B-C1B	-3.61	122.39	128.36
27	y	101	BCR	C33-C5-C6	-3.61	121.06	124.61
31	m	102	LMG	C1-O6-C5	-3.61	106.75	113.75
27	B	619	BCR	C3-C4-C5	-3.60	108.15	113.87
27	H	101	BCR	C24-C23-C22	-3.60	120.72	126.22
27	A	410	BCR	C16-C17-C18	-3.59	122.01	127.20
25	D	404	PL9	C22-C23-C24	-3.59	119.96	127.76
27	h	101	BCR	C15-C14-C13	-3.59	122.02	127.20
23	b	617	CLA	CMB-C2B-C1B	-3.58	122.44	128.36
27	c	515	BCR	C11-C10-C9	-3.58	122.03	127.20
27	d	405	BCR	C24-C23-C22	-3.56	120.79	126.22
23	c	504	CLA	CMB-C2B-C1B	-3.55	122.50	128.36
27	B	619	BCR	C33-C5-C6	-3.55	121.12	124.61
23	B	613	CLA	CMB-C2B-C1B	-3.53	122.52	128.36
27	c	515	BCR	C3-C4-C5	-3.53	108.26	113.87
27	B	617	BCR	C38-C26-C25	-3.52	121.15	124.61
30	f	102	SQD	O9-S-O7	-3.52	100.65	113.48
27	C	514	BCR	C38-C26-C25	-3.52	121.15	124.61
30	a	415	SQD	O9-S-O7	-3.50	100.72	113.48
30	A	413	SQD	O9-S-O7	-3.50	100.74	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	F	102	SQD	O9-S-O7	-3.49	100.75	113.48
23	C	507	CLA	CMB-C2B-C1B	-3.49	122.59	128.36
23	B	603	CLA	CMB-C2B-C1B	-3.49	122.59	128.36
23	d	402	CLA	CMB-C2B-C1B	-3.49	122.59	128.36
27	C	516	BCR	C16-C17-C18	-3.48	122.17	127.20
27	J	102	BCR	C27-C26-C25	-3.47	118.36	122.78
27	C	516	BCR	C3-C4-C5	-3.47	108.37	113.87
30	D	408	SQD	O9-S-O7	-3.46	100.87	113.48
28	b	623	DGD	C1D-O6D-C5D	-3.45	107.05	113.75
27	C	514	BCR	C28-C27-C26	-3.45	108.40	113.87
27	B	618	BCR	C4-C5-C6	-3.44	118.40	122.78
23	D	401	CLA	CMB-C2B-C1B	-3.43	122.69	128.36
30	d	408	SQD	O9-S-O7	-3.43	100.99	113.48
23	B	612	CLA	CMB-C2B-C1B	-3.43	122.70	128.36
23	C	508	CLA	CMB-C2B-C1B	-3.42	122.70	128.36
27	B	620	BCR	C11-C10-C9	-3.42	122.25	127.20
27	h	101	BCR	C24-C23-C22	-3.42	121.00	126.22
23	B	614	CLA	CMB-C2B-C1B	-3.41	122.72	128.36
25	d	404	PL9	C37-C38-C39	-3.41	120.35	127.76
27	c	514	BCR	C7-C6-C5	-3.40	113.58	121.37
23	A	407	CLA	CMB-C2B-C1B	-3.40	122.74	128.36
25	D	404	PL9	C12-C13-C14	-3.39	120.38	127.76
23	c	506	CLA	CMB-C2B-C1B	-3.39	122.75	128.36
23	c	508	CLA	CMB-C2B-C1B	-3.38	122.77	128.36
27	C	514	BCR	C11-C10-C9	-3.38	122.32	127.20
25	a	410	PL9	C22-C23-C24	-3.38	120.42	127.76
27	b	621	BCR	C33-C5-C6	-3.37	121.29	124.61
27	k	102	BCR	C20-C21-C22	-3.37	122.33	127.20
23	B	611	CLA	CMB-C2B-C1B	-3.37	122.80	128.36
28	A	411	DGD	C3G-C2G-C1G	-3.36	104.21	112.07
28	B	621	DGD	C1D-O6D-C5D	-3.36	107.23	113.75
27	c	514	BCR	C16-C17-C18	-3.35	122.35	127.20
25	d	404	PL9	C22-C23-C24	-3.35	120.47	127.76
23	A	404	CLA	CMB-C2B-C1B	-3.35	122.82	128.36
31	A	414	LMG	C1-O6-C5	-3.35	107.25	113.75
27	c	514	BCR	C35-C13-C14	-3.35	117.96	122.90
27	j	102	BCR	C33-C5-C6	-3.35	121.32	124.61
23	b	612	CLA	CMB-C2B-C1B	-3.33	122.85	128.36
23	A	405	CLA	O2D-CGD-O1D	-3.33	116.91	123.79
23	B	606	CLA	CMB-C2B-C1B	-3.33	122.86	128.36
23	B	608	CLA	CMB-C2B-C1B	-3.33	122.86	128.36
31	M	101	LMG	C1-O6-C5	-3.32	107.30	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	101	HEM	CBA-CAA-C2A	-3.32	106.58	112.53
25	D	404	PL9	C37-C38-C39	-3.32	120.55	127.76
27	J	102	BCR	C33-C5-C6	-3.31	121.35	124.61
30	b	601	SQD	O9-S-O7	-3.31	101.43	113.48
23	a	405	CLA	CMB-C2B-C1B	-3.30	122.91	128.36
23	C	503	CLA	CMB-C2B-C1B	-3.30	122.91	128.36
27	B	617	BCR	C11-C10-C9	-3.29	122.44	127.20
27	H	101	BCR	C16-C17-C18	-3.29	122.44	127.20
27	C	515	BCR	C11-C10-C9	-3.29	122.44	127.20
27	A	410	BCR	C20-C21-C22	-3.29	122.44	127.20
23	c	507	CLA	CMB-C2B-C1B	-3.29	122.93	128.36
23	B	616	CLA	CMB-C2B-C1B	-3.28	122.94	128.36
23	b	619	CLA	CMB-C2B-C1B	-3.28	122.94	128.36
27	C	514	BCR	C7-C6-C5	-3.26	113.90	121.37
27	b	622	BCR	C20-C21-C22	-3.26	122.50	127.20
27	T	101	BCR	C7-C8-C9	-3.24	121.27	126.22
34	f	101	HEM	CBA-CAA-C2A	-3.24	106.72	112.53
23	a	404	CLA	CMB-C2B-C1B	-3.23	123.02	128.36
25	A	408	PL9	C22-C23-C24	-3.23	120.74	127.76
23	b	607	CLA	CMB-C2B-C1B	-3.23	123.02	128.36
30	B	626	SQD	O9-S-O7	-3.23	101.72	113.48
23	B	607	CLA	CMB-C2B-C1B	-3.23	123.03	128.36
31	m	102	LMG	C6-C5-C4	-3.22	105.07	113.02
27	b	621	BCR	C16-C17-C18	-3.22	122.55	127.20
23	C	504	CLA	CMB-C2B-C1B	-3.22	123.04	128.36
23	b	606	CLA	CMB-C2B-C1B	-3.21	123.05	128.36
27	c	514	BCR	C28-C27-C26	-3.21	108.78	113.87
27	A	410	BCR	C11-C10-C9	-3.21	122.57	127.20
24	A	406	PHO	O2D-CGD-O1D	-3.21	117.17	123.79
23	B	606	CLA	O2D-CGD-O1D	-3.20	117.17	123.79
27	C	514	BCR	C20-C21-C22	-3.20	122.57	127.20
23	C	506	CLA	CMB-C2B-C1B	-3.18	123.11	128.36
23	D	403	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
23	b	612	CLA	O2D-CGD-O1D	-3.17	117.24	123.79
27	c	514	BCR	C20-C21-C22	-3.17	122.62	127.20
27	y	101	BCR	C24-C23-C22	-3.17	121.39	126.22
23	c	510	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
23	b	615	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
27	A	410	BCR	C24-C23-C22	-3.15	121.41	126.22
23	B	607	CLA	O2D-CGD-O1D	-3.15	117.29	123.79
31	M	101	LMG	C6-C5-C4	-3.15	105.25	113.02
30	a	401	SQD	O9-S-O7	-3.15	102.02	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	618	CLA	CMB-C2B-C1B	-3.15	123.16	128.36
31	c	519	LMG	C1-O6-C5	-3.14	107.66	113.75
23	b	610	CLA	CMB-C2B-C1B	-3.13	123.19	128.36
27	T	101	BCR	C11-C10-C9	-3.12	122.69	127.20
27	d	405	BCR	C38-C26-C25	-3.12	121.54	124.61
23	c	513	CLA	CMB-C2B-C1B	-3.12	123.20	128.36
27	T	102	BCR	C4-C5-C6	-3.12	118.81	122.78
28	a	413	DGD	C1D-O6D-C5D	-3.11	107.70	113.75
23	A	403	CLA	CMB-C2B-C1B	-3.10	123.24	128.36
27	c	514	BCR	C38-C26-C25	-3.10	121.56	124.61
27	T	101	BCR	C16-C17-C18	-3.10	122.72	127.20
27	H	101	BCR	C38-C26-C25	-3.09	121.57	124.61
27	D	405	BCR	C3-C4-C5	-3.08	108.97	113.87
27	h	101	BCR	C38-C26-C25	-3.08	121.58	124.61
31	D	407	LMG	C1-O6-C5	-3.08	107.77	113.75
27	B	619	BCR	C16-C17-C18	-3.08	122.75	127.20
25	d	404	PL9	C7-C8-C9	-3.07	121.49	126.70
23	C	502	CLA	CMB-C2B-C1B	-3.07	123.28	128.36
23	C	512	CLA	CMB-C2B-C1B	-3.07	123.29	128.36
27	C	516	BCR	C20-C21-C22	-3.07	122.77	127.20
27	T	101	BCR	C38-C26-C25	-3.06	121.60	124.61
23	a	406	CLA	CMB-C2B-C1B	-3.06	123.30	128.36
27	H	101	BCR	C15-C14-C13	-3.05	122.78	127.20
27	z	101	BCR	C20-C21-C22	-3.05	122.79	127.20
23	C	510	CLA	CMB-C2B-C1B	-3.05	123.32	128.36
31	C	520	LMG	C1-O6-C5	-3.05	107.83	113.75
23	d	403	CLA	O2D-CGD-O1D	-3.04	117.51	123.79
23	B	615	CLA	CMB-C2B-C1B	-3.03	123.35	128.36
30	A	417	SQD	O9-S-O7	-3.03	102.45	113.48
23	A	405	CLA	CMB-C2B-C1B	-3.03	123.36	128.36
23	b	607	CLA	O2D-CGD-O1D	-3.02	117.54	123.79
23	B	609	CLA	CMB-C2B-C1B	-3.02	123.36	128.36
23	D	401	CLA	O2D-CGD-O1D	-3.01	117.58	123.79
31	d	407	LMG	C1-C2-C3	-3.01	104.05	109.97
27	B	620	BCR	C7-C8-C9	-2.99	121.66	126.22
23	b	611	CLA	CMB-C2B-C1B	-2.99	123.42	128.36
23	c	512	CLA	O2D-CGD-O1D	-2.99	117.62	123.79
23	c	503	CLA	CMB-C2B-C1B	-2.98	123.43	128.36
23	B	605	CLA	CMB-C2B-C1B	-2.98	123.43	128.36
23	c	502	CLA	CMB-C2B-C1B	-2.96	123.46	128.36
23	b	605	CLA	CMB-C2B-C1B	-2.96	123.46	128.36
23	c	502	CLA	O2D-CGD-O1D	-2.96	117.67	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	101	BCR	C20-C21-C22	-2.96	122.92	127.20
31	a	402	LMG	C6-C5-C4	-2.96	105.72	113.02
23	C	507	CLA	O2D-CGD-O1D	-2.95	117.71	123.79
23	B	601	CLA	CMB-C2B-C1B	-2.95	123.49	128.36
25	d	404	PL9	C32-C33-C34	-2.94	121.37	127.76
27	b	621	BCR	C11-C10-C9	-2.94	122.95	127.20
23	B	602	CLA	CMB-C2B-C1B	-2.93	123.51	128.36
27	h	101	BCR	C10-C11-C12	-2.92	114.22	123.13
23	c	503	CLA	O2D-CGD-O1D	-2.92	117.76	123.79
23	a	406	CLA	O2D-CGD-O1D	-2.92	117.77	123.79
23	C	511	CLA	O2D-CGD-O1D	-2.91	117.77	123.79
23	a	409	CLA	CMB-C2B-C1B	-2.91	123.55	128.36
31	a	416	LMG	C1-O6-C5	-2.91	108.10	113.75
23	c	512	CLA	CMB-C2B-C1B	-2.90	123.56	128.36
23	C	510	CLA	O2D-CGD-O1D	-2.88	117.84	123.79
23	C	513	CLA	CMB-C2B-C1B	-2.88	123.60	128.36
25	d	404	PL9	C12-C13-C14	-2.88	121.50	127.76
23	c	504	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
23	c	501	CLA	O2D-CGD-O1D	-2.86	117.88	123.79
23	b	605	CLA	O2D-CGD-O1D	-2.86	117.89	123.79
27	B	619	BCR	C11-C10-C9	-2.85	123.07	127.20
27	D	405	BCR	C27-C26-C25	-2.85	119.15	122.78
27	C	515	BCR	C20-C21-C22	-2.85	123.08	127.20
27	H	101	BCR	C8-C7-C6	-2.85	118.77	127.32
23	c	510	CLA	O2D-CGD-O1D	-2.85	117.91	123.79
27	C	515	BCR	C28-C27-C26	-2.84	109.36	113.87
23	c	505	CLA	CMB-C2B-C1B	-2.84	123.66	128.36
23	B	604	CLA	O2D-CGD-O1D	-2.83	117.95	123.79
23	c	506	CLA	O2D-CGD-O1D	-2.83	117.95	123.79
23	C	505	CLA	O2D-CGD-O1D	-2.82	117.96	123.79
27	B	619	BCR	C24-C23-C22	-2.82	121.92	126.22
25	a	410	PL9	C12-C13-C14	-2.81	121.66	127.76
31	C	521	LMG	C1-O6-C5	-2.80	108.30	113.75
24	D	402	PHO	CBD-CHA-C4D	-2.80	105.32	108.46
31	D	407	LMG	C1-C2-C3	-2.79	104.47	109.97
27	c	514	BCR	C34-C9-C10	-2.79	118.78	122.90
27	h	101	BCR	C20-C21-C22	-2.79	123.17	127.20
31	A	418	LMG	C6-C5-C4	-2.79	106.14	113.02
31	k	103	LMG	C1-O6-C5	-2.79	108.33	113.75
24	a	407	PHO	O2D-CGD-O1D	-2.78	118.05	123.79
24	A	406	PHO	CBD-CHA-C4D	-2.78	105.35	108.46
23	c	511	CLA	O2D-CGD-O1D	-2.77	118.07	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	623	LMG	C1-O6-C5	-2.77	108.38	113.75
23	b	610	CLA	O2D-CGD-O1D	-2.77	118.08	123.79
23	b	608	CLA	CMB-C2B-C1B	-2.76	123.80	128.36
23	C	511	CLA	CMB-C2B-C1B	-2.76	123.81	128.36
27	C	515	BCR	C7-C8-C9	-2.75	122.02	126.22
27	c	515	BCR	C20-C21-C22	-2.75	123.22	127.20
23	C	509	CLA	CMB-C2B-C1B	-2.74	123.83	128.36
25	j	101	PL9	C22-C23-C24	-2.74	121.80	127.76
28	a	413	DGD	C3G-C2G-C1G	-2.73	105.67	112.07
27	H	101	BCR	C10-C11-C12	-2.73	114.80	123.13
27	B	617	BCR	C20-C21-C22	-2.73	123.25	127.20
23	c	501	CLA	CMB-C2B-C1B	-2.72	123.86	128.36
27	d	405	BCR	C3-C4-C5	-2.72	109.55	113.87
27	B	618	BCR	C21-C20-C19	-2.72	114.84	123.13
23	c	513	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
23	b	613	CLA	O2D-CGD-O1D	-2.72	118.18	123.79
24	a	408	PHO	O2D-CGD-O1D	-2.72	118.18	123.79
27	D	405	BCR	C38-C26-C25	-2.71	121.94	124.61
27	B	617	BCR	C3-C4-C5	-2.71	109.57	113.87
23	b	615	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
28	A	411	DGD	C4D-C3D-C2D	-2.71	105.74	110.79
23	d	403	CLA	CMB-C2B-C1B	-2.70	123.90	128.36
27	d	405	BCR	C27-C26-C25	-2.70	119.34	122.78
23	c	511	CLA	CMB-C2B-C1B	-2.70	123.90	128.36
27	J	102	BCR	C35-C13-C14	-2.70	118.92	122.90
23	b	614	CLA	O2D-CGD-O1D	-2.69	118.24	123.79
23	b	617	CLA	O2D-CGD-O1D	-2.69	118.25	123.79
25	j	101	PL9	C12-C13-C14	-2.68	121.94	127.76
23	c	508	CLA	O2D-CGD-O1D	-2.68	118.27	123.79
31	I	101	LMG	C1-O6-C5	-2.67	108.55	113.75
27	C	514	BCR	C34-C9-C10	-2.67	118.95	122.90
31	i	101	LMG	C1-O6-C5	-2.67	108.56	113.75
28	c	516	DGD	C1D-O6D-C5D	-2.67	108.56	113.75
27	C	515	BCR	C15-C16-C17	-2.67	117.49	123.39
23	b	613	CLA	CMB-C2B-C1B	-2.67	123.95	128.36
23	B	614	CLA	O2D-CGD-O1D	-2.67	118.28	123.79
23	C	503	CLA	O2D-CGD-O1D	-2.66	118.30	123.79
27	C	515	BCR	C38-C26-C25	-2.66	122.00	124.61
25	J	101	PL9	C12-C13-C14	-2.65	122.00	127.76
27	T	102	BCR	C21-C20-C19	-2.65	115.06	123.13
31	D	406	LMG	O8-C28-O10	-2.65	116.67	123.49
27	z	101	BCR	C38-C26-C25	-2.64	122.02	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	O2D-CGD-O1D	-2.63	118.35	123.79
23	b	618	CLA	O2D-CGD-O1D	-2.63	118.36	123.79
27	H	101	BCR	C3-C4-C5	-2.63	109.70	113.87
27	C	514	BCR	C16-C17-C18	-2.63	123.40	127.20
27	b	621	BCR	C27-C26-C25	-2.63	119.43	122.78
23	B	611	CLA	O2D-CGD-O1D	-2.62	118.38	123.79
28	A	411	DGD	O4D-C4D-C5D	-2.62	102.31	109.24
25	a	410	PL9	C32-C33-C34	-2.62	122.08	127.76
33	D	410	LMT	C1B-O1B-C4'	-2.61	111.17	118.01
23	A	403	CLA	O2D-CGD-O1D	-2.61	118.40	123.79
23	B	604	CLA	CMB-C2B-C1B	-2.61	124.04	128.36
25	A	408	PL9	C12-C13-C14	-2.61	122.09	127.76
25	a	410	PL9	C17-C18-C19	-2.60	122.10	127.76
25	D	404	PL9	C32-C33-C34	-2.60	122.11	127.76
31	d	406	LMG	O8-C28-O10	-2.60	116.78	123.49
23	C	512	CLA	O2D-CGD-O1D	-2.60	118.42	123.79
23	C	501	CLA	O2D-CGD-O1D	-2.60	118.42	123.79
23	A	404	CLA	O2D-CGD-O1D	-2.60	118.43	123.79
23	b	611	CLA	O2D-CGD-O1D	-2.59	118.43	123.79
23	C	506	CLA	O2D-CGD-O1D	-2.59	118.44	123.79
23	b	606	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
27	a	412	BCR	C34-C9-C10	-2.58	119.10	122.90
31	a	402	LMG	C1-O6-C5	-2.58	108.75	113.75
23	b	609	CLA	CMB-C2B-C1B	-2.57	124.11	128.36
27	h	101	BCR	C3-C4-C5	-2.57	109.79	113.87
23	B	605	CLA	O2D-CGD-O1D	-2.57	118.49	123.79
25	D	404	PL9	C7-C8-C9	-2.56	122.35	126.70
27	C	516	BCR	C11-C10-C9	-2.56	123.50	127.20
24	a	407	PHO	CBD-CHA-C4D	-2.56	105.60	108.46
27	z	101	BCR	C28-C27-C26	-2.56	109.81	113.87
27	T	101	BCR	C3-C4-C5	-2.55	109.81	113.87
23	C	505	CLA	CMB-C2B-C1B	-2.55	124.14	128.36
27	y	101	BCR	C20-C21-C22	-2.55	123.51	127.20
28	c	518	DGD	C4D-C3D-C2D	-2.55	106.04	110.79
27	D	405	BCR	C21-C20-C19	-2.54	115.37	123.13
23	b	620	CLA	O2D-CGD-O1D	-2.54	118.54	123.79
28	b	602	DGD	C6D-C5D-C4D	-2.54	106.28	112.03
23	a	405	CLA	O2D-CGD-O1D	-2.54	118.56	123.79
23	B	616	CLA	O2D-CGD-O1D	-2.53	118.56	123.79
23	B	608	CLA	O2D-CGD-O1D	-2.53	118.57	123.79
27	k	102	BCR	C35-C13-C14	-2.53	119.17	122.90
23	a	404	CLA	O2A-CGA-O1A	-2.53	116.97	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	O2D-CGD-O1D	-2.52	118.58	123.79
23	b	619	CLA	O2D-CGD-O1D	-2.52	118.59	123.79
27	C	514	BCR	C24-C23-C22	-2.52	122.38	126.22
23	B	609	CLA	O2D-CGD-O1D	-2.52	118.59	123.79
28	C	518	DGD	O4D-C4D-C5D	-2.51	102.58	109.24
23	C	504	CLA	O2D-CGD-O1D	-2.51	118.62	123.79
27	j	102	BCR	C39-C30-C25	-2.50	106.38	110.30
27	J	102	BCR	C1-C6-C5	-2.50	118.98	122.66
23	b	608	CLA	O2D-CGD-O1D	-2.50	118.63	123.79
27	D	405	BCR	C23-C24-C25	-2.50	119.82	127.32
27	a	412	BCR	C11-C10-C9	-2.50	123.59	127.20
27	C	515	BCR	C8-C7-C6	-2.50	119.82	127.32
23	B	604	CLA	O2A-CGA-O1A	-2.49	117.06	123.49
25	d	404	PL9	C42-C43-C44	-2.49	122.35	127.76
27	A	410	BCR	C34-C9-C10	-2.49	119.23	122.90
23	C	501	CLA	CMB-C2B-C1B	-2.48	124.25	128.36
23	B	615	CLA	O2D-CGD-O1D	-2.48	118.67	123.79
23	B	601	CLA	O2D-CGD-O1D	-2.47	118.69	123.79
23	a	409	CLA	O2D-CGD-O1D	-2.47	118.70	123.79
27	C	514	BCR	C35-C13-C14	-2.46	119.27	122.90
23	b	620	CLA	CMB-C2B-C1B	-2.46	124.30	128.36
23	c	505	CLA	O2D-CGD-O1D	-2.45	118.72	123.79
25	A	408	PL9	C32-C33-C34	-2.45	122.43	127.76
27	J	102	BCR	C36-C18-C17	-2.45	119.28	122.90
31	b	625	LMG	C1-O6-C5	-2.44	109.02	113.75
23	c	507	CLA	O2D-CGD-O1D	-2.44	118.76	123.79
23	c	509	CLA	CMB-C2B-C1B	-2.43	124.34	128.36
27	B	619	BCR	C27-C26-C25	-2.43	119.68	122.78
31	m	102	LMG	O4-C4-C3	-2.43	104.86	110.34
23	a	404	CLA	O2D-CGD-O1D	-2.43	118.77	123.79
23	a	405	CLA	CAA-C2A-C3A	-2.43	106.23	113.22
34	f	101	HEM	CAA-C2A-C1A	-2.43	124.38	127.01
27	z	101	BCR	C8-C7-C6	-2.42	120.04	127.32
27	y	101	BCR	C35-C13-C14	-2.42	119.33	122.90
27	b	621	BCR	C8-C7-C6	-2.42	120.05	127.32
25	d	404	PL9	C36-C34-C33	-2.42	116.47	121.05
34	f	101	HEM	C3B-C4B-NB	-2.41	107.01	111.63
27	T	102	BCR	C23-C24-C25	-2.41	120.08	127.32
33	b	626	LMT	C1B-O1B-C4'	-2.41	111.71	118.01
23	C	513	CLA	O2D-CGD-O1D	-2.41	118.81	123.79
28	C	518	DGD	C1D-O6D-C5D	-2.41	109.07	113.75
23	d	402	CLA	O2D-CGD-O1D	-2.41	118.82	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	F	101	HEM	CAA-C2A-C1A	-2.40	124.40	127.01
27	d	405	BCR	C23-C24-C25	-2.40	120.10	127.32
28	c	517	DGD	C1D-O6D-C5D	-2.40	109.08	113.75
25	A	408	PL9	C26-C24-C23	-2.40	116.50	121.05
23	B	602	CLA	O2D-CGD-O1D	-2.40	118.84	123.79
28	C	519	DGD	C4D-C3D-C2D	-2.40	106.32	110.79
25	J	101	PL9	C22-C23-C24	-2.39	122.57	127.76
27	h	101	BCR	C8-C7-C6	-2.39	120.15	127.32
27	d	405	BCR	C21-C20-C19	-2.39	115.86	123.13
27	J	102	BCR	C37-C22-C21	-2.38	119.38	122.90
27	T	102	BCR	C15-C14-C13	-2.38	123.75	127.20
31	e	101	LMG	C1-O6-C5	-2.38	109.12	113.75
27	c	514	BCR	C24-C23-C22	-2.38	122.59	126.22
23	C	508	CLA	O2D-CGD-O1D	-2.37	118.89	123.79
23	b	609	CLA	O2D-CGD-O1D	-2.37	118.89	123.79
25	D	404	PL9	C45-C44-C43	-2.37	118.85	123.50
31	A	418	LMG	C1-O6-C5	-2.37	109.15	113.75
23	D	403	CLA	O2D-CGD-O1D	-2.36	118.91	123.79
25	D	404	PL9	C27-C28-C29	-2.36	122.64	127.76
23	D	401	CLA	O2A-CGA-O1A	-2.35	117.42	123.49
24	a	407	PHO	C2B-C1B-NB	-2.35	106.20	109.73
27	j	102	BCR	C35-C13-C14	-2.35	119.43	122.90
27	j	102	BCR	C1-C6-C5	-2.35	119.21	122.66
25	d	404	PL9	C45-C44-C43	-2.35	118.89	123.50
27	d	405	BCR	C16-C15-C14	-2.34	118.21	123.39
31	b	625	LMG	C6-C5-C4	-2.34	107.25	113.02
25	A	408	PL9	C11-C9-C8	-2.34	116.62	121.05
27	a	412	BCR	C20-C21-C22	-2.34	123.82	127.20
25	d	404	PL9	C17-C18-C19	-2.33	122.69	127.76
31	b	624	LMG	C1-O6-C5	-2.33	109.23	113.75
23	C	512	CLA	O2A-CGA-O1A	-2.32	117.50	123.49
28	a	413	DGD	C6E-C5E-C4E	-2.32	107.29	113.02
27	b	622	BCR	C28-C27-C26	-2.32	110.18	113.87
31	m	102	LMG	O8-C9-C8	-2.32	102.44	108.69
24	a	408	PHO	CBD-CHA-C4D	-2.31	105.87	108.46
33	d	410	LMT	C1B-O1B-C4'	-2.31	111.96	118.01
28	b	602	DGD	O4D-C4D-C5D	-2.31	103.11	109.24
27	h	101	BCR	C15-C16-C17	-2.31	118.29	123.39
31	a	402	LMG	O3-C3-C4	-2.31	105.14	110.34
31	D	407	LMG	O8-C28-O10	-2.30	117.55	123.49
23	a	405	CLA	O2A-CGA-O1A	-2.30	117.57	123.49
27	z	101	BCR	C11-C10-C9	-2.29	123.88	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	O2A-CGA-O1A	-2.29	117.57	123.49
23	a	409	CLA	O2A-CGA-O1A	-2.29	117.58	123.49
27	B	618	BCR	C23-C24-C25	-2.29	120.44	127.32
27	a	412	BCR	C23-C24-C25	-2.29	120.44	127.32
27	B	619	BCR	C37-C22-C21	-2.29	119.52	122.90
25	a	410	PL9	C27-C28-C29	-2.29	122.79	127.76
27	z	101	BCR	C23-C24-C25	-2.28	120.47	127.32
23	c	509	CLA	O2D-CGD-O1D	-2.28	119.08	123.79
27	T	102	BCR	C24-C23-C22	-2.28	122.75	126.22
23	C	513	CLA	O2A-CGA-O1A	-2.28	117.62	123.49
28	a	413	DGD	O4D-C4D-C5D	-2.27	103.22	109.24
27	B	618	BCR	C31-C1-C6	-2.26	106.75	110.30
27	B	617	BCR	C23-C24-C25	-2.26	120.53	127.32
31	b	624	LMG	O4-C4-C3	-2.26	105.25	110.34
23	b	617	CLA	O2A-CGA-O1A	-2.26	117.67	123.49
30	B	626	SQD	C10-C9-C8	-2.25	105.02	113.29
34	F	101	HEM	C3B-C4B-NB	-2.25	107.33	111.63
31	A	418	LMG	O8-C28-O10	-2.25	117.69	123.49
27	B	617	BCR	C36-C18-C17	-2.25	119.58	122.90
23	c	512	CLA	O2A-CGA-O1A	-2.25	117.69	123.49
27	B	618	BCR	C15-C14-C13	-2.24	123.96	127.20
30	b	601	SQD	C10-C9-C8	-2.24	105.06	113.29
27	T	102	BCR	C16-C17-C18	-2.24	123.96	127.20
27	j	102	BCR	C37-C22-C21	-2.24	119.60	122.90
27	C	516	BCR	C15-C16-C17	-2.24	118.45	123.39
27	T	102	BCR	C27-C26-C25	-2.24	119.93	122.78
27	T	102	BCR	C15-C16-C17	-2.23	118.46	123.39
27	C	516	BCR	C21-C20-C19	-2.23	116.33	123.13
27	y	101	BCR	C11-C10-C9	-2.23	123.98	127.20
27	C	515	BCR	C10-C11-C12	-2.23	116.34	123.13
25	a	410	PL9	C7-C8-C9	-2.23	122.92	126.70
23	A	405	CLA	O2A-CGA-O1A	-2.22	117.75	123.49
24	D	402	PHO	C2B-C1B-NB	-2.22	106.39	109.73
31	b	625	LMG	O3-C3-C4	-2.22	105.33	110.34
27	D	405	BCR	C34-C9-C10	-2.22	119.62	122.90
31	E	101	LMG	O9-C10-C11	-2.22	114.83	123.72
27	c	515	BCR	C23-C24-C25	-2.22	120.66	127.32
31	e	101	LMG	C6-C5-C4	-2.21	107.56	113.02
27	y	101	BCR	C32-C1-C6	-2.20	106.85	110.30
27	B	619	BCR	C15-C16-C17	-2.20	118.52	123.39
24	D	402	PHO	O2A-CGA-O1A	-2.20	117.81	123.49
27	H	101	BCR	C7-C8-C9	-2.20	122.86	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	k	103	LMG	O8-C28-O10	-2.20	117.81	123.49
30	A	417	SQD	O2-C2-C3	-2.20	105.39	110.34
27	J	102	BCR	C11-C12-C13	-2.19	119.87	126.32
23	B	605	CLA	O2A-CGA-O1A	-2.19	117.84	123.49
27	j	102	BCR	C34-C9-C10	-2.19	119.67	122.90
27	B	618	BCR	C16-C17-C18	-2.19	124.04	127.20
23	B	601	CLA	O2A-CGA-O1A	-2.19	117.85	123.49
23	A	407	CLA	O2D-CGD-O1D	-2.18	119.29	123.79
24	A	406	PHO	CMB-C2B-C1B	-2.18	121.51	125.06
31	i	101	LMG	O8-C28-O10	-2.18	117.86	123.49
27	C	515	BCR	C23-C24-C25	-2.18	120.77	127.32
28	C	519	DGD	O1G-C1A-O1A	-2.18	117.87	123.49
28	a	413	DGD	C4D-C3D-C2D	-2.18	106.73	110.79
27	B	618	BCR	C34-C9-C10	-2.17	119.69	122.90
28	c	516	DGD	C6E-C5E-C4E	-2.17	107.66	113.02
23	B	616	CLA	OBD-CAD-CBD	-2.17	122.67	125.94
31	c	519	LMG	C6-C5-C4	-2.17	107.67	113.02
23	C	511	CLA	O2A-CGA-O1A	-2.16	117.91	123.49
31	B	622	LMG	O4-C4-C3	-2.16	105.47	110.34
31	I	101	LMG	C6-C5-C4	-2.16	107.68	113.02
27	T	102	BCR	C33-C5-C6	-2.16	122.48	124.61
31	E	101	LMG	C1-O6-C5	-2.16	109.56	113.75
27	k	102	BCR	C28-C27-C26	-2.16	110.45	113.87
27	T	101	BCR	C23-C24-C25	-2.15	120.86	127.32
23	A	403	CLA	O2A-CGA-O1A	-2.15	117.94	123.49
23	B	603	CLA	O2D-CGD-O1D	-2.15	119.35	123.79
24	D	402	PHO	O2D-CGD-O1D	-2.15	119.35	123.79
25	D	404	PL9	C42-C43-C44	-2.15	123.09	127.76
27	k	102	BCR	C32-C1-C6	-2.15	106.94	110.30
28	A	411	DGD	C6E-C5E-C4E	-2.14	107.73	113.02
23	b	605	CLA	O2A-CGA-O1A	-2.14	117.97	123.49
23	c	508	CLA	O2A-CGA-O1A	-2.14	117.97	123.49
27	B	619	BCR	C7-C8-C9	-2.14	122.95	126.22
27	c	515	BCR	C21-C20-C19	-2.14	116.61	123.13
23	b	613	CLA	O2A-CGA-O1A	-2.14	117.97	123.49
27	B	620	BCR	C28-C27-C26	-2.14	110.48	113.87
25	D	404	PL9	C36-C34-C33	-2.14	117.00	121.05
27	T	101	BCR	C28-C27-C26	-2.13	110.48	113.87
31	B	623	LMG	O3-C3-C4	-2.13	105.53	110.34
23	c	507	CLA	O2A-CGA-O1A	-2.13	117.99	123.49
23	b	620	CLA	OBD-CAD-CBD	-2.13	122.72	125.94
23	b	610	CLA	O2A-CGA-O1A	-2.13	118.00	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	520	LMG	O8-C28-O10	-2.12	118.01	123.49
27	B	620	BCR	C32-C1-C6	-2.12	106.97	110.30
31	B	623	LMG	O8-C28-O10	-2.12	118.02	123.49
23	b	619	CLA	O2A-CGA-O1A	-2.12	118.02	123.49
31	M	101	LMG	O8-C9-C8	-2.12	102.99	108.69
23	c	501	CLA	O2A-CGA-O1A	-2.12	118.03	123.49
23	C	504	CLA	O2A-CGA-O1A	-2.12	118.03	123.49
25	d	404	PL9	C27-C28-C29	-2.12	123.16	127.76
28	D	409	DGD	C1D-O6D-C5D	-2.11	109.64	113.75
28	c	517	DGD	O4D-C4D-C5D	-2.11	103.64	109.24
25	D	404	PL9	C17-C18-C19	-2.11	123.17	127.76
23	c	513	CLA	O2A-CGA-O1A	-2.11	118.05	123.49
25	a	410	PL9	C26-C24-C23	-2.11	117.05	121.05
31	D	406	LMG	C1-O6-C5	-2.11	109.66	113.75
23	B	612	CLA	O2D-CGD-O1D	-2.10	119.45	123.79
23	A	403	CLA	OBD-CAD-CBD	-2.10	122.76	125.94
23	B	605	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
27	C	516	BCR	C23-C24-C25	-2.10	121.02	127.32
27	y	101	BCR	C28-C27-C26	-2.10	110.54	113.87
31	d	406	LMG	C6-C5-C4	-2.10	107.84	113.02
27	C	514	BCR	C39-C30-C25	-2.09	107.02	110.30
27	J	102	BCR	C39-C30-C25	-2.09	107.02	110.30
28	B	627	DGD	C4D-C3D-C2D	-2.09	106.89	110.79
31	e	101	LMG	O9-C10-C11	-2.09	115.37	123.72
27	b	622	BCR	C31-C1-C6	-2.09	107.03	110.30
31	A	418	LMG	O3-C3-C4	-2.09	105.64	110.34
25	a	410	PL9	C11-C9-C8	-2.08	117.10	121.05
23	d	402	CLA	C4B-CHC-C1C	-2.08	124.79	129.26
31	M	101	LMG	O3-C3-C4	-2.08	105.66	110.34
27	b	621	BCR	C31-C1-C6	-2.08	107.05	110.30
27	y	101	BCR	C4-C5-C6	-2.07	120.14	122.78
29	a	414	LHG	C5-O7-C7	-2.07	112.92	117.89
31	e	101	LMG	O7-C10-O9	-2.07	118.12	123.67
24	a	408	PHO	CMB-C2B-C1B	-2.07	121.69	125.06
25	A	408	PL9	C27-C28-C29	-2.06	123.27	127.76
23	B	610	CLA	O2A-CGA-O1A	-2.06	118.16	123.49
23	D	403	CLA	O2A-CGA-O1A	-2.06	118.18	123.49
31	C	521	LMG	O3-C3-C4	-2.06	105.70	110.34
28	c	518	DGD	C6E-C5E-C4E	-2.06	107.94	113.02
29	A	415	LHG	C6-C5-C4	-2.06	107.26	112.07
27	b	621	BCR	C35-C13-C14	-2.06	119.86	122.90
27	H	101	BCR	C21-C20-C19	-2.05	116.87	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	625	LMG	O8-C28-O10	-2.05	118.19	123.49
27	b	622	BCR	C21-C20-C19	-2.05	116.87	123.13
23	B	612	CLA	OBD-CAD-CBD	-2.05	122.84	125.94
27	B	617	BCR	C40-C30-C25	-2.05	107.09	110.30
27	A	410	BCR	C23-C24-C25	-2.05	121.17	127.32
31	m	102	LMG	O3-C3-C4	-2.05	105.73	110.34
23	C	506	CLA	CAA-CBA-CGA	-2.04	107.33	113.32
27	B	618	BCR	C24-C23-C22	-2.04	123.10	126.22
27	B	619	BCR	C31-C1-C6	-2.04	107.11	110.30
28	D	409	DGD	C6D-O5D-C1E	-2.04	109.54	113.82
27	j	102	BCR	C15-C16-C17	-2.04	118.89	123.39
28	A	411	DGD	C6D-C5D-C4D	-2.04	107.41	112.03
23	c	511	CLA	O2A-CGA-O1A	-2.04	118.24	123.49
23	B	613	CLA	O2D-CGD-O1D	-2.04	119.59	123.79
23	A	404	CLA	O2A-CGA-O1A	-2.04	118.24	123.49
23	b	609	CLA	O2A-CGA-O1A	-2.03	118.24	123.49
27	a	412	BCR	C28-C27-C26	-2.03	110.64	113.87
28	B	627	DGD	C6D-C5D-C4D	-2.03	107.42	112.03
27	j	102	BCR	C11-C12-C13	-2.03	120.33	126.32
23	b	616	CLA	O2D-CGD-O1D	-2.03	119.59	123.79
23	C	501	CLA	O2A-CGA-O1A	-2.03	118.25	123.49
28	c	518	DGD	O1G-C1A-O1A	-2.03	118.26	123.49
27	J	102	BCR	C38-C26-C25	-2.03	122.61	124.61
27	k	102	BCR	C23-C24-C25	-2.03	121.23	127.32
23	B	608	CLA	O2A-CGA-O1A	-2.03	118.26	123.49
27	J	102	BCR	C30-C25-C26	-2.02	119.69	122.66
28	d	409	DGD	O2G-C1B-O1B	-2.02	118.25	123.67
27	B	620	BCR	C40-C30-C25	-2.02	107.14	110.30
24	a	407	PHO	O2A-CGA-O1A	-2.02	118.28	123.49
23	C	509	CLA	O2D-CGD-O1D	-2.02	119.62	123.79
27	c	515	BCR	C15-C16-C17	-2.01	118.94	123.39
27	z	101	BCR	C10-C11-C12	-2.01	117.01	123.13
23	B	607	CLA	O2A-CGA-O1A	-2.01	118.31	123.49
31	C	521	LMG	C6-C5-C4	-2.00	108.07	113.02
27	b	621	BCR	C37-C22-C21	-2.00	119.94	122.90
23	c	505	CLA	O2A-CGA-O1A	-2.00	118.33	123.49
23	C	512	CLA	O1D-CGD-CBD	2.00	127.49	124.62
27	B	617	BCR	C36-C18-C19	2.00	121.43	118.10
23	a	404	CLA	O1D-CGD-CBD	2.00	127.49	124.62
27	j	102	BCR	C33-C5-C4	2.00	117.22	113.43
28	C	517	DGD	O3G-C1D-C2D	2.00	110.57	108.04
23	a	406	CLA	O1D-CGD-CBD	2.00	127.50	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	O2D-CGD-CBD	2.01	114.05	111.30
28	C	517	DGD	C3G-O3G-C1D	2.01	118.04	113.82
23	c	512	CLA	C1D-CHD-C4C	2.01	125.64	122.60
23	C	503	CLA	O1D-CGD-CBD	2.01	127.50	124.62
27	H	101	BCR	C36-C18-C19	2.02	121.45	118.10
31	B	623	LMG	O6-C5-C4	2.02	113.47	109.68
23	c	502	CLA	O1D-CGD-CBD	2.02	127.51	124.62
24	D	402	PHO	CBD-CHA-C1A	2.02	131.12	126.36
25	D	404	PL9	C51-C49-C50	2.02	119.60	114.64
23	b	615	CLA	O2D-CGD-CBD	2.02	114.07	111.30
23	B	609	CLA	O2D-CGD-CBD	2.02	114.07	111.30
28	a	413	DGD	O6D-C1D-O3G	2.02	114.93	110.05
24	a	408	PHO	CHB-C1B-NB	2.03	128.45	124.66
25	a	410	PL9	C30-C29-C31	2.03	118.51	115.41
27	J	102	BCR	C33-C5-C4	2.03	117.28	113.43
23	c	510	CLA	O2D-CGD-CBD	2.03	114.08	111.30
23	C	512	CLA	O2D-CGD-CBD	2.03	114.08	111.30
23	c	501	CLA	CMD-C2D-C3D	2.03	129.06	125.09
30	A	413	SQD	O6-C1-C2	2.04	110.61	108.04
23	B	601	CLA	O1D-CGD-CBD	2.04	127.54	124.62
23	c	509	CLA	CMD-C2D-C3D	2.04	129.07	125.09
23	D	401	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	c	513	CLA	C1D-CHD-C4C	2.04	125.68	122.60
25	d	404	PL9	C45-C44-C46	2.04	118.52	115.41
23	b	612	CLA	CMD-C2D-C3D	2.04	129.08	125.09
31	b	625	LMG	O6-C5-C4	2.04	113.51	109.68
23	B	604	CLA	CMB-C2B-C3B	2.04	129.08	125.09
23	a	405	CLA	O1D-CGD-CBD	2.04	127.55	124.62
33	I	102	LMT	O1B-C4'-C3'	2.04	112.44	107.17
28	b	602	DGD	C1E-C2E-C3E	2.04	114.00	109.97
23	C	510	CLA	O2D-CGD-CBD	2.04	114.10	111.30
27	c	514	BCR	C12-C13-C14	2.04	122.28	118.98
23	C	510	CLA	C4A-NA-C1A	2.04	109.00	106.36
27	c	515	BCR	C2-C1-C6	2.04	113.60	110.36
23	C	505	CLA	CMB-C2B-C3B	2.05	129.09	125.09
23	c	507	CLA	C1D-CHD-C4C	2.05	125.71	122.60
27	B	619	BCR	C38-C26-C27	2.06	117.33	113.43
27	T	101	BCR	C33-C5-C4	2.06	117.33	113.43
31	C	521	LMG	C9-O8-C28	2.06	122.62	116.85
23	C	510	CLA	C1D-CHD-C4C	2.07	125.73	122.60
34	f	101	HEM	C2C-C1C-CHC	2.07	126.83	123.68
23	b	617	CLA	O1D-CGD-CBD	2.07	127.58	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	520	LMG	C3-C4-C5	2.07	113.81	110.20
27	h	101	BCR	C36-C18-C19	2.07	121.54	118.10
28	D	409	DGD	O2G-C1B-C2B	2.07	116.03	111.53
27	y	101	BCR	C35-C13-C12	2.07	121.55	118.10
27	B	617	BCR	C33-C5-C4	2.07	117.36	113.43
23	C	511	CLA	O2D-CGD-CBD	2.08	114.14	111.30
27	k	102	BCR	C35-C13-C12	2.08	121.55	118.10
23	b	606	CLA	O2D-CGD-CBD	2.08	114.15	111.30
27	C	516	BCR	C2-C1-C6	2.08	113.65	110.36
23	b	611	CLA	O1D-CGD-CBD	2.08	127.60	124.62
27	y	101	BCR	C38-C26-C27	2.08	117.37	113.43
23	b	607	CLA	C1D-CHD-C4C	2.08	125.75	122.60
23	A	404	CLA	CMD-C2D-C3D	2.08	129.16	125.09
23	d	403	CLA	CMB-C2B-C3B	2.08	129.16	125.09
33	D	410	LMT	O1'-C1'-C2'	2.08	110.67	108.04
28	C	519	DGD	O3D-C3D-C4D	2.08	115.03	110.34
23	C	510	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	a	407	PHO	CBD-CHA-C1A	2.09	131.28	126.36
23	B	611	CLA	CMD-C2D-C3D	2.09	129.18	125.09
27	b	621	BCR	C2-C1-C6	2.09	113.67	110.36
23	b	617	CLA	O2D-CGD-CBD	2.09	114.17	111.30
31	b	625	LMG	C3-C4-C5	2.09	113.85	110.20
23	C	511	CLA	CMD-C2D-C3D	2.10	129.19	125.09
23	B	603	CLA	C1D-CHD-C4C	2.10	125.77	122.60
30	b	601	SQD	C1-O5-C5	2.10	117.82	113.75
23	b	620	CLA	CMD-C2D-C3D	2.10	129.20	125.09
23	c	511	CLA	CMB-C2B-C3B	2.11	129.21	125.09
33	I	102	LMT	O1'-C1'-C2'	2.11	110.70	108.04
23	C	503	CLA	O2D-CGD-CBD	2.11	114.19	111.30
34	V	201	HEM	C2D-C3D-C4D	2.11	105.08	101.50
31	I	101	LMG	C8-O7-C10	2.11	122.95	117.89
23	A	407	CLA	CMD-C2D-C3D	2.11	129.22	125.09
31	m	102	LMG	C9-O8-C28	2.11	122.76	116.85
29	A	412	LHG	C6-O8-C23	2.12	122.77	116.85
29	A	412	LHG	O8-C23-C24	2.12	118.36	111.90
24	A	406	PHO	CHB-C1B-NB	2.12	128.63	124.66
23	d	402	CLA	CHB-C4A-NA	2.12	127.45	124.51
27	A	410	BCR	C33-C5-C4	2.13	117.46	113.43
24	D	402	PHO	C1B-NB-C4B	2.13	110.72	106.51
25	d	404	PL9	C51-C49-C50	2.13	119.88	114.64
28	c	516	DGD	O3G-C1D-C2D	2.14	110.74	108.04
23	B	616	CLA	CHB-C4A-NA	2.15	127.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	619	BCR	C33-C5-C4	2.15	117.50	113.43
23	A	405	CLA	C4A-NA-C1A	2.15	109.14	106.36
25	J	101	PL9	C10-C9-C11	2.15	118.69	115.41
25	D	404	PL9	C10-C9-C11	2.15	118.69	115.41
30	B	626	SQD	C1-O5-C5	2.15	117.92	113.75
23	B	614	CLA	O1D-CGD-CBD	2.16	127.71	124.62
27	c	515	BCR	C33-C5-C4	2.16	117.52	113.43
23	c	503	CLA	CMD-C2D-C3D	2.16	129.31	125.09
23	b	615	CLA	O1D-CGD-CBD	2.16	127.72	124.62
29	a	414	LHG	O8-C23-C24	2.16	118.49	111.90
23	B	611	CLA	O2D-CGD-CBD	2.16	114.27	111.30
27	C	514	BCR	C29-C30-C25	2.16	113.79	110.36
23	b	620	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	C	508	CLA	C1D-CHD-C4C	2.17	125.88	122.60
23	b	620	CLA	O1D-CGD-CBD	2.17	127.73	124.62
27	c	514	BCR	C29-C30-C25	2.17	113.80	110.36
23	b	608	CLA	CMB-C2B-C3B	2.17	129.33	125.09
27	B	618	BCR	C35-C13-C12	2.17	121.71	118.10
23	A	404	CLA	O2D-CGD-CBD	2.17	114.28	111.30
25	D	404	PL9	C30-C29-C31	2.17	118.73	115.41
27	a	412	BCR	C38-C26-C27	2.17	117.55	113.43
23	b	605	CLA	CMD-C2D-C3D	2.17	129.34	125.09
23	B	601	CLA	CMD-C2D-C3D	2.17	129.34	125.09
23	b	615	CLA	CMB-C2B-C3B	2.18	129.34	125.09
23	b	612	CLA	O2D-CGD-CBD	2.18	114.28	111.30
23	B	616	CLA	O1D-CGD-CBD	2.18	127.75	124.62
27	z	101	BCR	C33-C5-C4	2.18	117.57	113.43
31	k	103	LMG	C3-C4-C5	2.18	114.00	110.20
30	A	413	SQD	O5-C1-C2	2.18	114.76	110.28
23	c	501	CLA	CMB-C2B-C3B	2.19	129.37	125.09
31	B	622	LMG	C4-C3-C2	2.19	114.87	110.79
25	a	410	PL9	C10-C9-C11	2.19	118.75	115.41
30	F	102	SQD	O6-C1-C2	2.19	110.81	108.04
30	A	413	SQD	C44-O6-C1	2.19	118.43	113.82
31	b	624	LMG	C4-C3-C2	2.19	114.89	110.79
23	b	613	CLA	CHB-C4A-NA	2.20	127.55	124.51
31	M	101	LMG	C9-O8-C28	2.20	123.00	116.85
23	B	614	CLA	CHB-C4A-NA	2.20	127.55	124.51
23	C	511	CLA	CMB-C2B-C3B	2.20	129.39	125.09
23	B	609	CLA	CMD-C2D-C3D	2.20	129.40	125.09
27	h	101	BCR	C35-C13-C12	2.21	121.77	118.10
25	a	410	PL9	C15-C14-C16	2.21	118.78	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	O1D-CGD-CBD	2.21	127.79	124.62
23	b	618	CLA	O2D-CGD-CBD	2.21	114.33	111.30
23	c	512	CLA	O2D-CGD-CBD	2.21	114.34	111.30
23	A	403	CLA	CMB-C2B-C3B	2.21	129.42	125.09
23	A	405	CLA	CMD-C2D-C3D	2.22	129.42	125.09
23	A	403	CLA	CHB-C4A-NA	2.22	127.58	124.51
34	F	101	HEM	C2D-C3D-C4D	2.22	105.27	101.50
23	C	506	CLA	CMD-C2D-C3D	2.22	129.44	125.09
31	b	624	LMG	C3-C4-C5	2.23	114.08	110.20
24	a	407	PHO	C4A-NA-C1A	2.23	110.20	108.21
23	a	405	CLA	C4A-NA-C1A	2.23	109.24	106.36
23	C	504	CLA	CMD-C2D-C3D	2.23	129.45	125.09
25	D	404	PL9	C20-C19-C21	2.23	118.81	115.41
25	A	408	PL9	C10-C9-C11	2.23	118.81	115.41
25	A	408	PL9	C15-C14-C16	2.23	118.82	115.41
31	k	103	LMG	C7-O1-C1	2.23	118.51	113.82
23	B	606	CLA	CMD-C2D-C3D	2.24	129.46	125.09
23	C	506	CLA	O1D-CGD-CBD	2.24	127.83	124.62
23	b	609	CLA	CMB-C2B-C3B	2.24	129.46	125.09
23	B	607	CLA	O1D-CGD-CBD	2.24	127.83	124.62
23	C	510	CLA	CMB-C2B-C3B	2.24	129.47	125.09
23	c	510	CLA	C4A-NA-C1A	2.24	109.25	106.36
23	a	404	CLA	CMB-C2B-C3B	2.24	129.47	125.09
23	B	615	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	c	504	CLA	CMD-C2D-C3D	2.25	129.49	125.09
25	d	404	PL9	C10-C9-C11	2.25	118.84	115.41
24	a	407	PHO	C1B-NB-C4B	2.25	110.96	106.51
23	c	511	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	C	505	CLA	CBA-CAA-C2A	2.25	120.09	113.73
23	B	606	CLA	C4A-NA-C1A	2.25	109.27	106.36
30	f	102	SQD	O5-C1-C2	2.26	114.90	110.28
23	c	509	CLA	O1D-CGD-CBD	2.26	127.86	124.62
23	b	619	CLA	O1D-CGD-CBD	2.26	127.86	124.62
23	c	505	CLA	CBA-CAA-C2A	2.26	120.10	113.73
28	c	518	DGD	O2G-C1B-C2B	2.26	116.44	111.53
23	B	605	CLA	CMD-C2D-C3D	2.26	129.51	125.09
30	F	102	SQD	O48-C23-C24	2.26	118.79	111.90
24	A	406	PHO	C1B-NB-C4B	2.26	110.99	106.51
23	C	502	CLA	CHB-C4A-NA	2.27	127.64	124.51
23	c	507	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	a	409	CLA	O1D-CGD-CBD	2.27	127.88	124.62
28	b	623	DGD	C3G-O3G-C1D	2.27	118.59	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	101	LMG	C3-C4-C5	2.27	114.16	110.20
23	c	507	CLA	O1D-CGD-CBD	2.27	127.88	124.62
28	c	516	DGD	O3D-C3D-C4D	2.28	115.46	110.34
31	C	520	LMG	O1-C1-C2	2.28	110.92	108.04
23	B	601	CLA	CMB-C2B-C3B	2.28	129.55	125.09
31	a	416	LMG	O6-C5-C6	2.28	112.12	106.36
23	B	605	CLA	O1D-CGD-CBD	2.28	127.89	124.62
23	c	510	CLA	CMD-C2D-C3D	2.28	129.56	125.09
23	c	505	CLA	CMB-C2B-C3B	2.28	129.56	125.09
23	b	605	CLA	CMB-C2B-C3B	2.28	129.56	125.09
30	A	417	SQD	O48-C23-C24	2.29	118.87	111.90
27	h	101	BCR	C33-C5-C4	2.29	117.77	113.43
27	C	516	BCR	C33-C5-C4	2.29	117.77	113.43
23	B	610	CLA	O1D-CGD-CBD	2.29	127.90	124.62
23	B	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	C	502	CLA	CMB-C2B-C3B	2.29	129.57	125.09
23	b	612	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	b	605	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	c	513	CLA	O1D-CGD-CBD	2.29	127.91	124.62
28	d	409	DGD	C2G-O2G-C1B	2.30	123.40	117.89
23	C	513	CLA	O1D-CGD-CBD	2.30	127.91	124.62
23	b	612	CLA	C4A-NA-C1A	2.30	109.33	106.36
23	b	607	CLA	CMD-C2D-C3D	2.30	129.59	125.09
23	b	613	CLA	CMB-C2B-C3B	2.30	129.59	125.09
23	c	508	CLA	O2D-CGD-CBD	2.30	114.45	111.30
23	C	502	CLA	CMD-C2D-C3D	2.30	129.59	125.09
23	b	613	CLA	C4A-NA-C1A	2.30	109.33	106.36
27	H	101	BCR	C35-C13-C12	2.30	121.93	118.10
27	b	621	BCR	C33-C5-C4	2.30	117.80	113.43
31	b	624	LMG	O1-C1-C2	2.31	110.95	108.04
23	C	509	CLA	CMB-C2B-C3B	2.31	129.60	125.09
23	B	616	CLA	C4A-NA-C1A	2.31	109.34	106.36
31	e	101	LMG	C8-O7-C10	2.31	123.43	117.89
30	f	102	SQD	O48-C23-C24	2.31	118.95	111.90
27	h	101	BCR	C34-C9-C8	2.32	121.95	118.10
23	b	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
34	v	201	HEM	C2D-C3D-C4D	2.32	105.43	101.50
31	B	623	LMG	C3-C4-C5	2.32	114.24	110.20
23	C	502	CLA	O1D-CGD-CBD	2.32	127.95	124.62
23	b	610	CLA	CMD-C2D-C3D	2.33	129.64	125.09
25	j	101	PL9	C10-C9-C11	2.33	118.97	115.41
23	B	610	CLA	C4A-NA-C1A	2.33	109.37	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	406	LMG	O1-C1-C2	2.33	110.98	108.04
28	d	409	DGD	O2G-C1B-C2B	2.33	116.60	111.53
30	B	626	SQD	O47-C7-C8	2.33	116.60	111.53
31	d	407	LMG	C7-O1-C1	2.34	118.73	113.82
27	a	412	BCR	C34-C9-C8	2.34	121.99	118.10
31	M	101	LMG	O1-C1-C2	2.34	110.99	108.04
31	C	521	LMG	C3-C4-C5	2.34	114.28	110.20
27	D	405	BCR	C33-C5-C4	2.34	117.87	113.43
27	b	621	BCR	C38-C26-C27	2.34	117.87	113.43
23	B	615	CLA	CMB-C2B-C3B	2.35	129.68	125.09
30	A	413	SQD	O48-C23-C24	2.35	119.05	111.90
23	C	505	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	c	516	DGD	O1G-C1A-C2A	2.35	119.06	111.90
28	A	411	DGD	O3D-C3D-C4D	2.35	115.63	110.34
23	B	604	CLA	CHB-C4A-NA	2.35	127.76	124.51
31	c	519	LMG	C3-C4-C5	2.35	114.30	110.20
23	c	510	CLA	O1D-CGD-CBD	2.36	128.00	124.62
23	A	405	CLA	CHB-C4A-NA	2.36	127.77	124.51
23	D	403	CLA	CHB-C4A-NA	2.36	127.77	124.51
28	a	413	DGD	O3D-C3D-C4D	2.36	115.65	110.34
28	B	627	DGD	C1G-O1G-C1A	2.36	123.45	116.85
23	b	609	CLA	O1D-CGD-CBD	2.36	128.01	124.62
23	b	615	CLA	CHB-C4A-NA	2.36	127.78	124.51
31	i	101	LMG	C7-O1-C1	2.36	118.79	113.82
27	B	619	BCR	C2-C1-C6	2.37	114.11	110.36
34	f	101	HEM	C2D-C3D-C4D	2.37	105.51	101.50
23	A	403	CLA	CMD-C2D-C3D	2.37	129.71	125.09
27	C	515	BCR	C33-C5-C4	2.37	117.92	113.43
25	j	101	PL9	C20-C19-C21	2.37	119.03	115.41
23	b	616	CLA	O1D-CGD-CBD	2.37	128.02	124.62
23	b	614	CLA	C4A-NA-C1A	2.38	109.43	106.36
27	k	102	BCR	C38-C26-C27	2.38	117.94	113.43
23	c	508	CLA	CMD-C2D-C3D	2.38	129.74	125.09
23	C	509	CLA	O1D-CGD-CBD	2.38	128.03	124.62
23	B	606	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	c	512	CLA	O1D-CGD-CBD	2.38	128.04	124.62
23	C	505	CLA	CMD-C2D-C3D	2.38	129.75	125.09
27	C	514	BCR	C33-C5-C4	2.38	117.95	113.43
23	B	602	CLA	CMB-C2B-C3B	2.38	129.75	125.09
28	d	409	DGD	O5D-C6D-C5D	2.39	113.40	109.08
28	b	623	DGD	O1G-C1A-C2A	2.39	119.17	111.90
23	c	503	CLA	CHB-C4A-NA	2.39	127.82	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	a	406	CLA	CMB-C2B-C3B	2.39	129.76	125.09
23	B	602	CLA	CMD-C2D-C3D	2.39	129.76	125.09
23	C	510	CLA	O1D-CGD-CBD	2.39	128.05	124.62
23	D	401	CLA	C4A-NA-C1A	2.39	109.45	106.36
30	d	408	SQD	O48-C23-C24	2.39	119.19	111.90
28	B	627	DGD	C1E-C2E-C3E	2.39	114.69	109.97
23	D	401	CLA	CMD-C2D-C3D	2.40	129.78	125.09
25	d	404	PL9	C15-C14-C16	2.40	119.07	115.41
25	A	408	PL9	C30-C29-C31	2.40	119.08	115.41
23	B	603	CLA	O1D-CGD-CBD	2.40	128.07	124.62
23	c	501	CLA	O1D-CGD-CBD	2.40	128.07	124.62
23	d	403	CLA	CHB-C4A-NA	2.40	127.84	124.51
23	A	404	CLA	C4A-NA-C1A	2.40	109.47	106.36
28	C	517	DGD	C1G-O1G-C1A	2.40	123.57	116.85
23	c	503	CLA	CMB-C2B-C3B	2.41	129.79	125.09
28	C	519	DGD	O2G-C1B-C2B	2.41	116.76	111.53
31	i	101	LMG	C3-C4-C5	2.41	114.40	110.20
27	c	514	BCR	C33-C5-C4	2.41	118.00	113.43
23	C	511	CLA	O1D-CGD-CBD	2.41	128.08	124.62
31	C	520	LMG	C7-O1-C1	2.41	118.89	113.82
28	b	602	DGD	O6D-C1D-O3G	2.42	115.87	110.05
23	c	505	CLA	O1D-CGD-CBD	2.42	128.09	124.62
23	D	403	CLA	CMD-C2D-C3D	2.42	129.81	125.09
23	D	403	CLA	C4A-NA-C1A	2.42	109.48	106.36
23	A	403	CLA	O1D-CGD-CBD	2.42	128.09	124.62
23	B	611	CLA	C4A-NA-C1A	2.42	109.49	106.36
23	c	503	CLA	C4A-NA-C1A	2.43	109.50	106.36
23	B	613	CLA	C4A-NA-C1A	2.43	109.50	106.36
23	B	612	CLA	O1D-CGD-CBD	2.43	128.10	124.62
23	B	605	CLA	CMB-C2B-C3B	2.43	129.84	125.09
23	b	610	CLA	CMB-C2B-C3B	2.43	129.85	125.09
23	b	616	CLA	CMD-C2D-C3D	2.44	129.85	125.09
28	c	517	DGD	O6E-C1E-C2E	2.44	115.28	110.28
23	C	507	CLA	C4A-NA-C1A	2.44	109.52	106.36
23	c	510	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	b	605	CLA	C4A-NA-C1A	2.44	109.52	106.36
30	D	408	SQD	O48-C23-C24	2.44	119.35	111.90
28	A	411	DGD	O1G-C1A-C2A	2.45	119.36	111.90
23	C	507	CLA	CMD-C2D-C3D	2.45	129.88	125.09
28	B	621	DGD	O2G-C1B-C2B	2.46	116.86	111.53
23	c	512	CLA	CMB-C2B-C3B	2.46	129.89	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	k	103	LMG	O1-C1-C2	2.46	111.15	108.04
23	a	404	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	k	102	BCR	C33-C5-C4	2.46	118.10	113.43
28	d	409	DGD	O3D-C3D-C4D	2.46	115.88	110.34
28	C	517	DGD	O1G-C1A-C2A	2.46	119.41	111.90
23	a	406	CLA	CMD-C2D-C3D	2.46	129.91	125.09
23	c	504	CLA	O1D-CGD-CBD	2.47	128.16	124.62
31	C	521	LMG	C7-O1-C1	2.47	119.00	113.82
23	A	403	CLA	C4A-NA-C1A	2.47	109.55	106.36
28	B	627	DGD	O6D-C1D-O3G	2.47	116.00	110.05
23	C	512	CLA	CMD-C2D-C3D	2.47	129.92	125.09
23	B	614	CLA	C4A-NA-C1A	2.47	109.55	106.36
31	I	101	LMG	C7-O1-C1	2.47	119.02	113.82
25	J	101	PL9	C15-C14-C16	2.48	119.19	115.41
27	B	620	BCR	C38-C26-C27	2.48	118.12	113.43
25	j	101	PL9	C15-C14-C16	2.48	119.19	115.41
30	b	601	SQD	O6-C1-C2	2.48	111.17	108.04
23	B	612	CLA	C4A-NA-C1A	2.48	109.56	106.36
23	A	407	CLA	CHB-C4A-NA	2.48	127.94	124.51
31	e	101	LMG	O7-C10-C11	2.48	116.92	111.53
23	c	513	CLA	CMB-C2B-C3B	2.48	129.94	125.09
23	B	615	CLA	C4A-NA-C1A	2.48	109.57	106.36
30	F	102	SQD	O5-C1-C2	2.48	115.37	110.28
23	b	605	CLA	O1D-CGD-CBD	2.49	128.18	124.62
23	A	407	CLA	C4A-NA-C1A	2.49	109.58	106.36
29	a	417	LHG	O8-C23-C24	2.49	119.49	111.90
23	a	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
30	a	415	SQD	O48-C23-C24	2.49	119.50	111.90
30	a	401	SQD	O48-C23-C24	2.49	119.50	111.90
23	c	506	CLA	O2D-CGD-CBD	2.49	114.72	111.30
23	a	409	CLA	CMB-C2B-C3B	2.50	129.97	125.09
23	b	615	CLA	C4A-NA-C1A	2.50	109.59	106.36
25	a	410	PL9	C20-C19-C21	2.50	119.22	115.41
33	b	603	LMT	O1B-C4'-C3'	2.50	113.62	107.17
23	b	613	CLA	CMD-C2D-C3D	2.50	129.97	125.09
23	C	503	CLA	CMD-C2D-C3D	2.50	129.98	125.09
23	c	507	CLA	C4A-NA-C1A	2.50	109.59	106.36
23	a	406	CLA	O2D-CGD-CBD	2.50	114.73	111.30
27	d	405	BCR	C33-C5-C4	2.50	118.18	113.43
23	b	618	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	C	501	CLA	CHB-C4A-NA	2.51	127.98	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CMB-C2B-C3B	2.51	129.99	125.09
23	b	609	CLA	CMD-C2D-C3D	2.51	129.99	125.09
23	B	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	D	405	BCR	C29-C30-C25	2.51	114.34	110.36
28	B	627	DGD	O1G-C1A-C2A	2.51	119.55	111.90
23	c	501	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	A	405	CLA	CMB-C2B-C3B	2.51	130.00	125.09
23	b	611	CLA	CMB-C2B-C3B	2.51	130.01	125.09
23	b	609	CLA	CHB-C4A-NA	2.52	127.99	124.51
30	b	601	SQD	O47-C7-C8	2.52	117.00	111.53
23	a	409	CLA	CMD-C2D-C3D	2.52	130.01	125.09
23	b	620	CLA	C4A-NA-C1A	2.52	109.61	106.36
23	b	614	CLA	O2D-CGD-CBD	2.52	114.76	111.30
29	a	414	LHG	C6-O8-C23	2.52	123.91	116.85
23	B	611	CLA	CHB-C4A-NA	2.53	128.00	124.51
23	b	607	CLA	C4A-NA-C1A	2.53	109.62	106.36
23	C	513	CLA	CMB-C2B-C3B	2.53	130.03	125.09
23	b	619	CLA	CMD-C2D-C3D	2.53	130.04	125.09
27	b	622	BCR	C38-C26-C27	2.53	118.22	113.43
23	B	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	C	512	CLA	CMB-C2B-C3B	2.53	130.04	125.09
23	b	609	CLA	C4A-NA-C1A	2.53	109.63	106.36
23	c	506	CLA	CMD-C2D-C3D	2.54	130.06	125.09
31	m	102	LMG	O1-C1-C2	2.55	111.26	108.04
23	c	513	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	c	515	BCR	C38-C26-C27	2.55	118.27	113.43
23	C	503	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	b	608	CLA	O1D-CGD-CBD	2.55	128.28	124.62
23	c	502	CLA	CMB-C2B-C3B	2.55	130.08	125.09
28	B	621	DGD	O1G-C1A-C2A	2.56	119.69	111.90
23	c	502	CLA	O2D-CGD-CBD	2.56	114.81	111.30
25	D	404	PL9	C15-C14-C16	2.56	119.32	115.41
31	I	101	LMG	O1-C1-C2	2.56	111.28	108.04
23	b	613	CLA	O2D-CGD-CBD	2.56	114.81	111.30
23	c	508	CLA	C4A-NA-C1A	2.57	109.68	106.36
23	C	502	CLA	C4A-NA-C1A	2.57	109.68	106.36
23	C	501	CLA	C4A-NA-C1A	2.57	109.68	106.36
23	C	508	CLA	C4A-NA-C1A	2.57	109.68	106.36
23	c	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	B	601	CLA	CHB-C4A-NA	2.57	128.07	124.51
31	M	101	LMG	O8-C28-C29	2.57	119.73	111.90
23	b	618	CLA	CMB-C2B-C3B	2.57	130.12	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	CMB-C2B-C3B	2.57	130.12	125.09
25	d	404	PL9	C20-C19-C21	2.57	119.34	115.41
31	a	402	LMG	O1-C1-C2	2.58	111.29	108.04
28	a	413	DGD	O1G-C1A-C2A	2.58	119.76	111.90
23	A	404	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	B	616	CLA	CMB-C2B-C3B	2.58	130.14	125.09
23	d	403	CLA	C4A-NA-C1A	2.58	109.70	106.36
23	c	506	CLA	CHB-C4A-NA	2.58	128.09	124.51
28	C	517	DGD	O3D-C3D-C4D	2.58	116.16	110.34
31	E	101	LMG	O7-C10-C11	2.58	117.14	111.53
23	C	513	CLA	C4A-NA-C1A	2.59	109.70	106.36
23	C	512	CLA	CHB-C4A-NA	2.59	128.09	124.51
28	c	518	DGD	O3D-C3D-C4D	2.59	116.16	110.34
23	c	507	CLA	CMB-C2B-C3B	2.59	130.15	125.09
23	C	511	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	b	606	CLA	C4A-NA-C1A	2.59	109.71	106.36
23	C	503	CLA	C4A-NA-C1A	2.59	109.71	106.36
25	A	408	PL9	C20-C19-C21	2.59	119.37	115.41
23	c	501	CLA	C4A-NA-C1A	2.59	109.71	106.36
23	a	409	CLA	C4A-NA-C1A	2.60	109.71	106.36
28	a	413	DGD	C3D-C4D-C5D	2.60	114.72	110.20
23	B	612	CLA	CMD-C2D-C3D	2.60	130.17	125.09
23	B	616	CLA	CMD-C2D-C3D	2.60	130.17	125.09
25	d	404	PL9	C40-C39-C41	2.60	119.38	115.41
23	c	506	CLA	C4A-NA-C1A	2.60	109.72	106.36
27	C	516	BCR	C38-C26-C27	2.60	118.36	113.43
28	A	411	DGD	C3D-C4D-C5D	2.60	114.73	110.20
23	C	509	CLA	C4A-NA-C1A	2.60	109.72	106.36
27	b	621	BCR	C29-C30-C25	2.60	114.48	110.36
23	C	505	CLA	O1D-CGD-CBD	2.60	128.35	124.62
28	c	517	DGD	O1G-C1A-C2A	2.61	119.84	111.90
23	B	607	CLA	O2D-CGD-CBD	2.61	114.88	111.30
30	b	601	SQD	O5-C5-C4	2.61	114.58	109.68
23	c	513	CLA	C4A-NA-C1A	2.61	109.73	106.36
23	D	403	CLA	CMB-C2B-C3B	2.61	130.19	125.09
23	B	609	CLA	C4A-NA-C1A	2.61	109.73	106.36
23	c	503	CLA	O2D-CGD-CBD	2.61	114.88	111.30
23	a	409	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	C	506	CLA	C4A-NA-C1A	2.61	109.74	106.36
23	C	504	CLA	C4A-NA-C1A	2.61	109.74	106.36
31	b	624	LMG	C7-O1-C1	2.61	119.31	113.82
23	b	614	CLA	CHB-C4A-NA	2.61	128.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C4A-NA-C1A	2.62	109.74	106.36
30	B	626	SQD	O48-C23-C24	2.62	119.88	111.90
27	B	619	BCR	C29-C30-C25	2.62	114.51	110.36
23	c	510	CLA	CMB-C2B-C3B	2.62	130.22	125.09
23	B	604	CLA	C4A-NA-C1A	2.62	109.75	106.36
23	b	610	CLA	O1D-CGD-CBD	2.62	128.38	124.62
29	A	415	LHG	O8-C23-C24	2.62	119.89	111.90
30	b	601	SQD	O48-C23-C24	2.63	119.90	111.90
30	B	626	SQD	O5-C5-C4	2.63	114.61	109.68
23	C	504	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	B	602	CLA	C4A-NA-C1A	2.63	109.76	106.36
23	b	610	CLA	C4A-NA-C1A	2.63	109.76	106.36
23	c	511	CLA	C4A-NA-C1A	2.63	109.76	106.36
23	b	616	CLA	C4A-NA-C1A	2.63	109.76	106.36
23	b	619	CLA	C4A-NA-C1A	2.64	109.77	106.36
23	C	507	CLA	CHB-C4A-NA	2.64	128.16	124.51
31	E	101	LMG	C8-O7-C10	2.64	124.22	117.89
31	i	101	LMG	O1-C1-C2	2.64	111.38	108.04
23	C	508	CLA	CMB-C2B-C3B	2.65	130.26	125.09
23	B	608	CLA	O1D-CGD-CBD	2.65	128.41	124.62
23	c	508	CLA	CMB-C2B-C3B	2.65	130.26	125.09
23	B	609	CLA	CMB-C2B-C3B	2.65	130.26	125.09
23	c	511	CLA	O1D-CGD-CBD	2.65	128.42	124.62
33	i	102	LMT	O1'-C1'-C2'	2.65	111.39	108.04
23	c	502	CLA	C4A-NA-C1A	2.66	109.79	106.36
23	B	608	CLA	CMB-C2B-C3B	2.66	130.29	125.09
31	i	101	LMG	O8-C28-C29	2.66	120.00	111.90
30	f	102	SQD	O5-C5-C4	2.66	114.68	109.68
30	A	413	SQD	O5-C5-C4	2.66	114.68	109.68
23	C	508	CLA	O1D-CGD-CBD	2.66	128.44	124.62
27	B	618	BCR	C29-C30-C25	2.66	114.58	110.36
23	B	606	CLA	CMB-C2B-C3B	2.66	130.30	125.09
23	C	503	CLA	CMB-C2B-C3B	2.66	130.30	125.09
23	c	502	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	b	607	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	b	611	CLA	C4A-NA-C1A	2.67	109.81	106.36
28	b	602	DGD	C1G-O1G-C1A	2.67	124.32	116.85
23	B	608	CLA	C4A-NA-C1A	2.67	109.81	106.36
23	b	606	CLA	CMD-C2D-C3D	2.67	130.31	125.09
23	B	608	CLA	CHB-C4A-NA	2.67	128.21	124.51
23	c	512	CLA	C4A-NA-C1A	2.68	109.82	106.36
23	B	604	CLA	O1D-CGD-CBD	2.68	128.46	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	623	DGD	O2G-C1B-C2B	2.68	117.35	111.53
28	b	602	DGD	O1G-C1A-C2A	2.68	120.06	111.90
23	C	506	CLA	CMB-C2B-C3B	2.68	130.33	125.09
23	b	612	CLA	O1D-CGD-CBD	2.68	128.47	124.62
23	C	513	CLA	CHB-C4A-NA	2.68	128.22	124.51
33	B	628	LMT	O1B-C4'-C3'	2.70	114.12	107.17
23	B	603	CLA	C4A-NA-C1A	2.70	109.84	106.36
30	a	415	SQD	O5-C5-C4	2.70	114.74	109.68
23	B	603	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	b	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
28	c	518	DGD	O6D-C5D-C6D	2.70	112.13	106.61
30	F	102	SQD	C44-O6-C1	2.71	119.50	113.82
31	b	625	LMG	C7-O1-C1	2.71	119.52	113.82
23	b	616	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	C	505	CLA	C4A-NA-C1A	2.71	109.87	106.36
30	a	415	SQD	C44-O6-C1	2.71	119.52	113.82
23	c	509	CLA	CHB-C4A-NA	2.71	128.27	124.51
30	f	102	SQD	O6-C1-C2	2.72	111.47	108.04
30	F	102	SQD	O5-C5-C4	2.72	114.79	109.68
23	C	506	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	C	508	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	B	601	CLA	C4A-NA-C1A	2.73	109.88	106.36
23	d	402	CLA	CMB-C2B-C3B	2.73	130.42	125.09
23	c	504	CLA	CMB-C2B-C3B	2.73	130.42	125.09
28	C	518	DGD	O1G-C1A-C2A	2.73	120.22	111.90
31	D	407	LMG	O8-C28-C29	2.73	120.22	111.90
27	C	516	BCR	C29-C30-C25	2.73	114.69	110.36
23	b	612	CLA	CMB-C2B-C3B	2.73	130.43	125.09
31	d	406	LMG	C3-C4-C5	2.74	114.97	110.20
23	b	619	CLA	CHB-C4A-NA	2.74	128.30	124.51
31	m	102	LMG	O8-C28-C29	2.74	120.26	111.90
23	B	605	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	a	404	CLA	C4A-NA-C1A	2.75	109.91	106.36
23	c	508	CLA	CHB-C4A-NA	2.75	128.32	124.51
23	B	605	CLA	C4A-NA-C1A	2.75	109.92	106.36
27	H	101	BCR	C33-C5-C4	2.75	118.65	113.43
23	b	606	CLA	CMB-C2B-C3B	2.76	130.48	125.09
28	D	409	DGD	O1G-C1A-C2A	2.76	120.32	111.90
23	c	504	CLA	CHB-C4A-NA	2.76	128.34	124.51
27	T	102	BCR	C29-C30-C25	2.77	114.74	110.36
23	c	504	CLA	C4A-NA-C1A	2.77	109.94	106.36
31	D	406	LMG	C3-C4-C5	2.77	115.02	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	C	512	CLA	C4A-NA-C1A	2.77	109.94	106.36
25	D	404	PL9	C40-C39-C41	2.77	119.64	115.41
23	B	607	CLA	CMB-C2B-C3B	2.78	130.52	125.09
23	c	506	CLA	CMB-C2B-C3B	2.78	130.53	125.09
31	B	622	LMG	C7-O1-C1	2.78	119.67	113.82
23	A	407	CLA	CMB-C2B-C3B	2.78	130.53	125.09
27	T	102	BCR	C33-C5-C4	2.78	118.71	113.43
27	c	515	BCR	C29-C30-C25	2.79	114.78	110.36
28	b	602	DGD	O2G-C1B-C2B	2.79	117.60	111.53
23	A	404	CLA	CMB-C2B-C3B	2.79	130.55	125.09
23	B	612	CLA	CMB-C2B-C3B	2.80	130.56	125.09
31	a	402	LMG	O8-C28-C29	2.80	120.42	111.90
23	c	502	CLA	CMD-C2D-C3D	2.80	130.56	125.09
23	b	606	CLA	CHB-C4A-NA	2.80	128.38	124.51
28	C	518	DGD	O6E-C1E-C2E	2.80	116.02	110.28
27	d	405	BCR	C29-C30-C25	2.80	114.80	110.36
27	b	622	BCR	C2-C1-C6	2.80	114.80	110.36
23	c	512	CLA	CHB-C4A-NA	2.81	128.39	124.51
27	B	618	BCR	C33-C5-C4	2.81	118.75	113.43
23	b	617	CLA	C4A-NA-C1A	2.82	110.00	106.36
28	b	602	DGD	C3G-O3G-C1D	2.82	119.74	113.82
23	b	607	CLA	CMB-C2B-C3B	2.82	130.61	125.09
23	b	619	CLA	CMB-C2B-C3B	2.83	130.62	125.09
23	a	406	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	C	504	CLA	CMB-C2B-C3B	2.83	130.62	125.09
27	y	101	BCR	C33-C5-C4	2.83	118.80	113.43
23	C	509	CLA	CHB-C4A-NA	2.84	128.44	124.51
31	I	101	LMG	O8-C28-C29	2.84	120.57	111.90
28	b	623	DGD	O3D-C3D-C4D	2.85	116.75	110.34
31	B	622	LMG	O8-C28-C29	2.85	120.59	111.90
23	a	406	CLA	C4A-NA-C1A	2.86	110.05	106.36
23	b	618	CLA	C4A-NA-C1A	2.86	110.06	106.36
28	d	409	DGD	O1G-C1A-C2A	2.87	120.63	111.90
23	b	617	CLA	CHB-C4A-NA	2.87	128.48	124.51
31	E	101	LMG	O8-C28-C29	2.87	120.65	111.90
31	b	624	LMG	O8-C28-C29	2.87	120.66	111.90
27	D	405	BCR	C38-C26-C27	2.88	118.88	113.43
23	B	614	CLA	CMB-C2B-C3B	2.88	130.72	125.09
34	f	101	HEM	CMD-C2D-C3D	2.88	127.09	114.35
25	J	101	PL9	C20-C19-C21	2.88	119.81	115.41
23	c	509	CLA	C4A-NA-C1A	2.88	110.09	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CMB-C2B-C3B	2.89	130.73	125.09
27	j	102	BCR	C38-C26-C27	2.89	118.90	113.43
23	B	613	CLA	CMB-C2B-C3B	2.89	130.74	125.09
31	e	101	LMG	O8-C28-C29	2.89	120.72	111.90
28	C	519	DGD	O6D-C5D-C6D	2.90	112.53	106.61
31	A	418	LMG	O8-C28-C29	2.90	120.74	111.90
23	b	607	CLA	O2D-CGD-CBD	2.90	115.28	111.30
31	I	101	LMG	O7-C10-C11	2.91	117.84	111.53
28	c	518	DGD	O3G-C1D-C2D	2.91	111.71	108.04
23	B	606	CLA	O1D-CGD-CBD	2.91	128.80	124.62
28	C	519	DGD	O1G-C1A-C2A	2.92	120.80	111.90
27	J	102	BCR	C38-C26-C27	2.93	118.98	113.43
27	T	102	BCR	C2-C1-C6	2.93	115.00	110.36
34	F	101	HEM	CMD-C2D-C3D	2.93	127.31	114.35
27	B	620	BCR	C2-C1-C6	2.93	115.01	110.36
31	d	406	LMG	C7-O1-C1	2.94	119.99	113.82
27	B	618	BCR	C2-C1-C6	2.94	115.02	110.36
31	d	407	LMG	O8-C28-C29	2.94	120.87	111.90
27	B	618	BCR	C38-C26-C27	2.95	119.02	113.43
30	f	102	SQD	C44-O6-C1	2.95	120.01	113.82
23	C	507	CLA	O2D-CGD-CBD	2.95	115.35	111.30
31	A	418	LMG	C7-O1-C1	2.95	120.02	113.82
30	a	415	SQD	O6-C1-C2	2.95	111.77	108.04
31	a	416	LMG	O8-C28-C29	2.96	120.90	111.90
23	c	505	CLA	C4A-NA-C1A	2.96	110.19	106.36
28	c	516	DGD	C1G-O1G-C1A	2.97	125.15	116.85
31	E	101	LMG	O1-C1-C2	2.97	111.79	108.04
23	D	401	CLA	CMB-C2B-C3B	2.97	130.90	125.09
23	b	617	CLA	CMB-C2B-C3B	2.98	130.91	125.09
31	D	407	LMG	O7-C10-C11	2.98	118.00	111.53
31	i	101	LMG	O7-C10-C11	2.98	118.00	111.53
34	V	201	HEM	CMD-C2D-C3D	2.99	127.57	114.35
27	d	405	BCR	C38-C26-C27	2.99	119.10	113.43
31	a	402	LMG	C7-O1-C1	2.99	120.11	113.82
23	C	511	CLA	C4A-NA-C1A	3.00	110.23	106.36
30	D	408	SQD	O5-C5-C4	3.00	115.31	109.68
31	A	418	LMG	O1-C1-C2	3.00	111.83	108.04
28	A	411	DGD	O6D-C5D-C6D	3.00	112.75	106.61
31	e	101	LMG	C7-O1-C1	3.00	120.13	113.82
28	c	518	DGD	O1G-C1A-C2A	3.00	121.05	111.90
23	d	402	CLA	C4A-NA-C1A	3.00	110.24	106.36
30	d	408	SQD	O5-C5-C4	3.01	115.33	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	CLA	O1D-CGD-CBD	3.01	128.94	124.62
31	b	625	LMG	O8-C28-C29	3.01	121.07	111.90
23	B	607	CLA	C4A-NA-C1A	3.01	110.25	106.36
23	d	402	CLA	O1D-CGD-CBD	3.01	128.94	124.62
23	C	507	CLA	CMB-C2B-C3B	3.02	131.00	125.09
31	D	406	LMG	C7-O1-C1	3.03	120.17	113.82
31	d	406	LMG	O8-C28-C29	3.03	121.12	111.90
34	v	201	HEM	CMD-C2D-C3D	3.03	127.74	114.35
28	d	409	DGD	C3G-O3G-C1D	3.04	120.19	113.82
31	c	519	LMG	O8-C28-C29	3.04	121.18	111.90
31	d	407	LMG	O7-C10-C11	3.07	118.19	111.53
31	B	623	LMG	O8-C28-C29	3.07	121.26	111.90
23	d	403	CLA	O2D-CGD-CBD	3.07	115.52	111.30
27	T	102	BCR	C38-C26-C27	3.08	119.26	113.43
31	E	101	LMG	C7-O1-C1	3.08	120.30	113.82
23	B	607	CLA	CHB-C4A-NA	3.09	128.78	124.51
31	C	520	LMG	O8-C28-C29	3.10	121.33	111.90
34	F	101	HEM	C3B-C4B-CHC	3.10	127.53	123.16
23	B	610	CLA	CMB-C2B-C3B	3.11	131.17	125.09
30	A	417	SQD	C1-C2-C3	3.12	116.12	109.97
31	A	418	LMG	C3-C4-C5	3.12	115.63	110.20
28	C	517	DGD	O2G-C1B-C2B	3.12	118.31	111.53
23	b	616	CLA	CMB-C2B-C3B	3.13	131.20	125.09
27	c	514	BCR	C1-C6-C7	3.13	124.58	115.82
31	A	414	LMG	O8-C28-C29	3.13	121.43	111.90
27	B	620	BCR	C33-C5-C4	3.15	119.40	113.43
31	e	101	LMG	O1-C1-C2	3.16	112.04	108.04
30	A	413	SQD	O47-C7-C8	3.17	118.42	111.53
31	A	414	LMG	C7-O1-C1	3.18	120.50	113.82
28	B	621	DGD	O3D-C3D-C4D	3.18	117.50	110.34
27	J	102	BCR	C29-C30-C25	3.18	115.40	110.36
27	C	514	BCR	C1-C6-C7	3.19	124.76	115.82
28	c	516	DGD	O2G-C1B-C2B	3.20	118.48	111.53
30	b	601	SQD	C44-O6-C1	3.20	120.55	113.82
28	B	627	DGD	C3G-O3G-C1D	3.22	120.58	113.82
31	C	521	LMG	O8-C28-C29	3.22	121.71	111.90
27	j	102	BCR	C29-C30-C25	3.23	115.47	110.36
31	D	407	LMG	C7-O1-C1	3.24	120.62	113.82
31	k	103	LMG	O8-C28-C29	3.25	121.82	111.90
23	b	614	CLA	CMB-C2B-C3B	3.26	131.46	125.09
30	A	417	SQD	C44-O6-C1	3.27	120.68	113.82
27	b	622	BCR	C33-C5-C4	3.27	119.63	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	413	DGD	O6D-C5D-C6D	3.27	113.29	106.61
25	D	404	PL9	C25-C24-C26	3.30	120.45	115.41
30	a	401	SQD	O5-C1-C2	3.31	117.07	110.28
29	A	412	LHG	O7-C7-C8	3.32	118.73	111.53
25	J	101	PL9	C25-C24-C26	3.32	120.48	115.41
23	A	405	CLA	O2D-CGD-CBD	3.33	115.86	111.30
30	B	626	SQD	C44-O6-C1	3.33	120.81	113.82
30	a	401	SQD	C1-C2-C3	3.33	116.54	109.97
31	k	103	LMG	O7-C10-C11	3.33	118.77	111.53
29	a	414	LHG	O7-C7-C8	3.34	118.79	111.53
28	c	518	DGD	O5D-C1E-C2E	3.35	112.27	108.04
31	D	406	LMG	O8-C28-C29	3.37	122.16	111.90
31	a	402	LMG	C3-C4-C5	3.38	116.09	110.20
24	D	402	PHO	O1D-CGD-CBD	3.39	129.47	124.62
34	v	201	HEM	CMC-C2C-C3C	3.41	125.04	116.53
34	f	101	HEM	C3B-C4B-CHC	3.41	127.97	123.16
30	A	417	SQD	O5-C1-C2	3.42	117.29	110.28
30	a	415	SQD	C1-O5-C5	3.42	120.39	113.75
24	a	407	PHO	O1D-CGD-CBD	3.43	129.54	124.62
24	a	408	PHO	O1D-CGD-CBD	3.44	129.56	124.62
28	D	409	DGD	O5D-C1E-C2E	3.44	112.39	108.04
34	F	101	HEM	CMB-C2B-C3B	3.46	125.18	116.53
31	C	521	LMG	O1-C1-C2	3.46	112.42	108.04
25	A	408	PL9	C35-C34-C36	3.47	120.71	115.41
25	d	404	PL9	C35-C34-C36	3.47	120.71	115.41
24	A	406	PHO	O1D-CGD-CBD	3.49	129.62	124.62
28	b	602	DGD	C3D-C4D-C5D	3.50	116.30	110.20
28	D	409	DGD	C3G-O3G-C1D	3.50	121.17	113.82
31	M	101	LMG	C3-C4-C5	3.50	116.30	110.20
31	C	520	LMG	O7-C10-C11	3.50	119.14	111.53
30	a	401	SQD	C44-O6-C1	3.51	121.19	113.82
34	f	101	HEM	CMB-C2B-C3B	3.51	125.29	116.53
27	j	102	BCR	C2-C1-C6	3.51	115.92	110.36
28	C	518	DGD	O2G-C1B-C2B	3.52	119.17	111.53
31	c	519	LMG	O1-C1-C2	3.52	112.48	108.04
28	C	518	DGD	O3G-C1D-C2D	3.53	112.50	108.04
30	a	415	SQD	O47-C7-C8	3.54	119.22	111.53
30	A	417	SQD	C1-O5-C5	3.55	120.64	113.75
31	B	622	LMG	O1-C1-C2	3.56	112.53	108.04
27	J	102	BCR	C2-C1-C6	3.57	116.01	110.36
30	a	401	SQD	O5-C5-C4	3.59	116.43	109.68
25	j	101	PL9	C25-C24-C26	3.60	120.90	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	V	201	HEM	CMC-C2C-C3C	3.60	125.51	116.53
30	f	102	SQD	C1-O5-C5	3.60	120.73	113.75
31	c	519	LMG	O7-C10-C11	3.60	119.35	111.53
30	A	417	SQD	O6-C1-C2	3.60	112.59	108.04
28	c	518	DGD	C2G-O2G-C1B	3.62	126.57	117.89
30	A	417	SQD	O5-C5-C4	3.62	116.47	109.68
25	D	404	PL9	C35-C34-C36	3.63	120.94	115.41
28	c	517	DGD	O2G-C1B-C2B	3.63	119.41	111.53
30	a	401	SQD	C1-O5-C5	3.63	120.79	113.75
30	a	401	SQD	O47-C7-C8	3.64	119.44	111.53
31	A	418	LMG	O7-C10-C11	3.65	119.45	111.53
29	a	417	LHG	O7-C7-C8	3.65	119.46	111.53
28	c	516	DGD	O5D-C1E-C2E	3.65	112.66	108.04
28	B	627	DGD	C3D-C4D-C5D	3.65	116.57	110.20
31	a	402	LMG	O7-C10-C11	3.66	119.49	111.53
28	B	627	DGD	O2G-C1B-C2B	3.66	119.49	111.53
31	b	625	LMG	O7-C10-C11	3.67	119.51	111.53
31	D	406	LMG	O7-C10-C11	3.69	119.54	111.53
27	j	102	BCR	C31-C1-C2	3.69	121.99	108.79
27	J	102	BCR	C31-C1-C2	3.70	122.03	108.79
25	A	408	PL9	C25-C24-C26	3.72	121.09	115.41
30	D	408	SQD	C1-O5-C5	3.72	120.97	113.75
30	d	408	SQD	C1-O5-C5	3.72	120.97	113.75
30	A	413	SQD	C1-O5-C5	3.73	120.98	113.75
30	A	417	SQD	O47-C7-C8	3.74	119.67	111.53
28	C	519	DGD	C2G-O2G-C1B	3.75	126.89	117.89
31	C	521	LMG	O7-C10-C11	3.76	119.70	111.53
29	A	415	LHG	O7-C7-C8	3.77	119.72	111.53
31	d	406	LMG	O7-C10-C11	3.78	119.74	111.53
31	a	416	LMG	O7-C10-C11	3.82	119.82	111.53
30	F	102	SQD	C1-O5-C5	3.82	121.16	113.75
30	f	102	SQD	O47-C7-C8	3.83	119.85	111.53
31	A	414	LMG	O7-C10-C11	3.83	119.86	111.53
25	d	404	PL9	C25-C24-C26	3.87	121.31	115.41
25	a	410	PL9	C25-C24-C26	3.89	121.35	115.41
31	B	622	LMG	O7-C10-C11	3.91	120.03	111.53
28	c	517	DGD	O3G-C1D-C2D	3.93	113.01	108.04
31	M	101	LMG	O7-C10-C11	3.94	120.09	111.53
31	m	102	LMG	O7-C10-C11	3.94	120.10	111.53
34	v	201	HEM	CAD-C3D-C4D	3.95	126.39	112.47
27	c	514	BCR	C8-C7-C6	3.95	139.18	127.32
31	b	624	LMG	O7-C10-C11	3.95	120.12	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	F	102	SQD	O47-C7-C8	3.96	120.12	111.53
28	a	413	DGD	O2G-C1B-C2B	3.96	120.13	111.53
28	D	409	DGD	O2D-C2D-C1D	3.96	118.71	110.02
30	D	408	SQD	O47-C7-C8	3.98	120.18	111.53
31	m	102	LMG	C3-C4-C5	3.99	117.16	110.20
31	B	623	LMG	O7-C10-C11	4.00	120.22	111.53
25	a	410	PL9	C35-C34-C36	4.00	121.52	115.41
30	f	102	SQD	O9-S-C6	4.01	110.32	106.94
31	B	623	LMG	O1-C1-C2	4.02	113.12	108.04
28	A	411	DGD	O2G-C1B-C2B	4.03	120.29	111.53
34	F	101	HEM	CAD-C3D-C4D	4.05	126.75	112.47
30	d	408	SQD	O7-S-C6	4.05	110.36	106.94
28	C	519	DGD	O5D-C1E-C2E	4.06	113.17	108.04
34	f	101	HEM	CAD-C3D-C4D	4.08	126.86	112.47
28	d	409	DGD	O5D-C1E-C2E	4.10	113.22	108.04
34	V	201	HEM	CAD-C3D-C4D	4.11	126.96	112.47
28	C	517	DGD	O5D-C1E-C2E	4.16	113.29	108.04
27	C	514	BCR	C8-C7-C6	4.18	139.88	127.32
31	b	625	LMG	O1-C1-C2	4.19	113.33	108.04
28	d	409	DGD	O2D-C2D-C1D	4.23	119.30	110.02
28	b	602	DGD	O5D-C1E-C2E	4.23	113.39	108.04
31	a	416	LMG	C7-O1-C1	4.26	122.77	113.82
30	d	408	SQD	O47-C7-C8	4.28	120.83	111.53
30	a	401	SQD	O6-C1-C2	4.44	113.64	108.04
34	V	201	HEM	CMB-C2B-C3B	4.49	127.73	116.53
34	v	201	HEM	CMB-C2B-C3B	4.53	127.84	116.53
34	f	101	HEM	CMC-C2C-C3C	4.69	128.24	116.53
34	F	101	HEM	CMC-C2C-C3C	4.71	128.28	116.53
30	B	626	SQD	O9-S-C6	4.80	110.98	106.94
30	D	408	SQD	O7-S-C6	4.84	111.02	106.94
30	d	408	SQD	C44-O6-C1	4.93	124.17	113.82
34	f	101	HEM	CAD-C3D-C2D	5.01	127.63	113.22
30	A	413	SQD	O7-S-C6	5.08	111.23	106.94
31	D	407	LMG	O1-C1-C2	5.11	114.49	108.04
28	C	519	DGD	C3G-O3G-C1D	5.11	124.56	113.82
34	V	201	HEM	CAD-C3D-C2D	5.13	127.96	113.22
34	F	101	HEM	CAD-C3D-C2D	5.14	127.98	113.22
28	B	627	DGD	O5D-C1E-C2E	5.14	114.53	108.04
34	v	201	HEM	CAD-C3D-C2D	5.20	128.17	113.22
30	D	408	SQD	C44-O6-C1	5.21	124.76	113.82
28	a	413	DGD	C3G-O3G-C1D	5.36	125.08	113.82
30	a	401	SQD	O7-S-C6	5.37	111.47	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	417	SQD	O7-S-C6	5.38	111.47	106.94
28	A	411	DGD	C3G-O3G-C1D	5.53	125.44	113.82
30	a	415	SQD	O9-S-C6	5.54	111.61	106.94
31	d	407	LMG	O1-C1-C2	5.54	115.04	108.04
30	b	601	SQD	O9-S-C6	5.55	111.62	106.94
30	a	415	SQD	O7-S-C6	5.62	111.68	106.94
28	c	518	DGD	C3G-O3G-C1D	5.64	125.67	113.82
30	F	102	SQD	O9-S-C6	5.73	111.77	106.94
30	A	413	SQD	O9-S-C6	5.80	111.83	106.94
30	F	102	SQD	O7-S-C6	5.80	111.83	106.94
30	D	408	SQD	O9-S-C6	5.88	111.90	106.94
28	d	409	DGD	O3G-C1D-C2D	6.51	116.26	108.04
27	J	102	BCR	C31-C1-C6	6.54	120.55	110.30
30	d	408	SQD	O9-S-C6	6.58	112.49	106.94
30	B	626	SQD	O7-S-C6	6.59	112.50	106.94
27	j	102	BCR	C31-C1-C6	6.60	120.66	110.30
28	D	409	DGD	O3G-C1D-C2D	6.75	116.57	108.04
30	f	102	SQD	O7-S-C6	6.84	112.71	106.94
30	b	601	SQD	O7-S-C6	7.12	112.94	106.94
30	d	408	SQD	O6-C1-C2	7.44	117.43	108.04
30	D	408	SQD	O6-C1-C2	7.74	117.82	108.04
27	c	514	BCR	C7-C8-C9	8.04	138.47	126.22
27	C	514	BCR	C7-C8-C9	8.25	138.79	126.22

All (210) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	616	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	c	502	CLA	NC
23	c	502	CLA	ND
23	c	502	CLA	NA
23	b	618	CLA	NC
23	b	618	CLA	ND
23	b	618	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA

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Mol	Chain	Res	Type	Atom
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	b	620	CLA	NC
23	b	620	CLA	ND
23	b	620	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	ND
23	a	405	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	601	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	D	403	CLA	NC
23	D	403	CLA	ND
23	D	403	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	ND
23	b	617	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	503	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	c	509	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	a	404	CLA	NC
23	a	404	CLA	ND
23	a	404	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	C	506	CLA	NC
23	C	506	CLA	ND
23	C	506	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND
23	b	612	CLA	NA
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	B	609	CLA	NC
23	B	609	CLA	ND
23	B	609	CLA	NA
23	c	501	CLA	NC
23	c	501	CLA	ND
23	c	501	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	ND
23	a	406	CLA	NA

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Mol	Chain	Res	Type	Atom
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	505	CLA	NA
23	D	401	CLA	NC
23	D	401	CLA	ND
23	D	401	CLA	NA
23	A	403	CLA	NC
23	A	403	CLA	ND
23	A	403	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA

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Mol	Chain	Res	Type	Atom
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	d	402	CLA	NC
23	d	402	CLA	ND
23	d	402	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	ND
23	A	407	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	609	CLA	NA
23	C	501	CLA	NC
23	C	501	CLA	ND
23	C	501	CLA	NA

All (12) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
30	d	408	SQD	C45-O47-C7-C8

There are no ring outliers.

85 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	403	CLA	12	0
23	A	404	CLA	23	0
23	A	405	CLA	15	0
24	A	406	PHO	5	0
23	A	407	CLA	2	0
25	A	408	PL9	2	0
27	A	410	BCR	7	0
28	A	411	DGD	1	0
29	A	412	LHG	4	0
30	A	413	SQD	5	0
31	A	414	LMG	3	0
29	A	415	LHG	3	0
30	A	417	SQD	7	0
31	A	418	LMG	2	0
23	B	601	CLA	2	0
23	B	602	CLA	6	0
23	B	603	CLA	14	0
23	B	604	CLA	9	0
23	B	605	CLA	13	0
23	B	606	CLA	12	0
23	B	607	CLA	19	0
23	B	608	CLA	12	0
23	B	609	CLA	16	0
23	B	610	CLA	6	0
23	B	611	CLA	9	0
23	B	612	CLA	13	0
23	B	613	CLA	13	0
23	B	614	CLA	5	0
23	B	615	CLA	2	0
23	B	616	CLA	7	0
27	B	617	BCR	4	0
27	B	618	BCR	10	0
27	B	619	BCR	6	0
27	B	620	BCR	4	0
31	B	622	LMG	3	0
31	B	623	LMG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	624	LMT	1	0
30	B	626	SQD	2	0
28	B	627	DGD	2	0
33	B	628	LMT	2	0
33	B	629	LMT	2	0
23	C	501	CLA	7	0
23	C	502	CLA	2	0
23	C	503	CLA	6	0
23	C	504	CLA	7	0
23	C	505	CLA	6	0
23	C	506	CLA	4	0
23	C	507	CLA	9	0
23	C	508	CLA	4	0
23	C	509	CLA	3	0
23	C	510	CLA	9	0
23	C	511	CLA	11	0
23	C	512	CLA	5	0
23	C	513	CLA	4	0
27	C	514	BCR	9	0
27	C	515	BCR	8	0
27	C	516	BCR	5	0
28	C	517	DGD	8	0
28	C	518	DGD	8	0
28	C	519	DGD	5	0
31	C	520	LMG	3	0
31	C	521	LMG	2	0
23	D	401	CLA	7	0
24	D	402	PHO	6	0
23	D	403	CLA	3	0
25	D	404	PL9	12	0
27	D	405	BCR	3	0
31	D	406	LMG	2	0
31	D	407	LMG	6	0
30	D	408	SQD	5	0
28	D	409	DGD	2	0
33	D	410	LMT	1	0
31	E	101	LMG	1	0
34	F	101	HEM	5	0
30	F	102	SQD	2	0
27	H	101	BCR	7	0
31	I	101	LMG	2	0
33	I	102	LMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	J	101	PL9	1	0
27	J	102	BCR	4	0
31	M	101	LMG	2	0
33	M	102	LMT	1	0
27	T	101	BCR	6	0
27	T	102	BCR	6	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	335/360 (93%)	0.16	10 (2%) 54 48	43, 64, 104, 149	0
1	a	335/360 (93%)	-0.07	4 (1%) 81 75	44, 65, 106, 149	0
2	B	490/510 (96%)	0.40	30 (6%) 25 25	46, 69, 103, 159	0
2	b	490/510 (96%)	0.36	35 (7%) 19 21	47, 71, 104, 159	0
3	C	447/461 (96%)	0.11	7 (1%) 74 68	54, 79, 106, 132	0
3	c	447/461 (96%)	0.26	12 (2%) 58 53	56, 81, 105, 135	0
4	D	340/352 (96%)	0.01	5 (1%) 76 70	44, 66, 103, 137	0
4	d	340/352 (96%)	-0.04	2 (0%) 90 87	45, 66, 102, 134	0
5	E	82/84 (97%)	0.12	2 (2%) 62 57	68, 92, 125, 130	0
5	e	82/84 (97%)	0.44	4 (4%) 33 32	70, 92, 125, 129	0
6	F	35/45 (77%)	0.08	2 (5%) 27 27	68, 84, 119, 139	0
6	f	35/45 (77%)	0.40	1 (2%) 55 50	73, 85, 120, 141	0
7	H	65/66 (98%)	0.87	10 (15%) 3 8	77, 94, 122, 138	0
7	h	65/66 (98%)	0.65	5 (7%) 16 19	73, 93, 120, 144	0
8	I	35/38 (92%)	0.21	1 (2%) 55 50	65, 79, 107, 118	0
8	i	35/38 (92%)	0.09	0 100 100	66, 81, 106, 120	0
9	J	34/40 (85%)	0.06	1 (2%) 55 50	69, 85, 95, 112	0
9	j	34/40 (85%)	-0.21	1 (2%) 55 50	74, 88, 95, 116	0
10	K	37/46 (80%)	0.19	1 (2%) 58 53	77, 87, 101, 122	0
10	k	37/46 (80%)	0.33	3 (8%) 15 18	73, 88, 108, 123	0
11	L	37/37 (100%)	0.04	0 100 100	48, 62, 128, 156	0
11	l	37/37 (100%)	-0.08	0 100 100	52, 60, 126, 158	0
12	M	34/36 (94%)	0.14	2 (5%) 26 26	56, 71, 110, 164	0
12	m	34/36 (94%)	0.30	3 (8%) 12 16	55, 69, 108, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.91	35 (14%) 3 9	50, 78, 122, 169	0
13	o	243/272 (89%)	0.67	22 (9%) 11 15	52, 78, 121, 167	0
14	T	32/32 (100%)	0.32	5 (15%) 3 8	55, 67, 158, 174	0
14	t	32/32 (100%)	-0.04	0 100 100	54, 69, 159, 168	0
15	U	97/134 (72%)	1.02	12 (12%) 5 11	56, 71, 92, 108	0
15	u	97/134 (72%)	0.83	6 (6%) 24 24	55, 71, 91, 111	0
16	V	137/163 (84%)	0.39	8 (5%) 26 27	53, 71, 86, 101	0
16	v	137/163 (84%)	0.81	12 (8%) 12 16	59, 72, 88, 95	0
17	g	28/46 (60%)	0.88	6 (21%) 1 6	95, 108, 126, 132	0
17	y	28/46 (60%)	0.35	1 (3%) 46 43	89, 107, 126, 131	0
18	X	37/41 (90%)	1.04	8 (21%) 1 6	76, 93, 124, 140	0
18	x	37/41 (90%)	1.03	10 (27%) 1 5	75, 90, 126, 141	0
19	Z	62/62 (100%)	1.18	10 (16%) 3 8	87, 104, 168, 185	0
19	z	62/62 (100%)	0.79	4 (6%) 22 23	88, 105, 172, 187	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.33	280 (5%) 29 30	43, 75, 115, 187	0

All (280) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	170	GLY	6.1
2	B	129	GLY	5.7
10	k	14	ALA	4.4
13	o	84	ASN	4.4
15	U	54	LYS	4.3
2	b	483	ASP	4.2
7	H	2	ALA	4.0
4	d	295	SER	4.0
15	U	113	THR	3.9
15	u	107	GLU	3.8
13	O	90	GLU	3.8
7	H	4	ARG	3.7
2	B	128	THR	3.7
2	B	378	LYS	3.7
14	T	28	ARG	3.6
13	o	46	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	130	GLU	3.6
2	B	379	ALA	3.6
18	X	47	GLN	3.5
2	b	482	ILE	3.5
2	b	302	TRP	3.5
13	o	30	THR	3.5
14	T	31	LYS	3.5
1	A	11	ALA	3.4
19	Z	62	VAL	3.4
7	H	64	ALA	3.4
19	z	1	MET	3.4
13	O	157	PRO	3.3
2	B	294	SER	3.3
16	v	131	ARG	3.3
13	O	269	ILE	3.3
18	x	47	GLN	3.3
2	b	405	GLU	3.3
5	e	84	LYS	3.3
2	b	70	GLY	3.3
2	B	127	ARG	3.3
2	B	132	ALA	3.2
3	C	183	GLY	3.2
13	O	223	ILE	3.2
3	C	184	GLY	3.2
2	b	407	ASN	3.2
1	A	16	ARG	3.2
13	O	169	LYS	3.2
3	C	27	ASP	3.2
13	o	171	GLU	3.2
18	X	46	VAL	3.1
13	o	221	GLY	3.1
2	B	402	TYR	3.1
10	k	13	GLU	3.1
1	A	15	GLU	3.1
3	c	372	PRO	3.1
13	O	84	ASN	3.1
2	B	133	LEU	3.1
15	U	53	GLU	3.0
13	O	79	LYS	3.0
1	A	229	GLU	3.0
18	x	13	THR	3.0
9	j	7	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
19	Z	34	ASP	3.0
2	b	409	GLN	3.0
7	H	5	THR	3.0
1	A	12	ASN	3.0
2	B	477	ASP	3.0
1	A	10	SER	3.0
2	b	484	PRO	2.9
15	U	38	GLU	2.9
2	b	304	ALA	2.9
15	U	55	ILE	2.9
13	o	47	THR	2.9
19	Z	1	MET	2.9
13	O	222	GLN	2.9
13	O	119	LEU	2.9
13	o	55	ALA	2.9
15	u	113	THR	2.9
7	h	24	GLY	2.9
7	H	18	TYR	2.9
2	b	393	GLU	2.9
13	O	245	GLN	2.8
13	O	155	THR	2.8
2	b	294	SER	2.8
13	O	220	LYS	2.8
1	A	230	THR	2.8
17	y	42	ARG	2.8
3	C	332	GLN	2.8
1	a	80	GLY	2.8
13	o	158	ASN	2.8
17	g	27	MET	2.7
2	B	190	PHE	2.7
19	Z	54	VAL	2.7
18	x	11	THR	2.7
13	O	258	GLU	2.7
4	D	295	SER	2.7
18	X	17	LYS	2.7
4	d	227	GLU	2.7
13	o	32	THR	2.7
2	B	293	ALA	2.7
2	B	476	ARG	2.7
13	o	31	LEU	2.7
13	O	126	GLY	2.6
2	b	339	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	490	GLN	2.6
13	O	107	ILE	2.6
13	O	49	ASP	2.6
13	O	168	PHE	2.6
4	D	21	TRP	2.6
2	b	194	ASN	2.6
19	z	4	LEU	2.6
13	O	87	GLN	2.6
2	B	189	GLY	2.6
16	v	103	LYS	2.6
18	x	16	LEU	2.6
18	x	42	GLN	2.5
13	O	244	GLU	2.5
13	o	225	LEU	2.5
3	c	147	PHE	2.5
2	b	489	GLU	2.5
16	V	28	GLU	2.5
15	u	114	VAL	2.5
3	C	145	SER	2.5
7	H	66	GLY	2.5
2	b	408	GLY	2.5
19	Z	56	VAL	2.5
13	O	54	GLY	2.5
2	B	188	ASP	2.5
17	g	29	GLY	2.5
19	Z	57	LEU	2.5
2	b	403	GLY	2.5
12	m	5	GLN	2.5
2	B	295	GLY	2.5
13	O	171	GLU	2.5
17	g	21	GLN	2.5
13	O	50	ASP	2.5
15	U	112	PHE	2.5
16	v	44	THR	2.5
5	e	56	TYR	2.5
5	e	8	ARG	2.5
3	c	142	GLU	2.5
2	b	379	ALA	2.5
3	c	184	GLY	2.5
2	B	131	PRO	2.4
2	b	327	THR	2.4
2	b	404	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
18	x	46	VAL	2.4
3	C	28	GLN	2.4
7	H	63	LYS	2.4
13	O	89	ALA	2.4
15	U	50	ALA	2.4
16	v	27	ALA	2.4
18	x	20	PHE	2.4
3	C	258	GLY	2.4
13	O	221	GLY	2.4
13	o	238	ALA	2.4
18	x	12	ILE	2.4
2	B	347	ARG	2.4
13	o	229	LYS	2.4
16	v	93	ASP	2.4
2	b	340	TRP	2.4
15	U	123	GLU	2.4
16	V	96	GLU	2.4
3	c	144	SER	2.4
2	B	368	VAL	2.4
1	a	81	ALA	2.4
17	g	26	ALA	2.4
2	b	338	GLN	2.4
13	o	51	THR	2.4
3	c	146	PHE	2.4
2	B	162	PHE	2.4
16	v	130	MET	2.3
6	F	14	PRO	2.3
18	X	45	LYS	2.3
18	x	17	LYS	2.3
17	g	24	MET	2.3
13	O	156	GLN	2.3
7	h	4	ARG	2.3
2	B	121	GLU	2.3
2	B	478	VAL	2.3
13	O	48	LEU	2.3
12	M	2	GLU	2.3
13	o	168	PHE	2.3
1	A	242	GLU	2.3
13	o	228	ALA	2.3
16	v	36	VAL	2.3
3	c	373	ASN	2.3
15	U	39	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
7	h	66	GLY	2.3
15	u	106	ARG	2.3
10	k	15	TYR	2.3
3	c	363	GLY	2.3
1	A	14	TRP	2.3
13	o	49	ASP	2.3
12	m	7	GLY	2.3
16	V	49	GLU	2.3
2	B	353	GLU	2.2
7	H	3	ARG	2.2
14	T	29	ILE	2.2
12	m	4	ASN	2.2
16	V	77	SER	2.2
2	b	301	ALA	2.2
16	V	37	PRO	2.2
16	v	132	ASN	2.2
18	X	11	THR	2.2
2	b	84	THR	2.2
2	b	303	SER	2.2
2	b	297	THR	2.2
13	o	90	GLU	2.2
1	a	226	GLU	2.2
3	c	389	GLU	2.2
13	o	226	ASN	2.2
19	z	34	ASP	2.2
2	b	406	LEU	2.2
13	O	88	GLU	2.2
15	u	108	ASN	2.2
13	O	127	ILE	2.2
18	X	12	ILE	2.2
16	V	111	GLU	2.2
5	E	74	GLN	2.2
2	B	487	SER	2.2
2	b	295	GLY	2.1
9	J	7	ARG	2.1
14	T	27	PRO	2.1
19	Z	35	ARG	2.1
12	M	34	LYS	2.1
15	u	115	THR	2.1
16	v	31	PRO	2.1
2	B	126	PRO	2.1
4	D	24	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	b	378	LYS	2.1
3	c	145	SER	2.1
16	V	43	LYS	2.1
19	Z	38	GLN	2.1
7	h	27	THR	2.1
2	B	474	LEU	2.1
2	b	402	TYR	2.1
4	D	14	TRP	2.1
8	I	34	ARG	2.1
10	K	14	ALA	2.1
5	e	54	SER	2.1
18	X	13	THR	2.1
16	v	142	ALA	2.1
6	F	11	VAL	2.1
18	x	45	LYS	2.1
19	z	61	VAL	2.1
14	T	30	THR	2.1
1	a	75	ASN	2.1
7	H	9	ASP	2.1
2	b	373	LYS	2.1
15	U	65	PHE	2.1
13	O	55	ALA	2.1
13	O	113	VAL	2.1
2	B	488	PRO	2.1
2	b	305	ILE	2.1
2	B	124	ARG	2.1
13	o	152	VAL	2.1
2	b	296	ALA	2.1
2	b	300	GLU	2.1
5	E	57	ALA	2.1
13	o	220	LYS	2.1
7	h	26	GLY	2.1
19	Z	61	VAL	2.1
19	Z	45	GLY	2.1
13	O	116	ASP	2.1
16	v	145	ILE	2.1
1	A	13	LEU	2.0
13	O	58	ILE	2.0
16	V	40	SER	2.0
13	O	66	ILE	2.0
15	U	40	VAL	2.0
6	f	15	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
7	H	8	GLY	2.0
15	U	91	VAL	2.0
16	v	139	VAL	2.0
17	g	31	ALA	2.0
2	b	310	ALA	2.0
18	X	20	PHE	2.0
13	O	111	LEU	2.0
3	c	182	PHE	2.0
13	o	89	ALA	2.0
2	b	306	PRO	2.0
3	c	116	VAL	2.0
4	D	307	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
33	LMT	i	102	35/35	0.38	1.07	8.40	99,137,146,152	0
25	PL9	J	101	35/55	0.29	0.53	6.13	119,157,178,182	0
27	BCR	B	620	40/40	0.57	0.94	5.94	75,86,98,103	0
32	CL	A	416	1/1	0.44	1.00	5.65	49,49,49,49	0
27	BCR	C	514	40/40	0.84	1.01	4.74	73,80,87,94	0
27	BCR	c	514	40/40	0.80	1.11	4.58	76,82,88,89	0
27	BCR	z	101	40/40	0.67	1.31	4.55	86,96,112,115	0
31	LMG	C	521	45/55	0.33	1.12	4.29	84,119,143,175	0
33	LMT	B	629	35/35	0.48	0.67	4.22	70,137,165,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	DGD	D	409	63/66	0.56	0.74	4.05	104,127,181,188	0
23	CLA	b	605	65/65	0.50	0.91	4.01	88,108,124,137	0
31	LMG	c	519	45/55	0.55	0.97	3.91	86,119,142,171	0
33	LMT	b	627	35/35	0.56	0.88	3.73	100,140,152,154	0
23	CLA	C	513	65/65	0.75	0.92	3.68	95,109,142,149	0
27	BCR	C	515	40/40	0.80	1.03	3.65	85,92,115,116	0
23	CLA	c	511	65/65	0.82	0.69	3.57	75,91,102,108	0
28	DGD	d	409	63/66	0.59	0.62	3.54	106,128,181,190	0
22	BCT	d	401	4/4	0.86	0.48	3.49	87,91,92,94	0
27	BCR	j	102	40/40	0.49	0.51	3.47	110,128,180,184	0
33	LMT	I	102	35/35	0.65	0.68	3.46	99,135,144,145	0
23	CLA	B	612	65/65	0.90	0.51	3.44	61,72,82,86	0
23	CLA	c	507	65/65	0.82	0.66	3.40	83,93,105,111	0
23	CLA	b	607	65/65	0.83	0.78	3.37	68,82,92,103	0
27	BCR	b	622	40/40	0.66	0.65	3.37	72,83,94,96	0
23	CLA	c	501	65/65	0.85	0.81	3.36	67,82,92,94	0
23	CLA	c	513	65/65	0.66	1.06	3.31	93,109,142,148	0
23	CLA	D	403	65/65	0.86	0.87	3.30	74,87,123,124	0
31	LMG	E	101	44/55	0.45	0.66	3.29	87,123,132,139	0
27	BCR	y	101	40/40	0.68	0.78	3.25	79,86,106,109	0
33	LMT	D	410	31/35	0.60	0.95	3.25	83,133,154,159	0
33	LMT	B	625	35/35	0.72	0.76	3.21	95,139,149,152	0
23	CLA	c	503	65/65	0.83	0.81	3.14	77,89,97,103	0
23	CLA	B	601	65/65	0.53	1.00	3.09	92,108,131,137	0
23	CLA	B	604	65/65	0.83	0.58	3.07	59,67,104,124	0
28	DGD	B	627	52/66	0.72	0.50	3.05	75,105,178,180	0
23	CLA	B	609	65/65	0.90	0.73	3.05	74,89,104,106	0
23	CLA	c	512	65/65	0.77	1.05	2.97	83,104,146,152	0
23	CLA	C	512	65/65	0.83	0.84	2.97	89,101,144,149	0
27	BCR	c	515	40/40	0.78	0.79	2.93	75,86,95,101	0
27	BCR	H	101	40/40	0.70	1.03	2.90	83,96,130,131	0
23	CLA	B	605	65/65	0.87	0.66	2.89	58,78,86,92	0
31	LMG	i	101	43/55	0.72	0.67	2.78	84,120,162,177	0
30	SQD	d	408	43/54	0.64	0.74	2.73	67,109,152,157	0
33	LMT	B	628	35/35	0.39	0.62	2.70	72,126,141,144	0
23	CLA	b	613	65/65	0.81	0.73	2.68	65,93,104,114	0
33	LMT	d	410	31/35	0.39	0.87	2.68	83,134,157,157	0
23	CLA	C	509	65/65	0.86	0.63	2.60	62,81,95,98	0
31	LMG	a	402	42/55	0.66	0.51	2.56	72,100,119,143	0
23	CLA	B	610	65/65	0.84	0.68	2.44	69,81,88,92	0
23	CLA	A	407	65/65	0.84	0.49	2.31	56,66,127,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	B	603	65/65	0.89	0.66	2.27	65,81,94,109	0
33	LMT	b	603	35/35	0.61	0.48	2.26	73,119,136,138	0
31	LMG	I	101	43/55	0.74	0.56	2.24	73,118,166,178	0
33	LMT	b	604	35/35	0.68	0.49	2.24	69,133,158,160	0
25	PL9	j	101	35/55	0.32	0.43	2.21	120,160,178,182	0
32	CL	a	418	1/1	0.78	0.48	2.20	49,49,49,49	0
23	CLA	b	612	65/65	0.80	0.51	2.18	63,75,95,98	0
23	CLA	b	619	65/65	0.81	0.59	2.18	85,97,108,116	0
23	CLA	b	609	65/65	0.87	0.51	2.17	61,76,84,88	0
27	BCR	k	102	40/40	0.63	0.78	2.15	72,80,109,111	0
23	CLA	d	403	65/65	0.83	0.67	2.13	72,88,121,128	0
23	CLA	B	608	65/65	0.79	0.64	2.12	64,75,93,97	0
27	BCR	a	412	40/40	0.73	0.42	2.10	54,71,84,87	0
23	CLA	c	509	65/65	0.85	0.53	2.08	67,85,91,97	0
27	BCR	D	405	40/40	0.63	0.53	2.08	68,81,105,110	0
30	SQD	B	626	47/54	0.68	0.42	2.07	75,100,144,148	0
23	CLA	C	501	65/65	0.86	0.47	2.05	69,82,90,95	0
23	CLA	b	608	65/65	0.84	0.40	1.91	61,68,107,117	0
29	LHG	A	415	37/49	0.61	0.59	1.89	104,133,190,202	0
27	BCR	h	101	40/40	0.73	0.94	1.86	85,94,124,127	0
23	CLA	b	614	65/65	0.84	0.60	1.84	66,82,88,91	0
23	CLA	C	507	65/65	0.74	0.66	1.81	79,93,100,104	0
23	CLA	a	409	65/65	0.81	0.46	1.80	55,67,129,133	0
29	LHG	a	417	37/49	0.70	0.38	1.79	110,135,197,206	0
23	CLA	B	606	65/65	0.79	0.72	1.70	67,81,110,121	0
30	SQD	F	102	45/54	0.69	0.77	1.70	87,127,149,152	0
30	SQD	f	102	45/54	0.75	0.59	1.69	88,133,148,152	0
30	SQD	D	408	43/54	0.72	0.67	1.67	71,103,148,152	0
25	PL9	a	410	45/55	0.64	0.46	1.65	82,103,121,125	0
30	SQD	b	601	47/54	0.68	0.41	1.65	81,103,147,151	0
31	LMG	A	418	42/55	0.62	0.44	1.61	81,105,123,147	0
23	CLA	b	620	65/65	0.71	0.59	1.60	75,98,145,147	0
24	PHO	A	406	64/64	0.84	0.37	1.58	50,69,77,81	0
25	PL9	A	408	45/55	0.67	0.48	1.57	89,101,119,127	0
30	SQD	A	413	51/54	0.73	0.40	1.50	81,99,128,131	0
23	CLA	c	502	65/65	0.68	0.61	1.49	63,75,100,106	0
23	CLA	B	615	65/65	0.82	0.83	1.47	83,96,106,116	0
27	BCR	C	516	40/40	0.75	0.57	1.43	74,86,95,100	0
27	BCR	J	102	40/40	0.58	0.45	1.39	108,125,177,180	0
23	CLA	B	602	65/65	0.79	0.63	1.35	68,87,95,96	0
28	DGD	C	519	66/66	0.66	0.44	1.31	55,72,100,114	0
23	CLA	C	502	65/65	0.79	0.50	1.24	59,75,108,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	C	503	65/65	0.87	0.50	1.22	71,88,99,105	0
23	CLA	C	506	65/65	0.67	0.61	1.17	79,91,125,133	0
23	CLA	b	616	65/65	0.91	0.34	1.16	61,73,83,86	0
23	CLA	b	606	65/65	0.86	0.47	1.14	70,87,96,97	0
23	CLA	c	506	65/65	0.79	0.49	1.14	78,92,122,128	0
23	CLA	C	510	65/65	0.79	0.38	1.10	67,74,83,93	0
27	BCR	A	410	40/40	0.70	0.47	1.09	52,68,85,90	0
31	LMG	M	101	42/55	0.74	0.35	1.07	83,111,135,144	0
31	LMG	d	407	48/55	0.82	0.36	1.00	58,70,85,120	0
27	BCR	d	405	40/40	0.77	0.38	1.00	69,82,102,106	0
27	BCR	B	618	40/40	0.62	0.36	0.98	75,82,94,95	0
28	DGD	a	413	56/66	0.75	0.38	0.97	76,100,145,148	0
28	DGD	A	411	56/66	0.71	0.38	0.95	77,102,146,153	0
30	SQD	A	417	54/54	0.78	0.37	0.94	77,113,147,154	0
23	CLA	C	504	65/65	0.77	0.36	0.89	62,83,138,145	0
23	CLA	c	510	65/65	0.90	0.42	0.89	67,75,84,89	0
23	CLA	c	508	65/65	0.90	0.36	0.87	70,85,118,134	0
23	CLA	C	511	65/65	0.80	0.55	0.87	74,88,102,109	0
23	CLA	d	402	65/65	0.84	0.36	0.84	49,57,81,95	0
28	DGD	B	621	58/66	0.85	0.38	0.80	46,71,101,105	0
23	CLA	B	616	65/65	0.69	0.72	0.80	79,93,147,152	0
27	BCR	B	619	40/40	0.71	0.34	0.80	62,75,83,86	0
23	CLA	b	610	65/65	0.87	0.53	0.79	70,83,112,126	0
29	LHG	a	414	39/49	0.79	0.41	0.79	60,78,94,102	0
23	CLA	c	504	65/65	0.82	0.34	0.79	75,83,133,138	0
34	HEM	V	201	43/43	0.85	0.47	0.76	58,69,74,76	0
30	SQD	a	401	54/54	0.75	0.42	0.75	76,114,149,152	0
34	HEM	F	101	43/43	0.88	0.45	0.74	89,105,127,130	0
23	CLA	c	505	65/65	0.82	0.35	0.72	70,77,83,85	0
27	BCR	B	617	40/40	0.78	0.33	0.63	67,74,81,84	0
31	LMG	m	102	42/55	0.77	0.38	0.61	73,111,128,138	0
28	DGD	c	518	66/66	0.76	0.34	0.61	54,73,105,118	0
33	LMT	M	102	35/35	0.82	0.51	0.60	69,96,112,115	0
28	DGD	b	602	52/66	0.80	0.41	0.57	79,107,180,186	0
26	OEC	A	409	5/9	0.94	0.43	0.55	35,44,57,62	0
23	CLA	C	505	65/65	0.78	0.41	0.53	69,77,86,91	0
24	PHO	a	408	64/64	0.86	0.33	0.52	58,68,79,86	0
28	DGD	b	623	58/66	0.80	0.36	0.52	57,74,99,107	0
23	CLA	B	614	65/65	0.73	0.41	0.51	63,83,125,129	0
23	CLA	a	406	65/65	0.79	0.36	0.48	55,71,140,147	0
23	CLA	a	404	65/65	0.90	0.33	0.44	53,60,67,74	0
34	HEM	f	101	43/43	0.89	0.50	0.43	89,105,124,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	b	618	65/65	0.82	0.32	0.43	60,82,123,130	0
31	LMG	k	103	48/55	0.74	0.43	0.43	79,100,112,115	0
28	DGD	c	517	62/66	0.84	0.31	0.40	64,84,132,141	0
29	LHG	A	412	39/49	0.82	0.29	0.39	59,79,89,93	0
27	BCR	T	102	40/40	0.72	0.33	0.38	71,79,86,86	0
34	HEM	v	201	43/43	0.84	0.51	0.35	57,68,75,76	0
30	SQD	a	415	51/54	0.71	0.39	0.32	88,101,128,129	0
31	LMG	e	101	44/55	0.66	0.44	0.32	91,122,132,136	0
23	CLA	B	613	65/65	0.86	0.30	0.31	46,64,88,93	0
31	LMG	D	406	46/55	0.80	0.33	0.30	58,73,116,129	0
25	PL9	d	404	55/55	0.75	0.32	0.29	45,65,78,85	0
31	LMG	a	416	51/55	0.80	0.33	0.28	62,80,93,100	0
28	DGD	C	518	62/66	0.82	0.34	0.27	58,81,134,144	0
23	CLA	b	617	65/65	0.92	0.27	0.22	57,67,91,93	0
23	CLA	A	403	65/65	0.91	0.28	0.18	52,58,66,70	0
25	PL9	D	404	55/55	0.77	0.32	0.15	42,61,71,77	0
31	LMG	B	622	49/55	0.75	0.33	0.15	61,79,105,117	0
28	DGD	C	517	53/66	0.87	0.29	0.14	61,79,96,101	0
28	DGD	c	516	53/66	0.82	0.31	0.14	63,77,96,103	0
23	CLA	B	611	65/65	0.87	0.31	0.09	63,72,80,87	0
31	LMG	C	520	48/55	0.80	0.30	0.09	89,100,109,112	0
23	CLA	b	615	65/65	0.90	0.28	0.06	54,72,80,87	0
23	CLA	C	508	65/65	0.86	0.32	0.05	71,86,117,132	0
27	BCR	b	621	40/40	0.72	0.28	0.02	63,73,84,87	0
23	CLA	A	405	65/65	0.85	0.30	0.02	44,69,140,145	0
24	PHO	D	402	64/64	0.88	0.29	0.01	51,62,72,74	0
23	CLA	a	405	65/65	0.87	0.31	-0.03	44,53,69,73	0
26	OEC	a	411	5/9	0.92	0.35	-0.04	35,44,62,68	0
31	LMG	D	407	48/55	0.86	0.26	-0.08	54,72,81,120	0
27	BCR	T	101	40/40	0.79	0.32	-0.08	68,75,82,83	0
31	LMG	B	623	49/55	0.83	0.31	-0.15	58,76,84,87	0
22	BCT	A	402	4/4	0.87	0.33	-0.16	85,90,90,94	0
24	PHO	a	407	64/64	0.87	0.28	-0.19	53,63,70,73	0
23	CLA	D	401	65/65	0.88	0.27	-0.20	49,59,87,97	0
23	CLA	b	611	65/65	0.87	0.33	-0.21	54,64,89,92	0
31	LMG	b	624	49/55	0.85	0.27	-0.26	59,82,102,113	0
33	LMT	m	101	35/35	0.81	0.41	-0.35	68,93,112,114	0
31	LMG	b	625	49/55	0.81	0.32	-0.39	51,75,86,89	0
23	CLA	A	404	65/65	0.90	0.29	-0.42	44,54,67,74	0
23	CLA	B	607	65/65	0.86	0.28	-0.42	52,66,82,85	0
31	LMG	A	414	51/55	0.84	0.26	-0.45	63,77,92,95	0
31	LMG	d	406	46/55	0.89	0.24	-0.59	63,73,116,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	FE2	A	401	1/1	0.78	0.17	-1.38	64,64,64,64	0
21	FE2	a	403	1/1	0.87	0.16	-2.83	72,72,72,72	0
33	LMT	B	624	35/35	0.50	0.82	-	80,142,170,171	0
35	CA	K	101	1/1	0.62	0.53	-	86,86,86,86	0
35	CA	o	301	1/1	0.64	0.47	-	98,98,98,98	0
35	CA	O	301	1/1	0.35	0.47	-	112,112,112,112	0
33	LMT	b	626	35/35	0.62	0.67	-	76,139,174,176	0
35	CA	k	101	1/1	0.32	0.54	-	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.