



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2016 – 09:03 PM EST

PDB ID : 5TIS
Title : Room temperature XFEL structure of the native, doubly-illuminated photo-system II complex
Authors : Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Fuller, F.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Hussein, R.; Zhang, M.; Douthit, L.; Kubin, M.; de Lichtenberg, C.; Pham, L.V.; Nilsson, H.; Cheah, M.H.; Shevela, D.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Pastor, E.; Weninger, C.; Fransson, T.; Lassalle, L.; Braeuer, P.; Aller, P.; Docker, P.T.; Andi, B.; Orville, A.M.; Glowina, J.M.; Nelson, S.; Sikorski, M.; Zhu, D.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Watermann, D.G.; Evans, G.; Wernet, P.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2016-10-03
Resolution : 2.25 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692

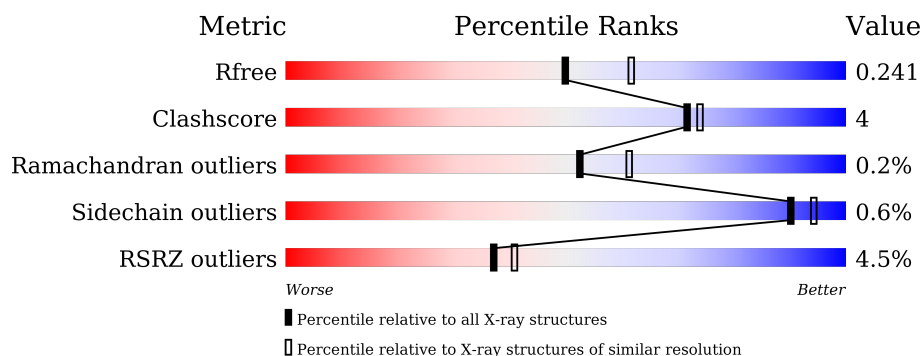
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

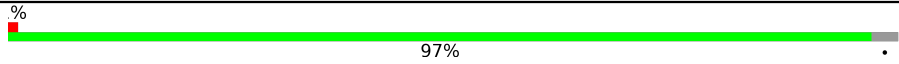

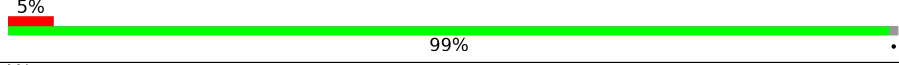

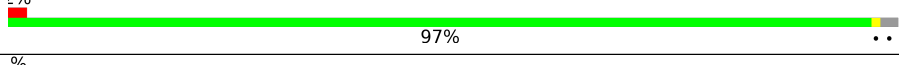
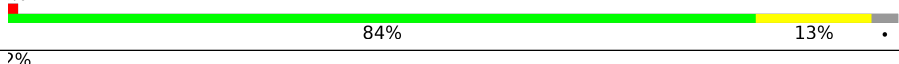
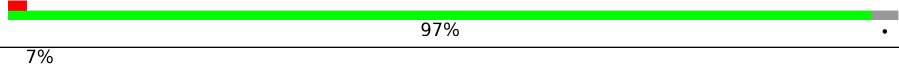

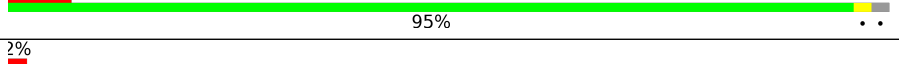


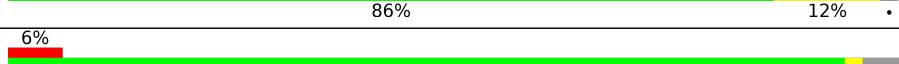
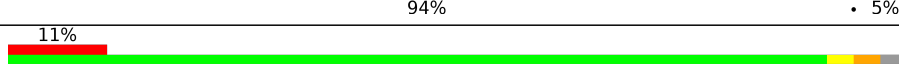
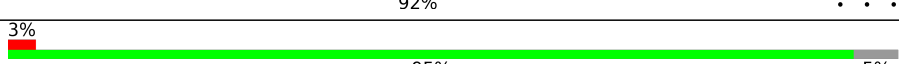
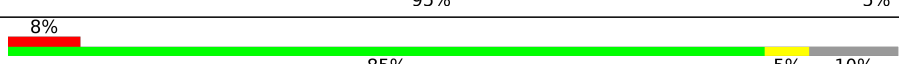
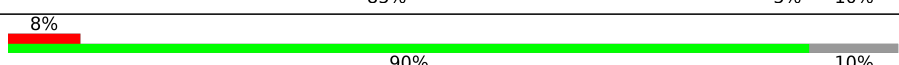
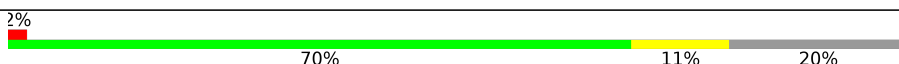
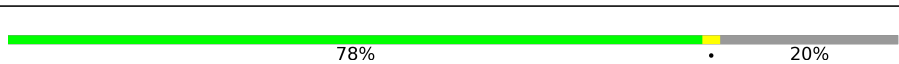
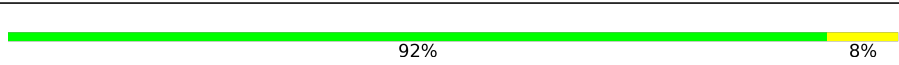
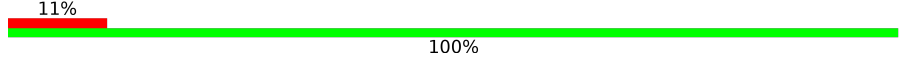

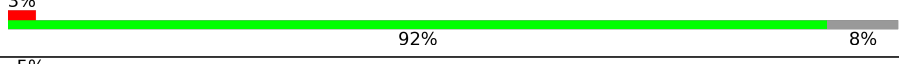
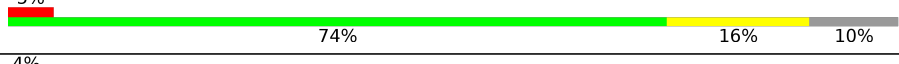
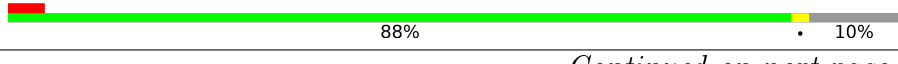

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; left: 0; top: -10px; width: 5px; height: 5px; background-color: red;"></div> <div style="position: absolute; left: 85%; top: -10px; width: 5px; height: 5px; background-color: yellow;"></div> <div style="position: absolute; left: 95%; top: -10px; width: 5px; height: 5px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 12% . </div> </div>

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EDS : rb-20028442
 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) : rb-20028442

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

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Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	613	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	X
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	X
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	615	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606[A]	X	-	-	-
25	CLA	b	606[B]	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-
28	PL9	A	611	-	-	-	X
28	PL9	a	612	-	-	-	X
29	SQD	B	625	-	-	-	X
29	SQD	D	409	-	-	-	X
30	LHG	A	618	-	-	-	X
30	LHG	a	617	-	-	-	X
30	LHG	d	406	-	-	-	X
31	UNL	A	615	-	-	-	X
31	UNL	A	617	-	-	-	X
31	UNL	B	627	-	-	-	X
31	UNL	C	522	-	-	-	X
31	UNL	D	410	-	-	-	X
31	UNL	M	101	-	-	-	X
31	UNL	M	102	-	-	-	X
31	UNL	a	619	-	-	-	X
31	UNL	c	525	-	-	-	X
31	UNL	d	409	-	-	-	X
31	UNL	j	801	-	-	-	X
31	UNL	m	103	-	-	-	X
31	UNL	t	102	-	-	-	X
32	LMG	B	621	-	-	-	X
32	LMG	B	626	-	-	-	X
32	LMG	C	521	-	-	-	X
32	LMG	b	620	-	-	-	X
32	LMG	c	520	-	-	-	X
32	LMG	d	408	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 51757 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2625	1719	431	460	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	5	0
			4005	2629	667	696	13			
2	b	504	Total	C	N	O	S	0	2	0
			3982	2613	665	691	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	1	0
			3494	2287	585	609	13			
3	c	451	Total	C	N	O	S	0	1	0
			3494	2286	587	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			
4	d	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			670	437	109	124			
5	e	82	Total	C	N	O	0	1	0
			671	438	108	125			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	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
			510	341	82	85	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total	C	N	O	S	0	0	0
			304	206	47	50	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			257	174	40	42	1			
9	j	36	Total	C	N	O	S	0	0	0
			257	174	40	42	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	33	Total	C	N	O	S	0	1	0
			269	178	39	51	1			
12	m	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1888	1179	320	385	4			
13	o	244	Total	C	N	O	S	0	2	0
			1888	1179	320	385	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	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
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1070	680	178	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	S	0	0	0
			281	188	45	48				
18	x	38	Total	C	N	O	S	0	1	0
			285	192	46	47				

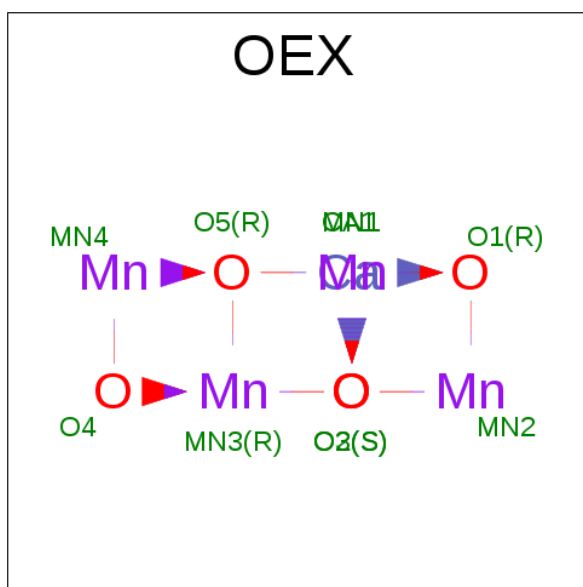
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			478	328	72	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	S	0	0	0
			273	186	47	40				
20	r	34	Total	C	N	O	S	0	0	0
			270	183	47	40				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

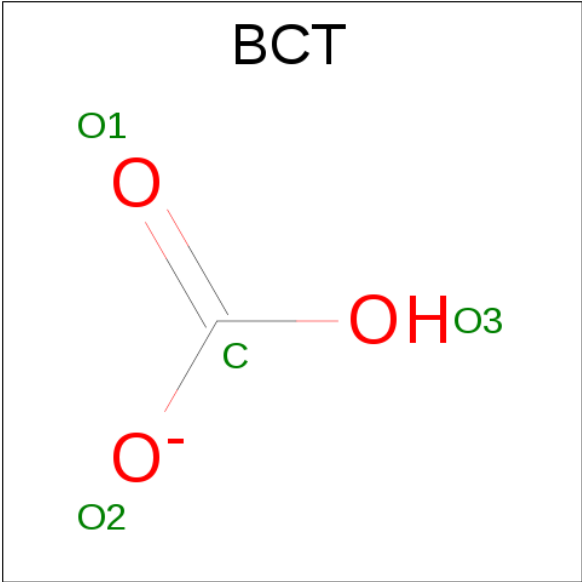
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

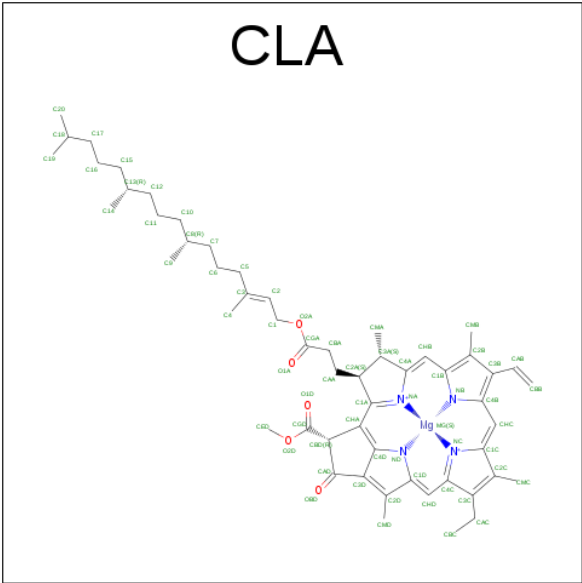
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	2	Total	Cl	0	0
			2	2		
23	a	2	Total	Cl	0	0
			2	2		

- Molecule 24 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O		0	0
			4	1	3			
24	a	1	Total	C	O		0	0
			4	1	3			

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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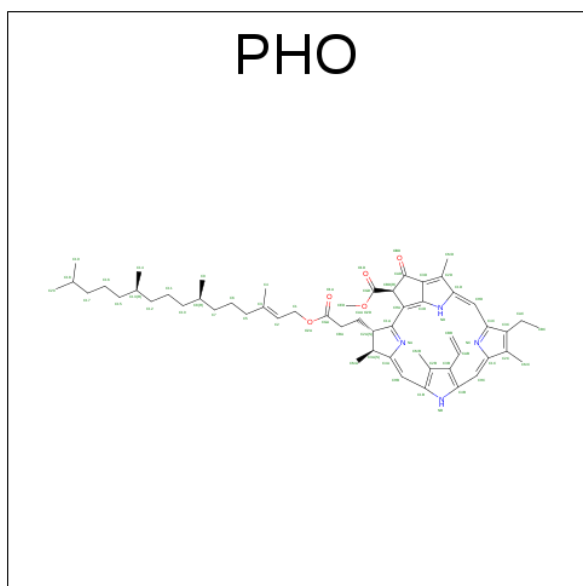
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total 129	C 110	Mg 1	N 8	O 10	0	1
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 64	C 54	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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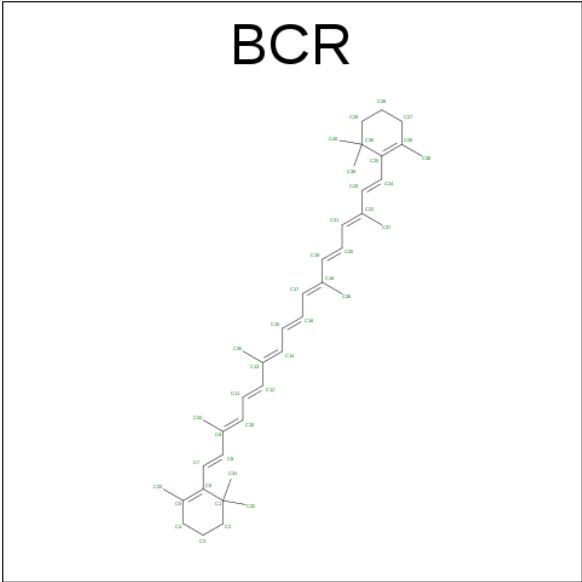
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 26 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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



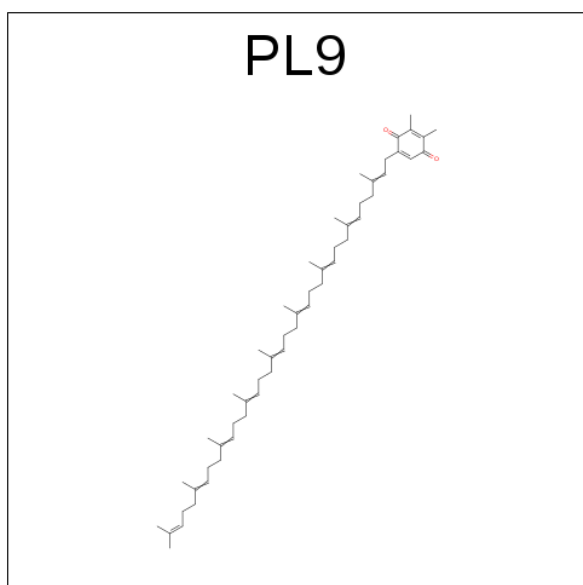
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	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	t	1	Total C 40 40	0	0

- Molecule 28 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: $C_{53}H_{80}O_2$).



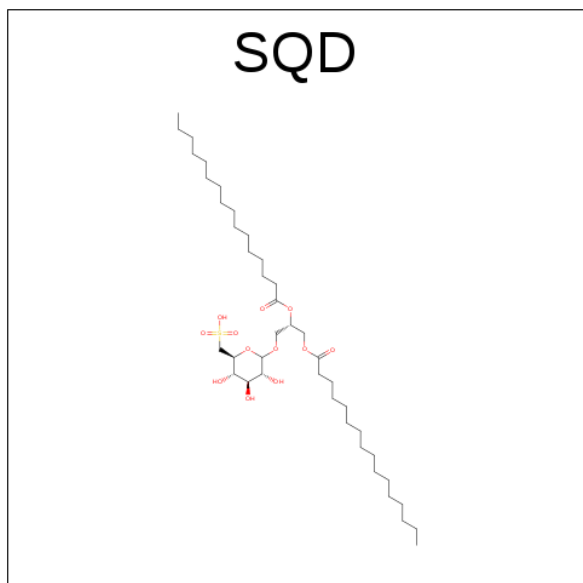
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	a	1	Total	C	O	0	0
			55	53	2		
28	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



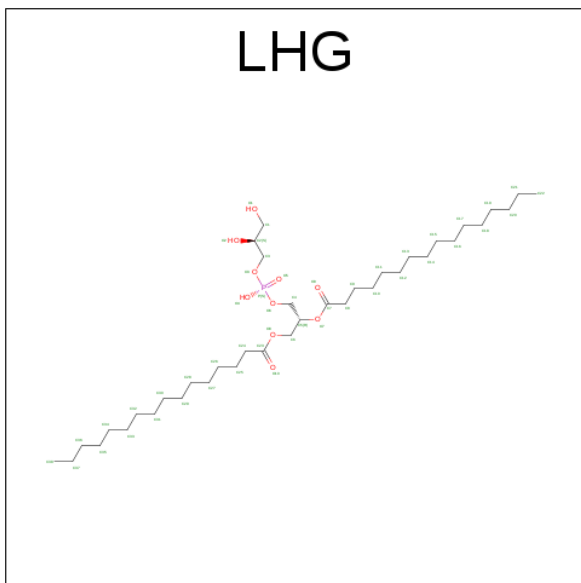
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	S	0	0
			52	39	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			54	41	12	1		
29	D	1	Total	C	O	S	0	0
			43	30	12	1		
29	D	1	Total	C	O	S	0	0
			47	34	12	1		
29	L	1	Total	C	O	S	0	0
			49	36	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	b	1	Total	C	O		0	0
			40	35	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).

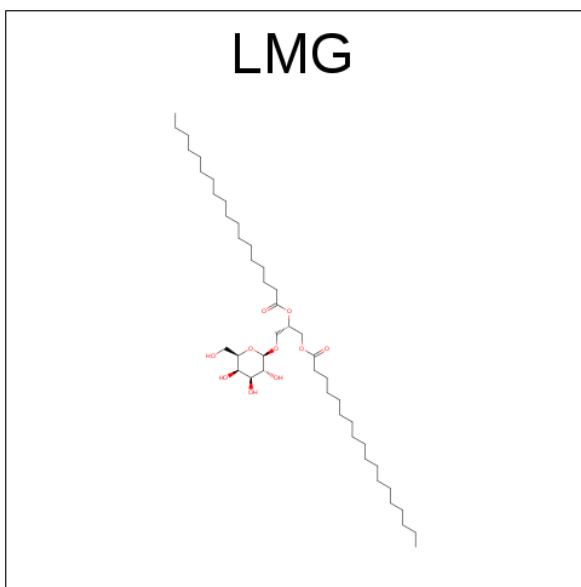


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			47	36	10	1		
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	B	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			39	28	10	1		
30	a	1	Total	C	O	P	0	0
			42	31	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

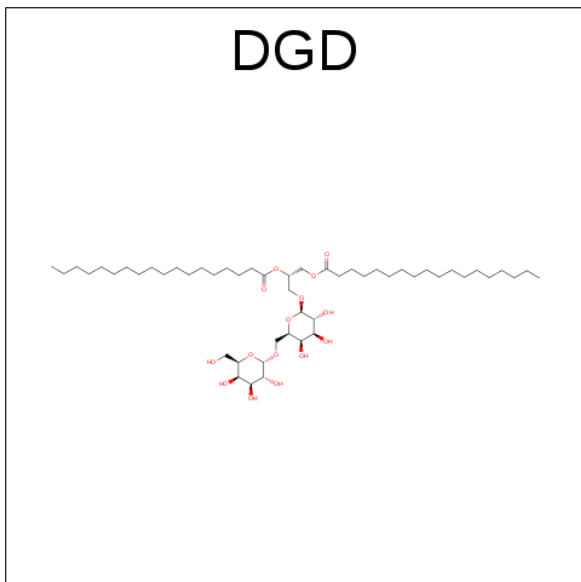
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	J	2	Total C O 23 21 2	0	0
31	i	1	Total C O 20 18 2	0	0
31	D	2	Total C 28 28	0	0
31	E	1	Total C O 12 10 2	0	0
31	H	1	Total C 7 7	0	0
31	B	2	Total C 26 26	0	0
31	I	2	Total C O 27 25 2	0	0
31	C	2	Total C O 33 31 2	0	0
31	a	2	Total C O 29 27 2	0	0
31	c	3	Total C O 40 34 6	0	0
31	x	1	Total C 16 16	0	0
31	A	2	Total C O 29 27 2	0	0
31	T	2	Total C 26 26	0	0
31	j	2	Total C O 27 25 2	0	0
31	d	1	Total C 17 17	0	0
31	t	1	Total C 18 18	0	0
31	m	2	Total C O 25 23 2	0	0
31	b	2	Total C 28 28	0	0
31	M	2	Total C O 32 30 2	0	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



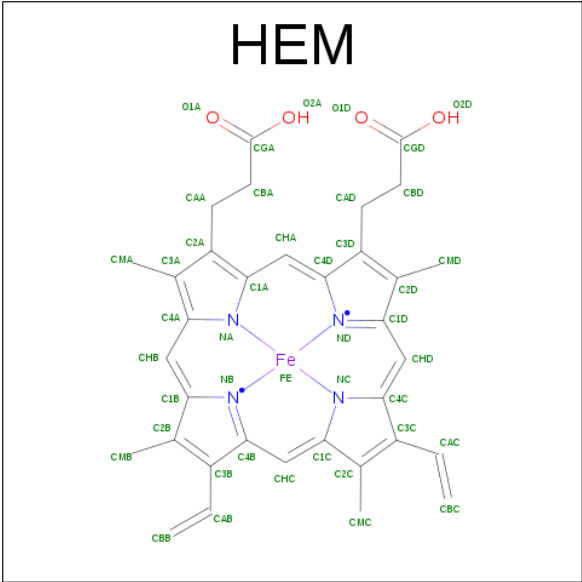
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	b	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			34	24	10		
32	d	1	Total	C	O	0	0
			51	41	10		
32	d	1	Total	C	O	0	0
			38	36	2		
32	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	C	1	Total	C	O	0	0
			62	47	15		
33	H	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	c	1	Total	C	O	0	0
			62	47	15		
33	h	1	Total	C	O	0	0
			62	47	15		

- 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	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	86	Total	O	0	0
			86	86		
35	B	109	Total	O	0	0
			109	109		
35	C	95	Total	O	0	0
			95	95		
35	D	82	Total	O	0	0
			82	82		
35	E	14	Total	O	0	0
			14	14		
35	F	3	Total	O	0	0
			3	3		
35	H	11	Total	O	0	0
			11	11		
35	I	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	5	Total 5	O 5	0	0
35	K	2	Total 2	O 2	0	0
35	L	3	Total 3	O 3	0	0
35	M	5	Total 5	O 5	0	0
35	O	72	Total 72	O 72	0	0
35	T	9	Total 9	O 9	0	0
35	U	22	Total 22	O 22	0	0
35	V	42	Total 42	O 42	0	0
35	X	5	Total 5	O 5	0	0
35	Z	3	Total 3	O 3	0	0
35	a	90	Total 90	O 90	0	0
35	b	129	Total 129	O 129	0	0
35	c	95	Total 95	O 95	0	0
35	d	87	Total 87	O 87	0	0
35	e	9	Total 9	O 9	0	0
35	f	2	Total 2	O 2	0	0
35	h	13	Total 13	O 13	0	0
35	i	6	Total 6	O 6	0	0
35	j	2	Total 2	O 2	0	0
35	k	4	Total 4	O 4	0	0
35	l	10	Total 10	O 10	0	0

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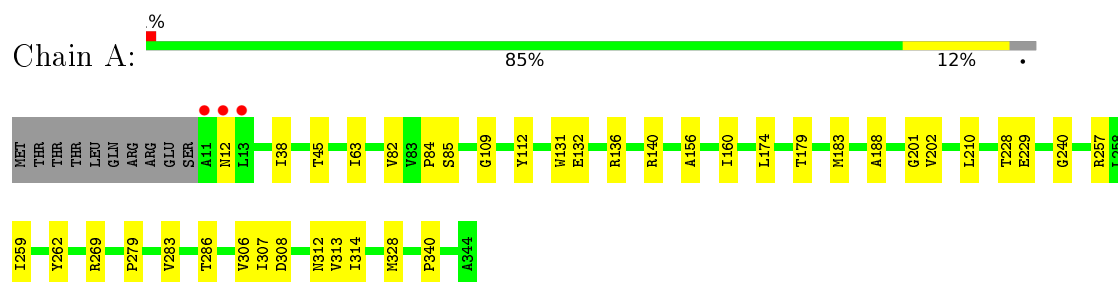
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	m	10	Total 10	O 10	0	0
35	o	69	Total 69	O 69	0	0
35	t	4	Total 4	O 4	0	0
35	u	34	Total 34	O 34	0	0
35	v	37	Total 37	O 37	0	0
35	y	1	Total 1	O 1	0	0
35	x	4	Total 4	O 4	0	0
35	z	1	Total 1	O 1	0	0
35	r	1	Total 1	O 1	0	0

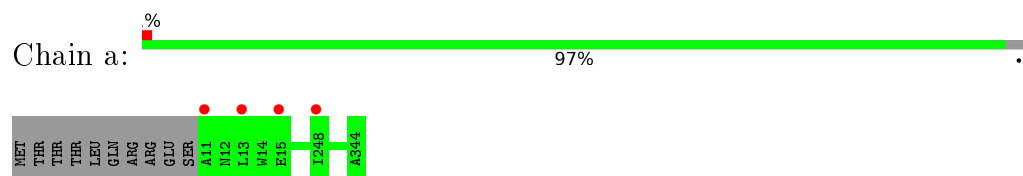
3 Residue-property plots [i](#)

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

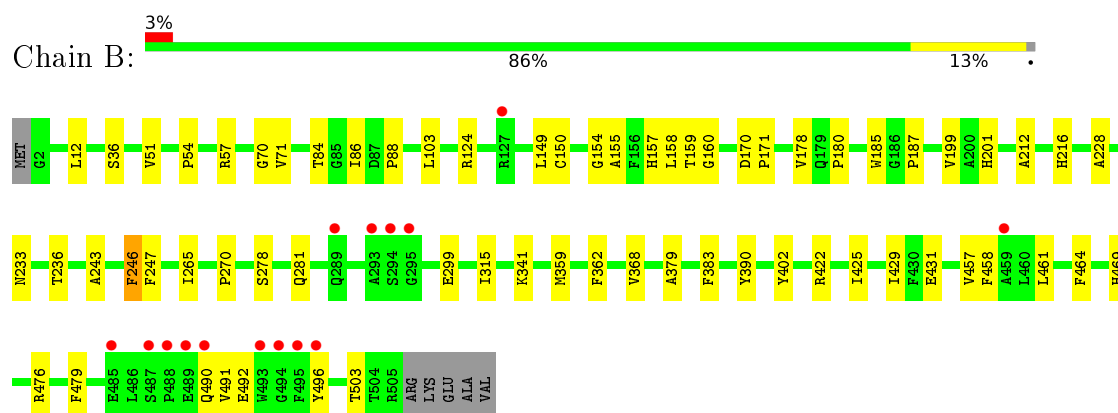
- Molecule 1: Photosystem II protein D1 1



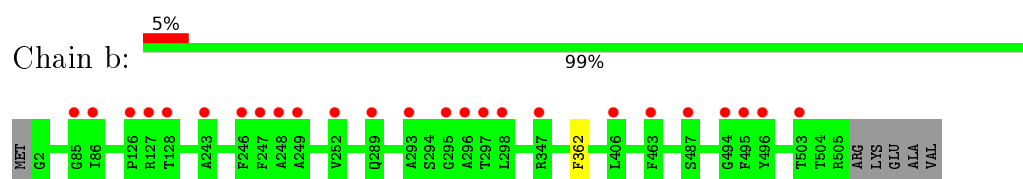
- Molecule 1: Photosystem II protein D1 1



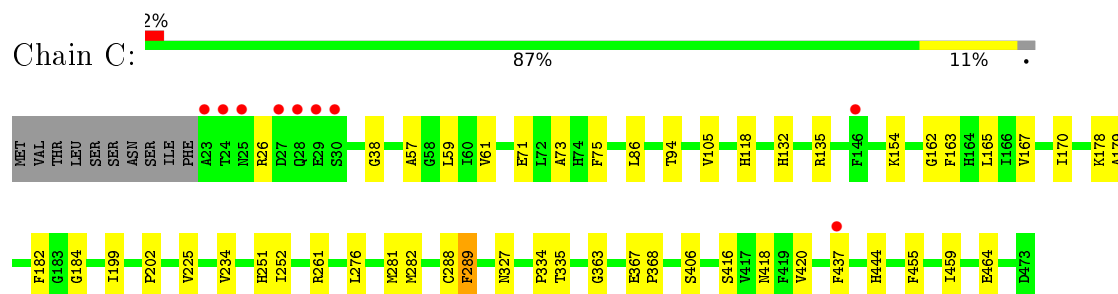
- Molecule 2: Photosystem II CP47 reaction center protein



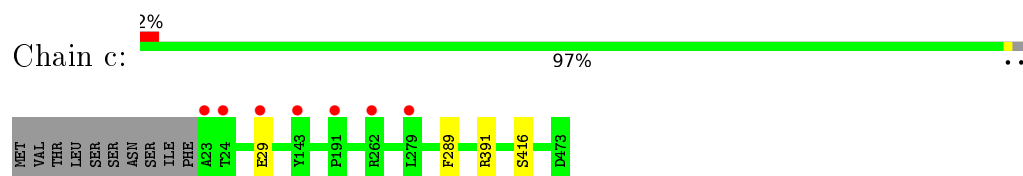
- Molecule 2: Photosystem II CP47 reaction center protein



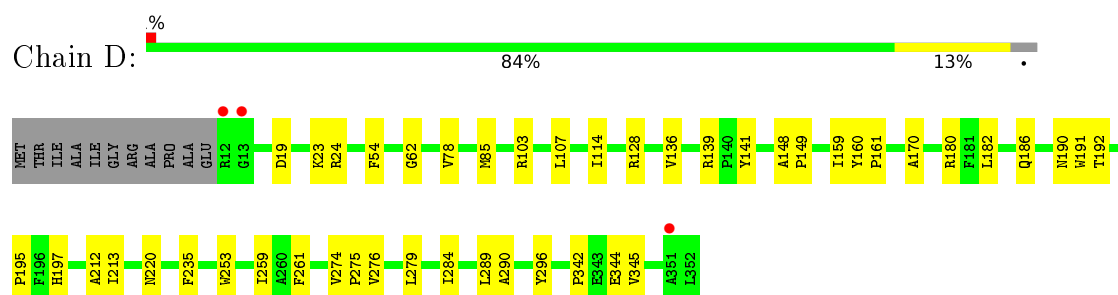
- Molecule 3: Photosystem II CP43 reaction center protein



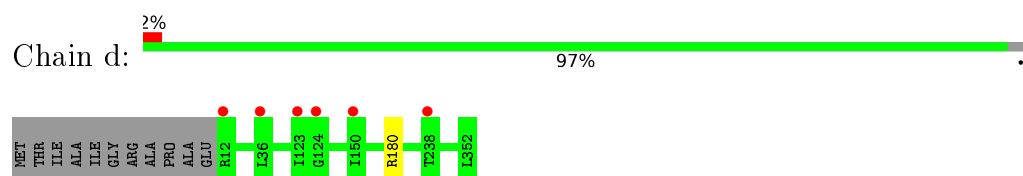
- Molecule 3: Photosystem II CP43 reaction center protein



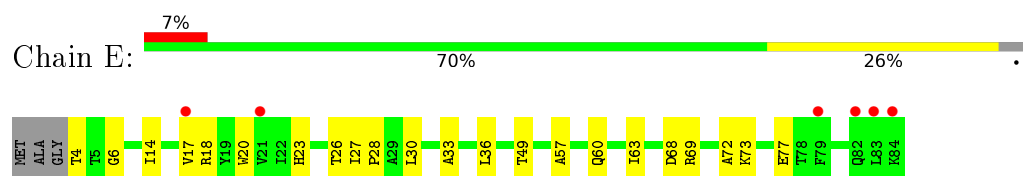
- Molecule 4: Photosystem II D2 protein



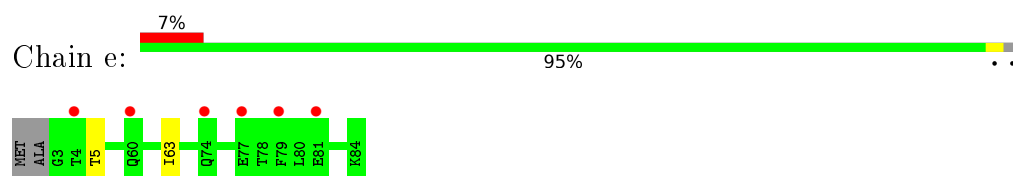
- Molecule 4: Photosystem II D2 protein



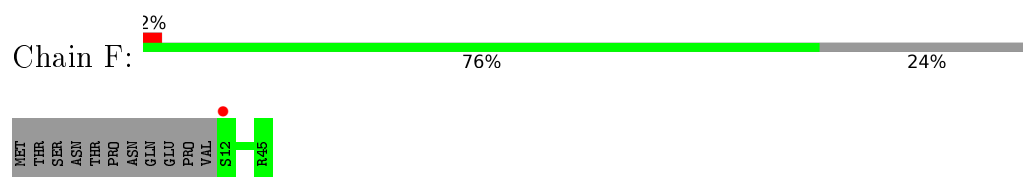
- Molecule 5: Cytochrome b559 subunit alpha



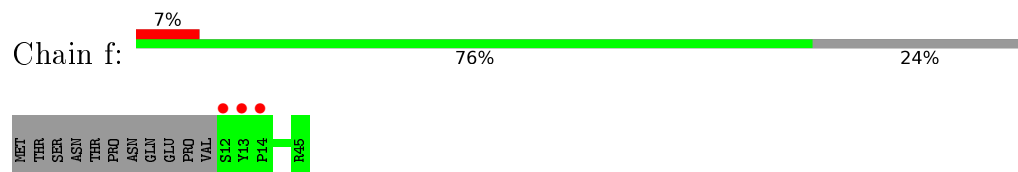
- Molecule 5: Cytochrome b559 subunit alpha



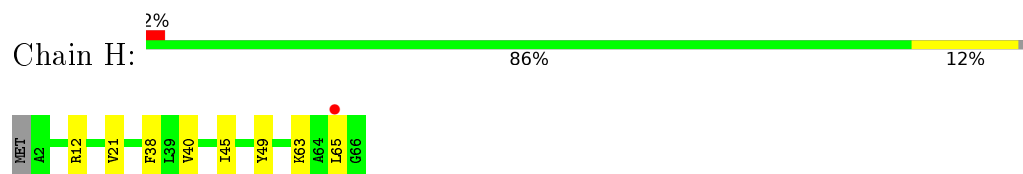
- Molecule 6: Cytochrome b559 subunit beta



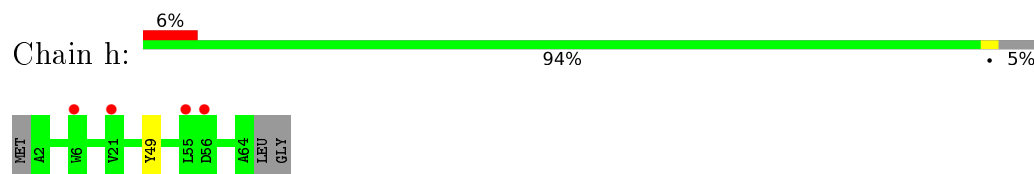
- Molecule 6: Cytochrome b559 subunit beta



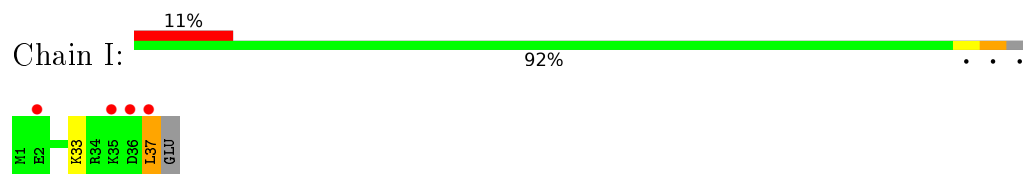
- Molecule 7: Photosystem II reaction center protein H



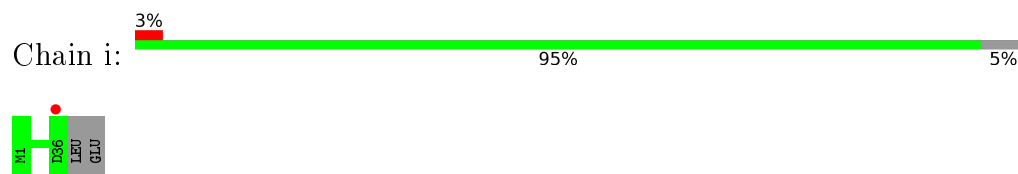
- Molecule 7: Photosystem II reaction center protein H



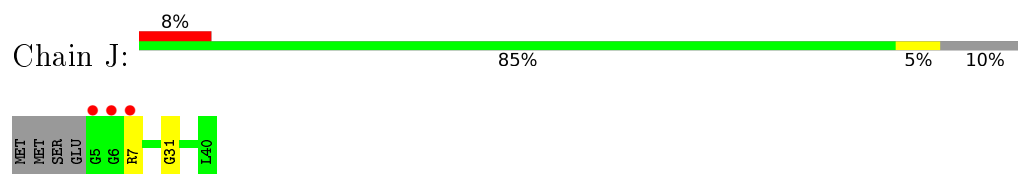
- Molecule 8: Photosystem II reaction center protein I



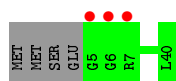
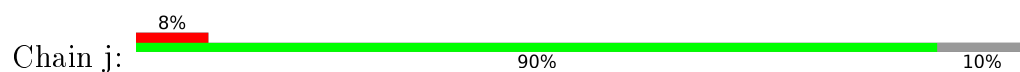
- Molecule 8: Photosystem II reaction center protein I



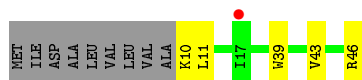
- Molecule 9: Photosystem II reaction center protein J



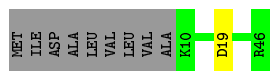
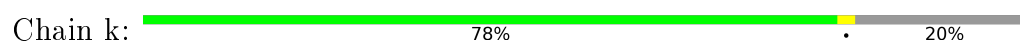
- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K



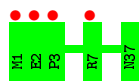
- Molecule 10: Photosystem II reaction center protein K



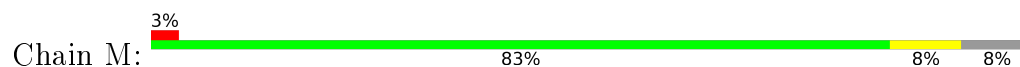
- Molecule 11: Photosystem II reaction center protein L



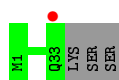
- Molecule 11: Photosystem II reaction center protein L



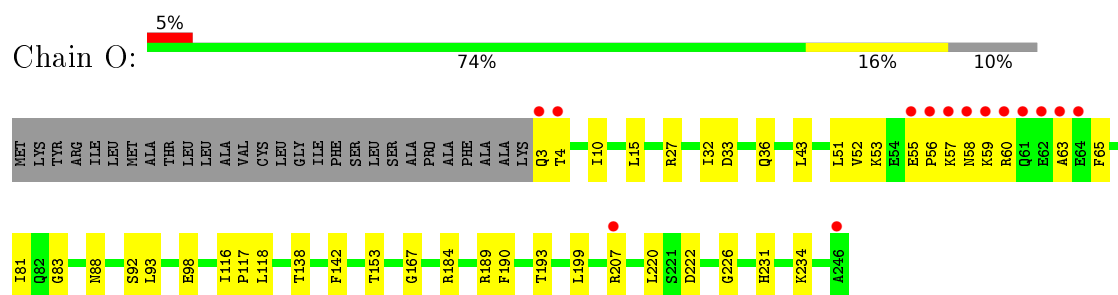
- Molecule 12: Photosystem II reaction center protein M



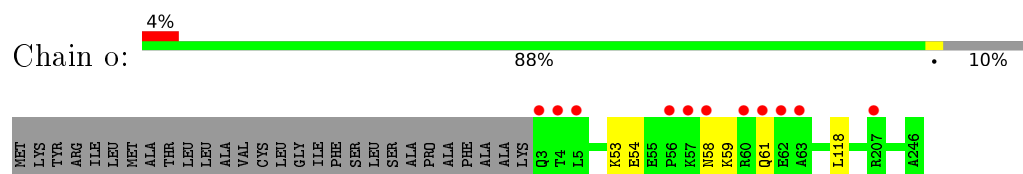
- Molecule 12: Photosystem II reaction center protein M



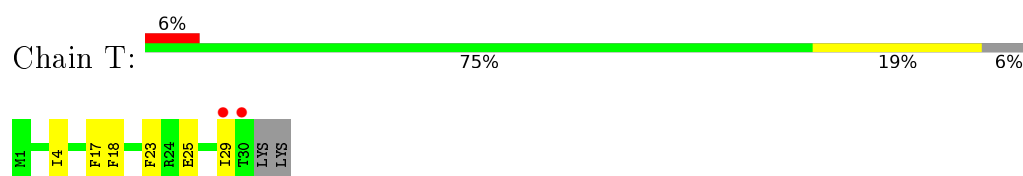
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



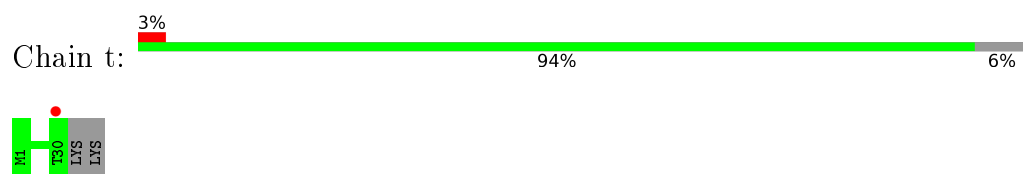
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



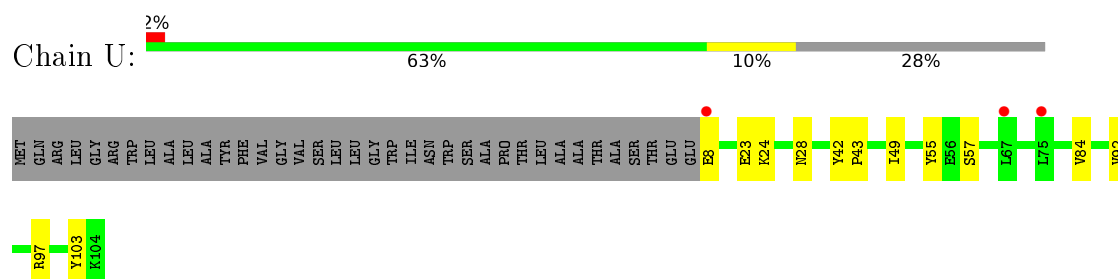
- Molecule 14: Photosystem II reaction center protein T



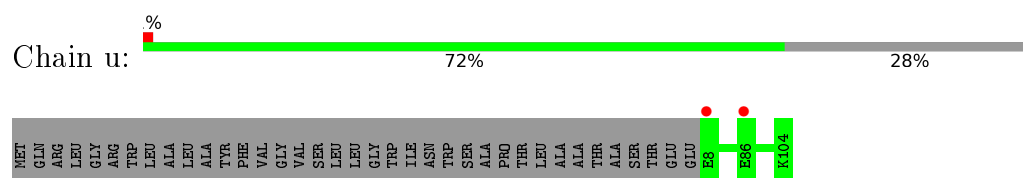
- Molecule 14: Photosystem II reaction center protein T



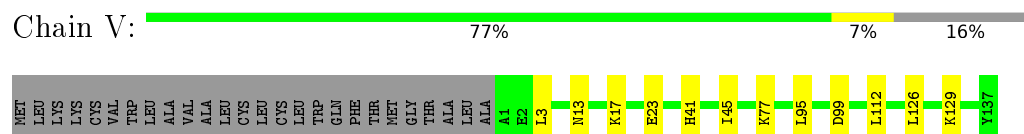
- Molecule 15: Photosystem II 12 kDa extrinsic protein



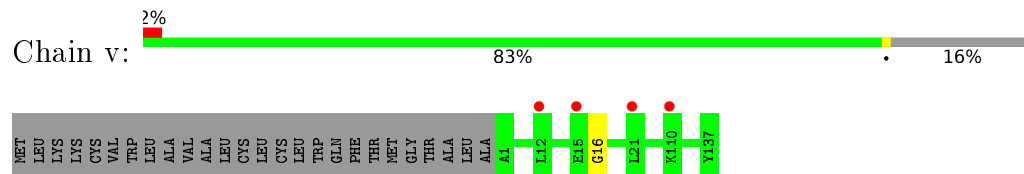
- Molecule 15: Photosystem II 12 kDa extrinsic protein



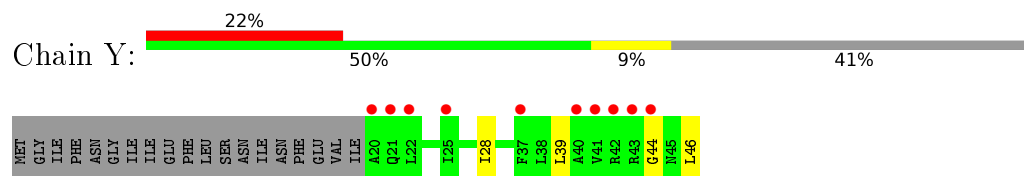
- Molecule 16: Cytochrome c-550



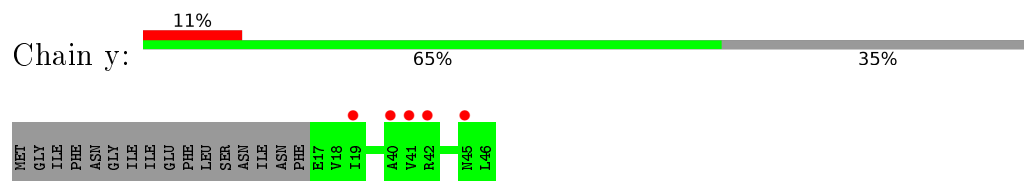
- Molecule 16: Cytochrome c-550



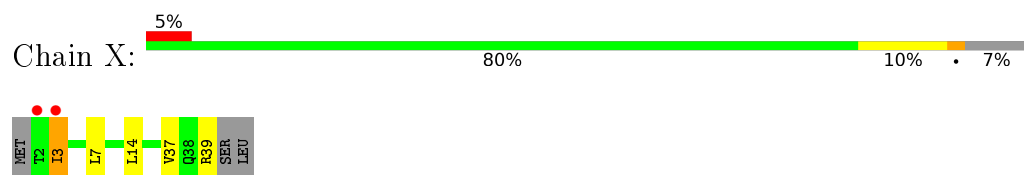
- Molecule 17: Photosystem II reaction center protein Ycf12



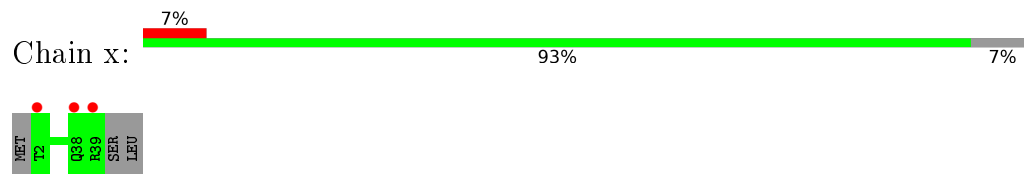
- Molecule 17: Photosystem II reaction center protein Ycf12



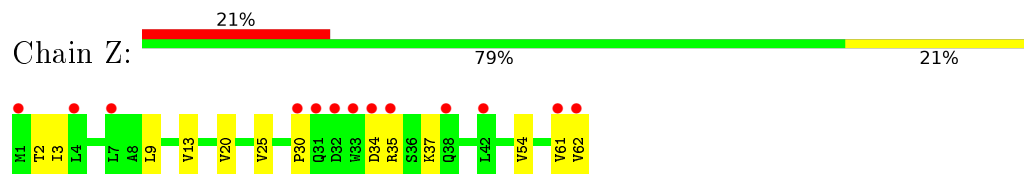
- Molecule 18: Photosystem II reaction center X protein



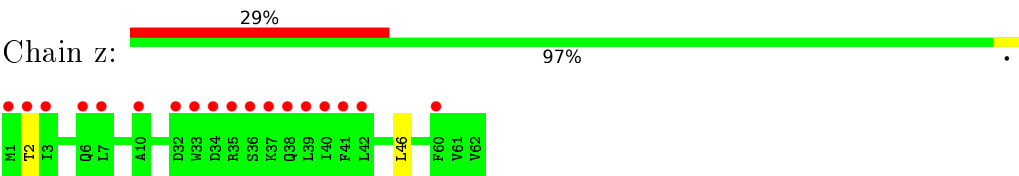
- Molecule 18: Photosystem II reaction center X protein



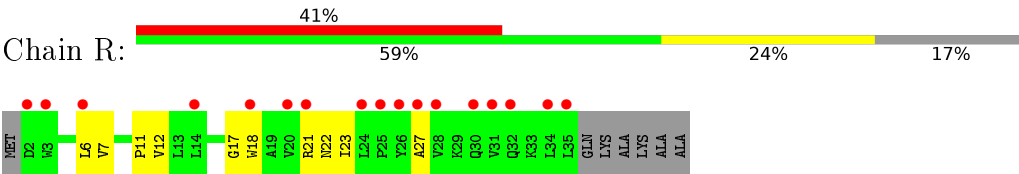
- Molecule 19: Photosystem II reaction center protein Z



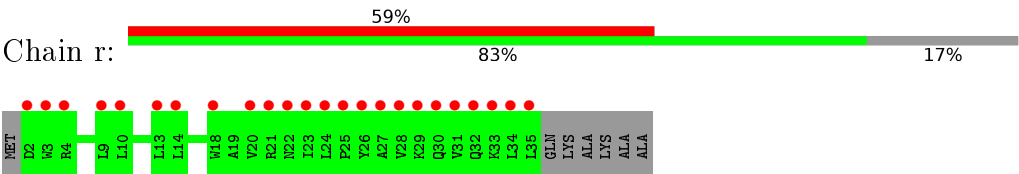
- Molecule 19: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II protein Y



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.87Å 223.14Å 310.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 2.25 44.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.28-2.25) 90.6 (44.28-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_2481)	Depositor
R, R_{free}	0.193 , 0.231 0.202 , 0.241	Depositor DCC
R_{free} test set	3426 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, PHO, DGD, CL, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, 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	0.25	0/2713	0.40	0/3700
1	a	0.25	0/2707	0.40	0/3692
2	B	0.25	0/4155	0.40	0/5661
2	b	0.25	0/4125	0.40	0/5621
3	C	0.25	0/3607	0.40	0/4911
3	c	0.25	0/3610	0.40	0/4914
4	D	0.26	0/2812	0.41	0/3832
4	d	0.25	0/2811	0.41	0/3830
5	E	0.23	0/689	0.37	0/940
5	e	0.30	1/693 (0.1%)	0.38	0/945
6	F	0.24	0/284	0.36	0/387
6	f	0.24	0/284	0.35	0/387
7	H	0.25	0/523	0.41	0/713
7	h	0.24	0/511	0.39	0/697
8	I	0.25	0/301	0.43	0/407
8	i	0.26	0/293	0.38	0/396
9	J	0.25	0/263	0.40	0/356
9	j	0.25	0/263	0.39	0/356
10	K	0.26	0/303	0.39	0/416
10	k	0.26	0/303	0.37	0/416
11	L	0.24	0/311	0.37	0/422
11	l	0.24	0/311	0.37	0/422
12	M	0.24	0/262	0.34	0/358
12	m	0.24	0/253	0.35	0/346
13	O	0.24	0/1925	0.46	0/2610
13	o	0.25	0/1925	0.47	0/2609
14	T	0.27	0/257	0.34	0/349
14	t	0.27	0/257	0.36	0/349
15	U	0.24	0/785	0.42	0/1064
15	u	0.24	0/785	0.42	0/1064
16	V	0.23	0/1085	0.41	0/1473
16	v	0.23	0/1094	0.40	0/1484

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.24	0/201	0.39	0/268
17	y	0.24	0/225	0.37	0/301
18	X	0.24	0/284	0.37	0/384
18	x	0.24	0/291	0.38	0/392
19	Z	0.24	0/490	0.35	0/669
19	z	0.24	0/489	0.36	0/669
20	R	0.22	0/279	0.40	0/383
20	r	0.22	0/276	0.36	0/379
All	All	0.25	1/43035 (0.0%)	0.40	0/58572

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	5.06	1.43	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2625	0	2524	32	0
1	a	2622	0	2519	0	0
2	B	4005	0	3865	54	0
2	b	3982	0	3842	0	0
3	C	3494	0	3417	45	0
3	c	3494	0	3420	0	0
4	D	2717	0	2621	38	0
4	d	2716	0	2621	0	0
5	E	670	0	655	17	0
5	e	671	0	657	0	0
6	F	275	0	282	0	0
6	f	275	0	282	0	0
7	H	510	0	532	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	498	0	518	0	0
8	I	304	0	322	3	0
8	i	296	0	311	0	0
9	J	257	0	268	2	0
9	j	257	0	268	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	304	0	316	6	0
11	l	304	0	316	0	0
12	M	269	0	280	1	0
12	m	260	0	275	0	0
13	O	1888	0	1865	24	0
13	o	1888	0	1865	0	0
14	T	258	0	261	7	0
14	t	258	0	261	0	0
15	U	774	0	773	9	0
15	u	774	0	773	0	0
16	V	1064	0	1073	7	0
16	v	1070	0	1086	0	0
17	Y	200	0	226	5	0
17	y	224	0	252	0	0
18	X	281	0	312	4	0
18	x	285	0	320	0	0
19	Z	479	0	516	9	0
19	z	478	0	516	0	0
20	R	273	0	305	6	0
20	r	270	0	296	0	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	4	0	1	0	0
24	a	4	0	1	0	0
25	A	249	0	264	17	0
25	B	1040	0	1152	65	0
25	C	845	0	936	57	0
25	D	130	0	144	9	0
25	a	260	0	288	0	0
25	b	1086	0	1187	0	0
25	c	839	0	919	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	d	130	0	144	0	0
26	A	64	0	74	4	0
26	D	64	0	74	0	0
26	a	128	0	148	0	0
27	A	40	0	56	2	0
27	B	120	0	168	12	0
27	C	80	0	112	8	0
27	D	40	0	56	4	0
27	H	40	0	56	4	0
27	K	40	0	56	2	0
27	T	40	0	56	5	0
27	Y	40	0	56	4	0
27	a	40	0	56	0	0
27	b	120	0	168	0	0
27	c	160	0	224	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	t	40	0	56	0	0
28	A	55	0	80	3	0
28	D	55	0	80	0	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	106	0	148	2	0
29	B	108	0	156	6	0
29	D	90	0	111	3	0
29	L	49	0	65	3	0
29	a	54	0	78	0	0
29	b	40	0	67	0	0
29	f	41	0	49	0	0
30	A	96	0	141	3	0
30	B	49	0	74	4	0
30	D	49	0	74	4	0
30	L	49	0	74	1	0
30	a	81	0	108	0	0
30	d	98	0	148	0	0
30	l	49	0	74	0	0
31	A	29	0	0	0	0
31	B	26	0	0	0	0
31	C	33	0	0	0	0
31	D	28	0	0	0	0
31	E	12	0	0	0	0
31	H	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	I	27	0	0	0	0
31	J	23	0	0	0	0
31	M	32	0	0	0	0
31	T	26	0	0	0	0
31	a	29	0	0	0	0
31	b	28	0	0	0	0
31	c	40	0	0	0	0
31	d	17	0	0	0	0
31	i	20	0	0	0	0
31	j	27	0	0	0	0
31	m	25	0	0	0	0
31	t	18	0	0	0	0
31	x	16	0	0	0	0
32	B	153	0	216	3	0
32	C	147	0	204	2	0
32	D	51	0	72	2	0
32	a	51	0	72	0	0
32	b	51	0	72	0	0
32	c	71	0	82	0	0
32	d	89	0	142	0	0
32	m	51	0	72	0	0
33	C	186	0	246	7	0
33	H	62	0	82	2	0
33	c	186	0	246	0	0
33	h	62	0	82	0	0
34	E	43	0	30	5	0
34	V	43	0	30	2	0
34	e	43	0	30	0	0
34	v	43	0	30	0	0
35	A	86	0	0	1	0
35	B	109	0	0	2	0
35	C	95	0	0	1	0
35	D	82	0	0	1	0
35	E	14	0	0	0	0
35	F	3	0	0	0	0
35	H	11	0	0	0	0
35	I	3	0	0	1	0
35	J	5	0	0	1	0
35	K	2	0	0	0	0
35	L	3	0	0	0	0
35	M	5	0	0	0	0
35	O	72	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	T	9	0	0	0	0
35	U	22	0	0	3	0
35	V	42	0	0	0	0
35	X	5	0	0	0	0
35	Z	3	0	0	0	0
35	a	90	0	0	0	0
35	b	129	0	0	0	0
35	c	95	0	0	0	0
35	d	87	0	0	0	0
35	e	9	0	0	0	0
35	f	2	0	0	0	0
35	h	13	0	0	0	0
35	i	6	0	0	0	0
35	j	2	0	0	0	0
35	k	4	0	0	0	0
35	l	10	0	0	0	0
35	m	10	0	0	0	0
35	o	69	0	0	0	0
35	r	1	0	0	0	0
35	t	4	0	0	0	0
35	u	34	0	0	0	0
35	v	37	0	0	0	0
35	x	4	0	0	0	0
35	y	1	0	0	0	0
35	z	1	0	0	0	0
All	All	51757	0	51380	383	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 4.

All (383) 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)
2:B:157:HIS:HE1	25:B:606:CLA:NA	1.78	0.81
2:B:359:MET:SD	35:B:703:HOH:O	32.98	0.75
3:C:165:LEU:HD21	25:C:507:CLA:HAB	1.67	0.74
5:E:17:VAL:H	9:J:7:ARG:HH21	2.15	0.74
15:U:55:TYR:OH	35:U:201:HOH:O	20.33	0.73
15:U:49:ILE:O	35:U:201:HOH:O	20.43	0.72
34:E:101:HEM:HBC2	34:E:101:HEM:HHD	1.72	0.72
5:E:23:HIS:HA	5:E:26:THR:HG22	4.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:E:101:HEM:HBB2	34:E:101:HEM:HHC	4.73	0.70
17:Y:44:GLY:HA2	19:Z:30:PRO:HD3	1.72	0.70
27:B:617:BCR:H383	29:B:624:SQD:H122	1.73	0.69
13:O:83:GLY:HA2	13:O:98:GLU:HG3	1.76	0.68
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.58	0.68
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.87	0.68
1:A:257:ARG:NH1	2:B:492[B]:GLU:O	2.22	0.67
25:A:607:CLA:H101	28:A:611:PL9:H203	1.76	0.66
26:A:608:PHO:HBC3	4:D:279:LEU:HD22	1.78	0.66
25:B:608:CLA:H161	25:D:402:CLA:H3A	30.20	0.65
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.78	0.64
25:B:604:CLA:H42	25:B:605:CLA:H2	3.08	0.64
25:C:504:CLA:H171	25:C:511:CLA:HBB2	1.79	0.63
2:B:216:HIS:HE1	25:B:609:CLA:NA	1.98	0.62
13:O:53:LYS:HE2	13:O:63:ALA:HB3	1.79	0.62
4:D:192:THR:HG23	25:D:402:CLA:HBC2	1.82	0.62
2:B:150:CYS:HB2	25:B:603:CLA:HMC3	1.92	0.61
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.83	0.61
2:B:187:PRO:HG3	25:B:601:CLA:HMD3	2.52	0.61
2:B:171:PRO:HD3	7:H:65:LEU:HB3	1.83	0.61
4:D:186:GLN:HB2	25:D:402:CLA:HBC1	1.83	0.60
2:B:103:LEU:HD21	25:B:605:CLA:HMC3	1.82	0.60
19:Z:9:LEU:HD23	19:Z:54:VAL:HG11	4.89	0.60
15:U:8:GLU:N	35:U:203:HOH:O	31.91	0.59
18:X:3:ILE:HA	18:X:7:LEU:HD23	1.83	0.59
5:E:14:ILE:O	5:E:20:TRP:NE1	2.55	0.59
25:C:506:CLA:H2	25:C:507:CLA:H203	14.62	0.59
25:B:603:CLA:H2	25:B:605:CLA:H91	1.85	0.59
13:O:51:LEU:HD12	13:O:234:LYS:HD2	2.55	0.59
9:J:31:GLY:O	35:J:201:HOH:O	2.17	0.58
29:B:624:SQD:H462	29:B:624:SQD:H92	1.86	0.58
17:Y:39:LEU:HD11	19:Z:25:VAL:HA	1.86	0.58
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.17	0.57
25:B:602:CLA:H43	7:H:45:ILE:HG22	5.61	0.57
8:I:37:LEU:O	35:I:201:HOH:O	2.17	0.57
11:L:14:ARG:NH2	14:T:23:PHE:O	3.03	0.57
2:B:124:ARG:O	7:H:12:ARG:NH2	2.44	0.57
3:C:202:PRO:HB3	3:C:234:VAL:HG23	1.86	0.57
25:B:604:CLA:H101	25:B:615:CLA:H42	1.86	0.57
33:C:518:DGD:HAF2	32:D:407:LMG:H201	12.07	0.57
16:V:77:LYS:HG2	16:V:95:LEU:HD12	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:HD21	25:B:604:CLA:H151	1.88	0.56
3:C:418:ASN:HD21	33:C:517:DGD:HD4	29.82	0.56
13:O:10:ILE:HG23	13:O:15:LEU:HB2	1.88	0.56
1:A:45:THR:HG21	29:A:616:SQD:H221	1.87	0.56
1:A:229:GLU:HG2	2:B:476:ARG:HH22	1.71	0.55
2:B:315:ILE:HD13	2:B:359:MET:HE3	5.29	0.55
19:Z:2:THR:OG1	19:Z:3:ILE:N	4.47	0.55
17:Y:28:ILE:HG23	27:Y:101:BCR:H10C	1.88	0.55
13:O:3:GLN:N	13:O:4:THR:HA	4.66	0.55
2:B:503:THR:HG23	18:X:39:ARG:HH21	5.61	0.54
2:B:457:VAL:HG13	4:D:284:ILE:HD12	4.58	0.54
25:C:502:CLA:H203	25:C:508:CLA:H152	1.89	0.54
1:A:210:LEU:HD13	25:A:607:CLA:H43	4.63	0.54
5:E:30:LEU:HD23	20:R:12:VAL:HG12	1.90	0.54
29:B:624:SQD:H442	14:T:23:PHE:CD2	37.03	0.54
1:A:12:ASN:ND2	35:A:705:HOH:O	2.40	0.54
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	1.89	0.54
14:T:18:PHE:HB2	27:T:101:BCR:HC8	2.05	0.54
3:C:178:LYS:NZ	3:C:184:GLY:O	2.40	0.53
25:C:505:CLA:H42	33:C:518:DGD:HB52	1.90	0.53
25:A:607:CLA:HAB	25:D:402:CLA:H72	1.89	0.53
2:B:469:HIS:CE1	25:B:611:CLA:NA	2.76	0.53
25:C:510:CLA:H91	25:C:513:CLA:HBD	1.91	0.53
35:B:707:HOH:O	4:D:24:ARG:NH2	72.37	0.53
25:B:601:CLA:HHD	27:H:101:BCR:H383	1.89	0.53
25:B:613:CLA:HBB1	25:B:613:CLA:HMB1	1.89	0.53
8:I:37:LEU:H	8:I:37:LEU:HD13	1.73	0.53
3:C:406:SER:HA	3:C:420:VAL:HG23	1.91	0.53
5:E:30:LEU:HD11	34:E:101:HEM:HAB	1.91	0.53
3:C:38:GLY:HA3	25:C:511:CLA:HMD3	15.97	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.52
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.92	0.52
25:D:403:CLA:H43	18:X:14:LEU:HA	1.92	0.52
34:E:101:HEM:HBB2	34:E:101:HEM:HMB1	1.90	0.52
2:B:341:LYS:HG3	2:B:429:ILE:HG22	1.91	0.52
25:B:610:CLA:H111	25:B:615:CLA:HAA1	2.94	0.52
25:C:502:CLA:H52	25:C:504:CLA:H91	1.91	0.52
3:C:276:LEU:HD21	25:C:508:CLA:HAB	13.68	0.52
1:A:183:MET:HA	25:A:606:CLA:HMD2	1.90	0.52
25:A:607:CLA:HMD3	4:D:182:LEU:HD11	1.92	0.52
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:ASP:OD1	4:D:23:LYS:NZ	3.68	0.51
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.92	0.51
25:B:608:CLA:HAC2	25:B:609:CLA:H142	1.92	0.51
25:C:514:CLA:HMC2	27:C:515:BCR:H372	1.92	0.51
1:A:38:ILE:HD13	29:A:616:SQD:H131	1.92	0.51
25:B:607:CLA:HBC3	27:B:618:BCR:HC8	1.93	0.51
3:C:199:ILE:HG21	3:C:234:VAL:HG21	1.93	0.51
3:C:327:ASN:ND2	35:C:610:HOH:O	48.65	0.51
25:C:504:CLA:HMD2	25:C:504:CLA:H201	1.91	0.51
3:C:59:LEU:HD13	25:C:511:CLA:HMD2	1.93	0.51
3:C:132:HIS:CE1	25:C:514:CLA:NA	2.79	0.50
3:C:38:GLY:HA3	25:C:512:CLA:HMD3	1.92	0.50
2:B:469:HIS:HE1	25:B:611:CLA:NA	2.08	0.50
3:C:251:HIS:HE1	25:C:506:CLA:NA	18.64	0.50
3:C:444:HIS:CE1	25:C:509:CLA:NA	2.79	0.50
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.50
15:U:57:SER:HA	15:U:84:VAL:HG11	1.93	0.49
25:B:614:CLA:H142	29:B:624:SQD:H381	1.94	0.49
2:B:458:PHE:HB3	25:B:604:CLA:HBC2	2.04	0.49
25:B:608:CLA:H143	25:D:403:CLA:HMB2	1.95	0.49
2:B:299:GLU:HG2	2:B:402:TYR:HD1	7.28	0.49
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.10	0.49
25:B:613:CLA:H52	30:B:623:LHG:H362	1.93	0.49
2:B:265:ILE:HD12	2:B:270:PRO:HA	3.94	0.49
2:B:212:ALA:HB2	25:B:609:CLA:HMC3	2.03	0.49
2:B:86:ILE:HD12	2:B:88:PRO:HD3	1.94	0.49
25:A:606:CLA:H143	26:A:608:PHO:H61	37.60	0.49
2:B:490:GLN:HG2	2:B:496:TYR:HE2	1.78	0.48
25:B:606:CLA:H72	27:B:619:BCR:H311	1.94	0.48
3:C:167:VAL:HG11	25:C:513:CLA:HBA1	1.95	0.48
1:A:201:GLY:HA3	1:A:286:THR:HB	2.01	0.48
1:A:63:ILE:HB	3:C:335:THR:HG21	1.95	0.48
25:A:609:CLA:H51	25:C:506:CLA:H191	1.95	0.48
3:C:163:PHE:CG	25:C:512:CLA:HAB	25.99	0.48
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.03	0.48
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.99	0.48
25:B:602:CLA:HMD2	7:H:38:PHE:HZ	1.81	0.48
3:C:444:HIS:CE1	25:C:508:CLA:NA	15.05	0.48
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.12	0.48
1:A:229:GLU:HG2	2:B:476:ARG:HH12	1.79	0.48
15:U:28:ASN:ND2	15:U:84:VAL:HG23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:614:CLA:H161	25:B:614:CLA:H202	1.70	0.48
25:C:503:CLA:H161	25:C:503:CLA:H141	1.71	0.48
15:U:23:GLU:HG3	15:U:24:LYS:HG2	1.96	0.48
25:B:609:CLA:H43	25:B:610:CLA:HBB2	2.57	0.47
25:B:603:CLA:HAB	25:B:605:CLA:H152	1.94	0.47
25:C:509:CLA:HMB3	25:C:510:CLA:HAA1	7.61	0.47
2:B:171:PRO:HB3	7:H:63:LYS:HA	1.99	0.47
1:A:240:GLY:HA3	14:T:29:ILE:HG23	1.95	0.47
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	1.96	0.47
3:C:132:HIS:HE1	25:C:513:CLA:NA	12.18	0.47
3:C:167:VAL:HG13	25:C:512:CLA:H102	28.06	0.47
3:C:26:ARG:O	10:K:46:ARG:NH2	4.29	0.47
1:A:262:TYR:HD1	30:A:618:LHG:H242	1.79	0.47
25:B:604:CLA:H62	25:B:604:CLA:H41	3.15	0.47
25:B:610:CLA:HBD	25:B:610:CLA:H143	1.95	0.47
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.47
2:B:341:LYS:HE3	2:B:431:GLU:HB2	1.95	0.47
1:A:131:TRP:CH2	25:C:506:CLA:HAA2	2.49	0.47
3:C:170[B]:ILE:HD11	25:C:513:CLA:H61	1.94	0.47
30:D:406:LHG:H191	14:T:17:PHE:HZ	4.29	0.47
3:C:73:ALA:HB2	10:K:11:LEU:HD13	1.96	0.47
2:B:154:GLY:HA2	2:B:158:LEU:HD12	2.42	0.47
4:D:85:MET:HE3	4:D:107:LEU:HD13	4.65	0.47
20:R:17:GLY:O	20:R:21:ARG:HG2	2.15	0.47
2:B:201:HIS:HE1	25:B:602:CLA:ND	2.13	0.47
25:B:614:CLA:H91	25:B:614:CLA:H111	1.61	0.47
25:C:514:CLA:H41	25:C:514:CLA:H61	1.71	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.47
11:L:14:ARG:NH2	29:L:101:SQD:O2	2.44	0.47
25:C:510:CLA:H61	25:C:510:CLA:H2	4.33	0.47
25:C:513:CLA:HBA1	25:C:513:CLA:H3A	1.55	0.47
13:O:189:ARG:NE	35:O:306:HOH:O	2.47	0.47
13:O:32:ILE:HG21	13:O:93:LEU:HD21	1.96	0.47
16:V:13:ASN:HD21	16:V:17:LYS:HD3	3.34	0.46
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.96	0.46
27:H:101:BCR:H20C	27:H:101:BCR:H361	1.88	0.46
1:A:131:TRP:CH2	25:C:505:CLA:HAA2	41.11	0.46
25:A:607:CLA:H162	30:A:618:LHG:H383	1.96	0.46
4:D:54:PHE:O	5:E:49:THR:OG1	2.25	0.46
2:B:71:VAL:HG23	25:B:606:CLA:HMA2	1.96	0.46
32:C:521:LMG:HC71	32:C:521:LMG:O2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.97	0.46
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.61	0.46
25:B:602:CLA:H162	25:B:602:CLA:H143	2.76	0.46
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.98	0.46
1:A:179:THR:O	1:A:183:MET:HG3	2.16	0.46
1:A:45:THR:HG21	29:B:625:SQD:H362	56.39	0.46
28:A:611:PL9:H513	29:D:408:SQD:H372	1.97	0.46
4:D:103:ARG:HG3	5:E:73:LYS:HZ3	3.54	0.46
11:L:14:ARG:HB3	14:T:25:GLU:HG3	1.98	0.46
1:A:308:ASP:OD1	1:A:312:ASN:N	2.48	0.46
25:C:509:CLA:H192	33:C:518:DGD:HAW1	1.97	0.46
2:B:383:PHE:N	4:D:344:GLU:O	2.57	0.46
25:A:606:CLA:HBD	25:A:613:CLA:HAC2	1.98	0.45
25:B:614:CLA:HBA2	25:B:614:CLA:H11	1.57	0.45
25:C:509:CLA:H62	25:C:509:CLA:H93	2.68	0.45
5:E:36:LEU:HD13	20:R:7:VAL:HG12	4.82	0.45
34:V:201:HEM:HBB2	34:V:201:HEM:HMB2	1.98	0.45
3:C:455:PHE:HD2	8:I:33:LYS:HG3	2.07	0.45
25:C:503:CLA:H193	25:C:503:CLA:HMD2	21.39	0.45
25:C:506:CLA:H72	25:C:506:CLA:H112	1.78	0.45
25:C:505:CLA:H43	27:C:515:BCR:HC7	33.35	0.45
25:B:607:CLA:HAC2	27:T:101:BCR:H272	32.50	0.45
25:B:615:CLA:H203	25:B:615:CLA:H162	1.77	0.45
3:C:61:VAL:HG12	3:C:118:HIS:O	2.22	0.45
27:C:516:BCR:H24C	27:C:516:BCR:H371	1.84	0.45
10:K:43:VAL:HB	10:K:46:ARG:HE	4.41	0.45
34:V:201:HEM:HBC2	34:V:201:HEM:HMC2	2.03	0.45
25:C:505:CLA:H122	25:C:505:CLA:H162	5.29	0.45
25:C:509:CLA:H151	25:C:509:CLA:H111	4.02	0.45
27:B:619:BCR:H382	29:B:625:SQD:H82	1.99	0.45
30:B:623:LHG:H351	30:B:623:LHG:H101	1.98	0.45
3:C:288:CYS:SG	33:C:517:DGD:HB32	2.56	0.45
3:C:281:MET:HG3	32:C:501:LMG:H412	1.99	0.45
33:C:519:DGD:HAE2	33:C:519:DGD:HA82	1.71	0.45
2:B:155:ALA:O	2:B:159:THR:OG1	2.29	0.45
3:C:179:ALA:HA	3:C:184:GLY:HA2	2.03	0.45
25:C:508:CLA:H141	25:C:508:CLA:H162	1.71	0.45
19:Z:34:ASP:HA	19:Z:37:LYS:HE2	4.51	0.45
19:Z:61:VAL:HG23	19:Z:62:VAL:HG23	1.99	0.45
25:B:605:CLA:H92	25:B:605:CLA:H61	1.78	0.45
30:B:623:LHG:H151	30:L:102:LHG:H282	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.01	0.44
16:V:99:ASP:N	16:V:99:ASP:OD1	2.51	0.44
1:A:132:GLU:O	1:A:136:ARG:HG2	2.21	0.44
25:A:607:CLA:H112	25:A:607:CLA:H91	1.70	0.44
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.09	0.44
25:B:614:CLA:H61	25:B:614:CLA:H41	1.55	0.44
25:C:508:CLA:O1A	25:C:510:CLA:H51	2.18	0.44
25:C:509:CLA:HBB1	25:C:509:CLA:HMB1	2.32	0.44
30:D:406:LHG:H261	11:L:22:LEU:HD22	1.99	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.44
5:E:73:LYS:NZ	5:E:77:GLU:OE1	2.49	0.44
2:B:278:SER:HB3	2:B:281:GLN:HB3	1.99	0.44
3:C:163:PHE:CD2	25:C:512:CLA:HAB	25.71	0.44
25:B:603:CLA:H41	25:B:603:CLA:H61	1.94	0.44
25:B:611:CLA:H112	25:B:611:CLA:H72	1.81	0.44
25:B:615:CLA:H2	25:B:615:CLA:H62	1.74	0.44
20:R:18:TRP:O	20:R:22:ASN:ND2	2.49	0.44
15:U:42:TYR:HA	15:U:43:PRO:HA	1.89	0.44
2:B:464:PHE:HD2	25:B:611:CLA:HAC2	5.87	0.44
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.13	0.44
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.99	0.44
25:A:606:CLA:H143	25:A:606:CLA:H161	2.65	0.44
3:C:459:ILE:HG21	3:C:464:GLU:HG3	2.15	0.44
25:C:504:CLA:H192	25:C:504:CLA:H161	1.79	0.44
25:C:502:CLA:HMD2	25:C:503:CLA:H101	2.00	0.44
27:K:101:BCR:H15C	27:K:101:BCR:H351	1.86	0.44
13:O:27:ARG:HG3	13:O:138:THR:HG21	2.50	0.44
25:B:602:CLA:H203	33:H:102:DGD:HBT2	6.32	0.43
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.98	0.43
25:B:605:CLA:H161	25:B:605:CLA:H141	1.77	0.43
25:A:606:CLA:H102	25:A:606:CLA:H62	1.82	0.43
25:B:614:CLA:H172	32:B:620:LMG:H421	2.00	0.43
27:B:618:BCR:H371	27:B:618:BCR:H24C	1.86	0.43
4:D:128:ARG:NH1	35:D:507:HOH:O	55.04	0.43
27:D:404:BCR:H15C	27:D:404:BCR:H351	1.91	0.43
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	3.60	0.43
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.02	0.43
16:V:3:LEU:HD23	16:V:23:GLU:HG3	5.29	0.43
25:D:402:CLA:H192	25:D:402:CLA:H162	2.25	0.43
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.28	0.43
13:O:58:ASN:O	13:O:60:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:HA	1:A:109:GLY:HA3	2.01	0.43
5:E:33:ALA:HB2	20:R:11:PRO:HG2	3.25	0.43
13:O:88:ASN:ND2	13:O:92:SER:O	2.47	0.43
25:B:601:CLA:H111	25:B:601:CLA:H91	4.10	0.43
30:B:623:LHG:O4	4:D:141:TYR:OH	2.20	0.43
3:C:57:ALA:O	3:C:61:VAL:HG23	2.18	0.43
25:B:614:CLA:H93	25:B:614:CLA:H61	4.69	0.43
25:C:510:CLA:H142	25:C:510:CLA:H111	1.72	0.43
25:A:606:CLA:H152	25:A:606:CLA:H112	1.85	0.43
1:A:202:VAL:HG11	25:A:607:CLA:C3D	2.49	0.43
1:A:340:PRO:HG3	15:U:103:TYR:CG	2.54	0.42
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.83	0.42
4:D:195:PRO:HG3	11:L:34:TYR:CE1	3.44	0.42
2:B:158:LEU:HB3	2:B:199:VAL:HG22	2.27	0.42
25:B:604:CLA:H61	25:B:604:CLA:H41	1.84	0.42
3:C:154:LYS:HE2	3:C:261:ARG:HB2	2.01	0.42
27:T:101:BCR:H11C	27:T:101:BCR:H341	1.96	0.42
15:U:92:VAL:HG12	15:U:97:ARG:HD2	2.17	0.42
2:B:247:PHE:HB2	25:B:608:CLA:HBC1	1.99	0.42
4:D:195:PRO:HG3	11:L:34:TYR:CZ	3.67	0.42
1:A:283:VAL:HA	1:A:286:THR:HG22	2.01	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.02	0.42
27:T:101:BCR:H351	27:T:101:BCR:H15C	1.85	0.42
1:A:308:ASP:OD1	1:A:312:ASN:HB2	2.76	0.42
25:B:610:CLA:H93	25:B:615:CLA:HBA1	3.84	0.42
3:C:367:GLU:N	3:C:368:PRO:HD2	2.68	0.42
25:C:505:CLA:H162	25:C:509:CLA:H121	2.01	0.42
4:D:159:ILE:HG23	33:H:102:DGD:HBF2	2.01	0.42
27:Y:101:BCR:HC21	19:Z:13:VAL:HG13	2.01	0.42
27:B:618:BCR:H351	27:B:618:BCR:H15C	1.86	0.42
27:B:619:BCR:H351	27:B:619:BCR:H15C	1.90	0.42
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.00	0.42
27:H:101:BCR:H24C	27:H:101:BCR:H371	3.88	0.42
20:R:23:ILE:HG22	20:R:27:ALA:HB2	2.00	0.42
25:B:601:CLA:HED3	32:B:621:LMG:HC61	2.01	0.42
25:C:511:CLA:H141	19:Z:20:VAL:HG13	20.89	0.42
4:D:342:PRO:O	4:D:345:VAL:HG22	2.20	0.42
13:O:56:PRO:HA	13:O:57:LYS:HA	4.12	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.75	0.42
29:L:101:SQD:H111	29:L:101:SQD:H141	1.65	0.42
1:A:156:ALA:HA	1:A:160:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:HIS:HE1	25:C:507:CLA:NA	2.17	0.42
25:C:504:CLA:C17	25:C:511:CLA:HBB2	2.48	0.42
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.02	0.42
1:A:269:ARG:HD2	4:D:235:PHE:HB2	2.01	0.42
25:B:601:CLA:H12	25:B:601:CLA:H52	1.79	0.42
25:B:613:CLA:H141	25:B:613:CLA:H161	1.71	0.42
25:B:615:CLA:H62	25:B:616:CLA:HBB1	2.02	0.42
27:D:404:BCR:H19C	32:D:407:LMG:H352	2.02	0.42
4:D:259:ILE:HD13	30:D:406:LHG:H281	2.01	0.42
5:E:57:ALA:H	5:E:60[B]:GLN:NE2	2.17	0.42
27:K:101:BCR:H371	27:K:101:BCR:H24C	1.82	0.42
25:B:614:CLA:H43	29:L:101:SQD:H112	23.77	0.42
27:A:610:BCR:H15C	27:A:610:BCR:H351	1.87	0.41
32:B:626:LMG:HC8	32:B:626:LMG:HC1	1.36	0.41
27:B:619:BCR:H361	27:B:619:BCR:H20C	1.84	0.41
3:C:75:PHE:HZ	3:C:105:VAL:HG21	2.08	0.41
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.01	0.41
12:M:17:VAL:HB	12:M:18:PRO:HD3	2.03	0.41
14:T:4:ILE:HD13	27:T:101:BCR:H401	2.01	0.41
26:A:608:PHO:H192	26:A:608:PHO:H162	4.13	0.41
27:D:404:BCR:H24C	27:D:404:BCR:H371	1.89	0.41
25:A:607:CLA:H122	25:A:607:CLA:H8	4.58	0.41
25:B:615:CLA:H61	25:B:615:CLA:H93	1.80	0.41
25:C:511:CLA:H62	25:C:511:CLA:H92	3.25	0.41
5:E:18:ARG:NH2	34:E:101:HEM:O2A	3.16	0.41
13:O:33:ASP:HB3	13:O:36:GLN:HB2	2.10	0.41
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.66	0.41
26:A:608:PHO:H3A	25:D:402:CLA:H142	2.01	0.41
13:O:117:PRO:HG2	13:O:222:ASP:HB3	2.02	0.41
27:C:516:BCR:H20C	27:C:516:BCR:H361	1.86	0.41
2:B:228:ALA:HB1	29:D:409:SQD:H91	2.03	0.41
27:H:101:BCR:H351	27:H:101:BCR:H15C	1.93	0.41
27:Y:101:BCR:H24C	27:Y:101:BCR:H371	1.90	0.41
28:A:611:PL9:H421	28:A:611:PL9:H38	1.74	0.41
2:B:233:ASN:O	2:B:236:THR:HG22	2.26	0.41
2:B:422:ARG:O	2:B:425:ILE:HG12	2.29	0.41
25:B:601:CLA:H62	25:B:601:CLA:H93	1.79	0.41
25:C:504:CLA:H101	25:C:504:CLA:H13	1.85	0.41
13:O:153:THR:HA	13:O:190:PHE:HE2	1.98	0.41
13:O:184:ARG:NH2	13:O:226:GLY:O	4.42	0.41
27:Y:101:BCR:H20C	27:Y:101:BCR:H361	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:VAL:HG12	1:A:314:ILE:HB	2.03	0.41
4:D:261:PHE:CZ	30:D:406:LHG:HC81	2.56	0.41
13:O:52:VAL:HG11	13:O:116:ILE:HD12	3.50	0.41
16:V:126:LEU:HB3	16:V:129:LYS:HB3	2.03	0.41
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.03	0.41
30:A:618:LHG:H261	30:A:618:LHG:H292	1.96	0.41
2:B:368:VAL:HG21	2:B:422:ARG:HG2	2.01	0.41
25:B:615:CLA:H111	25:B:615:CLA:H143	4.35	0.41
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.86	0.41
29:D:408:SQD:H332	29:D:408:SQD:H361	1.92	0.41
2:B:36:SER:OG	27:B:618:BCR:H362	2.21	0.41
25:C:507:CLA:HBA1	25:C:507:CLA:H3A	2.55	0.41
33:C:517:DGD:HAF2	33:C:517:DGD:HAE1	3.94	0.41
3:C:94:THR:HG22	25:C:502:CLA:HED1	2.02	0.41
25:D:403:CLA:H142	7:H:40:VAL:HG21	2.02	0.41
5:E:68:ASP:OD1	5:E:69:ARG:N	2.54	0.41
1:A:307:ILE:HG22	1:A:313:VAL:HA	2.03	0.41
25:B:612:CLA:H122	25:B:612:CLA:H8	1.97	0.41
27:B:617:BCR:H341	27:B:617:BCR:H11C	1.93	0.41
3:C:162:GLY:HA3	3:C:252:ILE:HG13	2.14	0.41
25:C:509:CLA:H141	25:C:509:CLA:H161	1.78	0.41
27:C:515:BCR:H20C	27:C:515:BCR:H361	1.83	0.41
27:D:404:BCR:H341	27:D:404:BCR:H11C	1.95	0.41
13:O:32:ILE:HA	13:O:32:ILE:HD13	2.08	0.41
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.03	0.40
25:B:609:CLA:H141	25:B:609:CLA:H162	1.81	0.40
25:B:609:CLA:H61	25:B:609:CLA:H92	1.89	0.40
27:B:617:BCR:H361	27:B:617:BCR:H20C	1.85	0.40
3:C:363:GLY:O	3:C:367:GLU:HG2	2.24	0.40
2:B:479[A]:PHE:O	4:D:139:ARG:NH2	2.55	0.40
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.56	0.40
13:O:55:GLU:OE2	13:O:231:HIS:NE2	2.54	0.40
16:V:41:HIS:HA	16:V:45:ILE:O	2.22	0.40
25:A:606:CLA:H162	25:A:606:CLA:H192	1.80	0.40
3:C:437:PHE:CZ	25:C:511:CLA:HMB3	2.56	0.40
4:D:274:VAL:HB	4:D:275:PRO:HD3	2.03	0.40
5:E:68:ASP:O	5:E:72:ALA:HB2	2.36	0.40
25:C:505:CLA:HBC2	27:C:515:BCR:H341	26.51	0.40
10:K:43:VAL:HB	10:K:46:ARG:HD3	2.02	0.40
25:C:508:CLA:H122	25:C:508:CLA:H162	4.09	0.40
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:39:TRP:NE1	17:Y:46:LEU:O	2.39	0.40
25:A:607:CLA:O1A	25:A:607:CLA:H2	3.64	0.40
27:A:610:BCR:H24C	27:A:610:BCR:H371	1.80	0.40
27:B:617:BCR:H15C	27:B:617:BCR:H351	1.86	0.40
3:C:135:ARG:HA	3:C:135:ARG:HD2	1.91	0.40
3:C:282:MET:HE2	25:C:508:CLA:H42	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	327 (98%)	5 (2%)	1 (0%)	46	52
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	504/510 (99%)	491 (97%)	13 (3%)	0	100	100
3	C	450/461 (98%)	439 (98%)	10 (2%)	1 (0%)	52	61
3	c	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	52	61
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	10
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	35/38 (92%)	32 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	30 (94%)	1 (3%)	1 (3%)	5	2
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	244/272 (90%)	235 (96%)	8 (3%)	1 (0%)	39	43
13	o	244/272 (90%)	229 (94%)	11 (4%)	4 (2%)	12	7
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	136/163 (83%)	130 (96%)	5 (4%)	1 (1%)	26	26
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	1 (3%)	1 (3%)	6	3
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	11	6
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	32/41 (78%)	31 (97%)	1 (3%)	0	100	100
All	All	5258/5700 (92%)	5108 (97%)	137 (3%)	13 (0%)	52	61

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	53	LYS
13	o	58	ASN
3	C	416	SER

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Mol	Chain	Res	Type
3	c	416	SER
13	o	59	LYS
19	z	2	THR
13	o	54	GLU
13	O	59	LYS
5	E	6	GLY
12	M	32	GLN
18	X	3	ILE
16	v	16	GLY
1	A	259	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	270 (100%)	1 (0%)	93	96
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	407/407 (100%)	403 (99%)	4 (1%)	82	89
2	b	403/407 (99%)	402 (100%)	1 (0%)	95	98
3	C	353/362 (98%)	352 (100%)	1 (0%)	94	97
3	c	353/362 (98%)	349 (99%)	4 (1%)	80	88
4	D	276/283 (98%)	275 (100%)	1 (0%)	93	96
4	d	276/283 (98%)	275 (100%)	1 (0%)	93	96
5	E	73/73 (100%)	72 (99%)	1 (1%)	74	84
5	e	73/73 (100%)	72 (99%)	1 (1%)	74	84
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	41	50
7	h	53/55 (96%)	52 (98%)	1 (2%)	65	75
8	I	33/34 (97%)	32 (97%)	1 (3%)	48	59
8	i	32/34 (94%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	29 (97%)	1 (3%)	45	56
10	k	30/37 (81%)	29 (97%)	1 (3%)	45	56
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	209/228 (92%)	207 (99%)	2 (1%)	82	89
13	o	209/228 (92%)	207 (99%)	2 (1%)	82	89
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	118/138 (86%)	118 (100%)	0	100	100
17	Y	20/37 (54%)	20 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	31/34 (91%)	31 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	75
19	z	52/52 (100%)	51 (98%)	1 (2%)	65	75
20	R	29/33 (88%)	28 (97%)	1 (3%)	44	54
20	r	28/33 (85%)	28 (100%)	0	100	100
All	All	4359/4654 (94%)	4331 (99%)	28 (1%)	90	94

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
2	B	51	VAL
2	B	84	THR
2	B	246	PHE
2	B	362	PHE

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Mol	Chain	Res	Type
3	C	289	PHE
4	D	180	ARG
5	E	4	THR
7	H	21	VAL
7	H	49	TYR
8	I	37	LEU
10	K	10	LYS
13	O	118	LEU
13	O	207	ARG
19	Z	35	ARG
20	R	6	LEU
2	b	362	PHE
3	c	29	GLU
3	c	289	PHE
3	c	391[A]	ARG
3	c	391[B]	ARG
4	d	180	ARG
5	e	5	THR
7	h	49	TYR
10	k	19	ASP
13	o	61	GLN
13	o	118	LEU
19	z	46	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	HIS
2	B	285	ASN
2	B	490	GLN
5	E	82	GLN
12	M	32	GLN
13	O	3	GLN
13	O	82	GLN
15	U	63	ASN
16	V	86	GLN
19	Z	31	GLN
1	a	312	ASN
2	b	216	HIS
2	b	223	GLN
2	b	394	GLN
2	b	409	GLN

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Mol	Chain	Res	Type
3	c	25	ASN
3	c	418	ASN
5	e	74	GLN
13	o	200	ASN
16	v	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.87	0	5,9,11	0.82	0
12	FME	M	1	12	8,9,10	0.86	0	5,9,11	0.95	0
14	FME	T	1	14	8,9,10	0.84	0	5,9,11	0.84	0
8	FME	i	1	8	8,9,10	0.88	0	5,9,11	0.90	0
12	FME	m	1	12	8,9,10	0.87	0	5,9,11	0.82	0
14	FME	t	1	14	8,9,10	0.89	0	5,9,11	0.98	0

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
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 33 are unknown and 6 are monoatomic - leaving 151 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	$\# Z > 2$
21	OEX	A	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
24	BCT	A	605	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	A	606	-	57,73,73	1.13	4 (7%)	61,113,113	1.09	3 (4%)
25	CLA	A	607	35	57,73,73	1.14	5 (8%)	61,113,113	1.10	5 (8%)
26	PHO	A	608	-	67,69,69	1.24	9 (13%)	86,99,99	1.08	8 (9%)
25	CLA	A	609	-	46,62,73	1.26	5 (10%)	47,99,113	1.25	7 (14%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
28	PL9	A	611	-	54,55,55	0.84	2 (3%)	68,69,69	1.44	13 (19%)
29	SQD	A	612	-	51,52,54	0.96	5 (9%)	60,63,65	1.85	9 (15%)
25	CLA	A	613	35	57,73,73	1.13	4 (7%)	61,113,113	1.08	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	A	614	-	46,46,48	0.62	1 (2%)	47,52,54	1.25	5 (10%)
29	SQD	A	616	-	53,54,54	0.95	5 (9%)	62,65,65	1.79	9 (14%)
30	LHG	A	618	-	48,48,48	0.63	1 (2%)	49,54,54	1.25	6 (12%)
25	CLA	B	601	35	57,73,73	1.14	5 (8%)	61,113,113	1.10	5 (8%)
25	CLA	B	602	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	4 (6%)
25	CLA	B	603	-	57,73,73	1.13	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	B	604	-	57,73,73	1.15	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	B	605	-	57,73,73	1.12	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	B	606	-	57,73,73	1.15	5 (8%)	61,113,113	1.11	5 (8%)
25	CLA	B	607	35	57,73,73	1.11	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	B	608	-	57,73,73	1.13	4 (7%)	61,113,113	1.08	5 (8%)
25	CLA	B	609	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	7 (11%)
25	CLA	B	610	35	57,73,73	1.13	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	B	611	-	57,73,73	1.14	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	B	612	-	57,73,73	1.12	4 (7%)	61,113,113	1.18	7 (11%)
25	CLA	B	613	-	57,73,73	1.11	4 (7%)	61,113,113	1.20	6 (9%)
25	CLA	B	614	-	57,73,73	1.12	4 (7%)	61,113,113	1.12	7 (11%)
25	CLA	B	615	-	57,73,73	1.15	4 (7%)	61,113,113	1.11	7 (11%)
25	CLA	B	616	-	57,73,73	1.13	6 (10%)	61,113,113	1.17	6 (9%)
27	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	4 (7%)
27	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	5 (8%)
27	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.21	4 (7%)
32	LMG	B	620	-	51,51,55	0.71	0	59,59,63	1.34	6 (10%)
32	LMG	B	621	-	51,51,55	0.71	0	59,59,63	1.32	7 (11%)
30	LHG	B	623	-	48,48,48	0.61	0	49,54,54	1.27	6 (12%)
29	SQD	B	624	-	53,54,54	0.95	5 (9%)	62,65,65	1.90	10 (16%)
29	SQD	B	625	-	53,54,54	0.95	5 (9%)	62,65,65	1.78	9 (14%)
32	LMG	B	626	-	51,51,55	0.71	1 (1%)	59,59,63	1.29	4 (6%)
32	LMG	C	501	-	48,48,55	0.72	0	56,56,63	1.29	5 (8%)
25	CLA	C	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	C	503	-	57,73,73	1.13	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	C	504	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	C	505	35	57,73,73	1.14	5 (8%)	61,113,113	1.12	5 (8%)
25	CLA	C	506	-	57,73,73	1.12	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	C	507	-	57,73,73	1.14	5 (8%)	61,113,113	1.14	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	C	508	35	57,73,73	1.12	4 (7%)	61,113,113	1.15	6 (9%)
25	CLA	C	509	-	57,73,73	1.13	5 (8%)	61,113,113	1.15	6 (9%)
25	CLA	C	510	-	57,73,73	1.12	4 (7%)	61,113,113	1.16	5 (8%)
25	CLA	C	511	-	57,73,73	1.13	4 (7%)	61,113,113	1.11	5 (8%)
25	CLA	C	512	3	57,73,73	1.14	5 (8%)	61,113,113	1.09	6 (9%)
25	CLA	C	513	-	57,73,73	1.14	4 (7%)	61,113,113	1.14	6 (9%)
25	CLA	C	514	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
27	BCR	C	515	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	4 (7%)
27	BCR	C	516	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
33	DGD	C	517	-	63,63,67	0.81	0	77,77,81	1.35	8 (10%)
33	DGD	C	518	-	63,63,67	0.86	1 (1%)	77,77,81	1.41	9 (11%)
33	DGD	C	519	-	63,63,67	0.85	1 (1%)	77,77,81	1.39	11 (14%)
32	LMG	C	520	-	48,48,55	0.74	0	56,56,63	1.33	7 (12%)
32	LMG	C	521	-	51,51,55	0.77	1 (1%)	59,59,63	1.34	6 (10%)
26	PHO	D	401	-	67,69,69	1.24	7 (10%)	86,99,99	1.07	7 (8%)
25	CLA	D	402	-	57,73,73	1.14	5 (8%)	61,113,113	1.07	5 (8%)
25	CLA	D	403	-	57,73,73	1.11	5 (8%)	61,113,113	1.19	7 (11%)
27	BCR	D	404	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
28	PL9	D	405	-	54,55,55	0.82	1 (1%)	68,69,69	1.45	12 (17%)
30	LHG	D	406	-	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
32	LMG	D	407	-	51,51,55	0.71	0	59,59,63	1.31	6 (10%)
29	SQD	D	408	-	42,43,54	1.06	5 (11%)	51,54,65	2.03	9 (17%)
29	SQD	D	409	-	46,47,54	1.02	5 (10%)	55,58,65	1.95	10 (18%)
34	HEM	E	101	5,6	24,50,50	2.03	5 (20%)	16,82,82	1.43	3 (18%)
27	BCR	H	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
33	DGD	H	102	-	63,63,67	0.87	1 (1%)	77,77,81	1.36	7 (9%)
27	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
29	SQD	L	101	-	48,49,54	0.99	4 (8%)	57,60,65	1.92	10 (17%)
30	LHG	L	102	-	48,48,48	0.61	1 (2%)	49,54,54	1.24	6 (12%)
27	BCR	T	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	6 (10%)
34	HEM	V	201	16	24,50,50	1.94	4 (16%)	16,82,82	1.42	2 (12%)
27	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	3 (5%)
21	OEX	a	601	1,3,35	0,15,15	0.00	-	0,32,32	0.00	-
24	BCT	a	605	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	a	606	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	607	35	57,73,73	1.14	5 (8%)	61,113,113	1.09	4 (6%)
26	PHO	a	608	-	67,69,69	1.23	7 (10%)	86,99,99	1.07	8 (9%)
26	PHO	a	609	-	67,69,69	1.24	7 (10%)	86,99,99	1.07	7 (8%)
25	CLA	a	610	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	6 (9%)
27	BCR	a	611	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	5 (8%)
28	PL9	a	612	-	54,55,55	0.83	2 (3%)	68,69,69	1.44	12 (17%)
29	SQD	a	613	-	53,54,54	0.94	5 (9%)	62,65,65	1.79	8 (12%)
32	LMG	a	614	-	51,51,55	0.72	0	59,59,63	1.34	7 (11%)
25	CLA	a	615	35	57,73,73	1.14	4 (7%)	61,113,113	1.07	4 (6%)
30	LHG	a	616	-	38,38,48	0.68	1 (2%)	39,44,54	1.17	3 (7%)
30	LHG	a	617	-	41,41,48	0.66	0	42,47,54	1.33	6 (14%)
25	CLA	b	601	35	57,73,73	1.15	5 (8%)	61,113,113	1.10	5 (8%)
25	CLA	b	602	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	5 (8%)
25	CLA	b	603	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	6 (9%)
25	CLA	b	604	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	b	605	-	57,73,73	1.14	5 (8%)	61,113,113	1.10	5 (8%)
25	CLA	b	606[A]	-	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	b	606[B]	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	b	607	35	57,73,73	1.12	4 (7%)	61,113,113	1.10	5 (8%)
25	CLA	b	608	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	6 (9%)
25	CLA	b	609	-	57,73,73	1.14	4 (7%)	61,113,113	1.11	6 (9%)
25	CLA	b	610	35	57,73,73	1.14	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	b	611	-	57,73,73	1.12	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	b	612	-	57,73,73	1.13	4 (7%)	61,113,113	1.16	6 (9%)
25	CLA	b	613	-	57,73,73	1.12	4 (7%)	61,113,113	1.17	7 (11%)
25	CLA	b	614	-	57,73,73	1.13	4 (7%)	61,113,113	1.13	5 (8%)
25	CLA	b	615	-	57,73,73	1.16	4 (7%)	61,113,113	1.09	5 (8%)
25	CLA	b	616	-	39,55,73	1.36	6 (15%)	42,91,113	1.31	5 (11%)
27	BCR	b	617	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	5 (8%)
27	BCR	b	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	5 (8%)
27	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	3 (5%)
32	LMG	b	620	-	51,51,55	0.71	0	59,59,63	1.35	7 (11%)
29	SQD	b	621	-	39,39,54	0.86	2 (5%)	41,41,65	1.15	2 (4%)
25	CLA	c	501	-	57,73,73	1.13	4 (7%)	61,113,113	1.14	5 (8%)
25	CLA	c	502	-	57,73,73	1.14	5 (8%)	61,113,113	1.11	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	503	-	57,73,73	1.14	4 (7%)	61,113,113	1.12	5 (8%)
25	CLA	c	504	35	52,68,73	1.19	4 (7%)	55,107,113	1.15	6 (10%)
25	CLA	c	505	-	57,73,73	1.12	4 (7%)	61,113,113	1.13	5 (8%)
25	CLA	c	506	-	57,73,73	1.14	4 (7%)	61,113,113	1.09	6 (9%)
25	CLA	c	507	35	57,73,73	1.14	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	508	-	56,72,73	1.14	5 (8%)	59,111,113	1.17	6 (10%)
25	CLA	c	509	-	57,73,73	1.13	4 (7%)	61,113,113	1.15	7 (11%)
25	CLA	c	510	-	57,73,73	1.14	5 (8%)	61,113,113	1.14	5 (8%)
25	CLA	c	511	3	57,73,73	1.13	4 (7%)	61,113,113	1.10	6 (9%)
25	CLA	c	512	-	57,73,73	1.15	5 (8%)	61,113,113	1.13	6 (9%)
25	CLA	c	513	-	57,73,73	1.13	5 (8%)	61,113,113	1.12	5 (8%)
27	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	5 (8%)
27	BCR	c	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	4 (7%)
33	DGD	c	516	-	63,63,67	0.82	1 (1%)	77,77,81	1.42	9 (11%)
33	DGD	c	517	-	63,63,67	0.88	1 (1%)	77,77,81	1.38	8 (10%)
33	DGD	c	518	-	63,63,67	0.83	0	77,77,81	1.37	9 (11%)
32	LMG	c	519	-	37,37,55	0.84	0	45,45,63	1.35	7 (15%)
32	LMG	c	520	-	34,34,55	0.85	0	42,42,63	1.24	4 (9%)
27	BCR	c	521	-	41,41,41	1.12	3 (7%)	56,56,56	1.17	3 (5%)
27	BCR	c	522	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	4 (7%)
25	CLA	d	401	-	57,73,73	1.14	4 (7%)	61,113,113	1.07	7 (11%)
25	CLA	d	402	-	57,73,73	1.14	5 (8%)	61,113,113	1.08	5 (8%)
27	BCR	d	403	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	5 (8%)
28	PL9	d	404	-	54,55,55	0.86	3 (5%)	68,69,69	1.42	15 (22%)
30	LHG	d	405	-	48,48,48	0.60	0	49,54,54	1.28	6 (12%)
30	LHG	d	406	-	48,48,48	0.60	0	49,54,54	1.24	6 (12%)
32	LMG	d	407	-	51,51,55	0.72	0	59,59,63	1.34	7 (11%)
32	LMG	d	408	-	33,36,55	0.13	0	32,35,63	1.38	3 (9%)
34	HEM	e	101	5,6	24,50,50	2.12	4 (16%)	16,82,82	1.43	2 (12%)
29	SQD	f	101	-	40,41,54	1.08	5 (12%)	49,52,65	1.90	9 (18%)
27	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	6 (10%)
33	DGD	h	102	-	63,63,67	0.86	0	77,77,81	1.36	9 (11%)
30	LHG	l	101	-	48,48,48	0.61	0	49,54,54	1.24	6 (12%)
32	LMG	m	102	-	51,51,55	0.71	0	59,59,63	1.37	7 (11%)
27	BCR	t	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	v	201	16	24,50,50	1.93	5 (20%)	16,82,82	1.37	3 (18%)

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
21	OEX	A	601	1,3,35	-	0/0/68/68	0/0/6/6
24	BCT	A	605	22	-	0/0/0/0	0/0/0/0
25	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	607	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	A	608	-	-	0/53/103/103	0/1/6/6
25	CLA	A	609	-	3/3/17/25	0/24/122/135	0/0/9/9
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
28	PL9	A	611	-	-	0/53/73/73	0/1/1/1
29	SQD	A	612	-	-	0/47/67/69	0/1/1/1
25	CLA	A	613	35	3/3/20/25	0/37/135/135	0/0/9/9
30	LHG	A	614	-	-	0/51/51/53	0/0/0/0
29	SQD	A	616	-	-	0/49/69/69	0/1/1/1
30	LHG	A	618	-	-	0/53/53/53	0/0/0/0
25	CLA	B	601	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	607	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
32	LMG	B	620	-	-	0/46/66/70	0/1/1/1
32	LMG	B	621	-	-	0/46/66/70	0/1/1/1
30	LHG	B	623	-	-	0/53/53/53	0/0/0/0
29	SQD	B	624	-	-	0/49/69/69	0/1/1/1
29	SQD	B	625	-	-	0/49/69/69	0/1/1/1
32	LMG	B	626	-	-	0/46/66/70	0/1/1/1
32	LMG	C	501	-	-	0/43/63/70	0/1/1/1
25	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	505	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	514	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	BCR	C	516	-	-	0/29/63/63	0/2/2/2
33	DGD	C	517	-	-	0/51/91/95	0/2/2/2
33	DGD	C	518	-	-	0/51/91/95	0/2/2/2
33	DGD	C	519	-	-	0/51/91/95	0/2/2/2
32	LMG	C	520	-	-	0/43/63/70	0/1/1/1
32	LMG	C	521	-	-	1/46/66/70	0/1/1/1
26	PHO	D	401	-	-	0/53/103/103	0/1/6/6
25	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	D	404	-	-	0/29/63/63	0/2/2/2
28	PL9	D	405	-	-	0/53/73/73	0/1/1/1
30	LHG	D	406	-	-	0/53/53/53	0/0/0/0
32	LMG	D	407	-	-	0/46/66/70	0/1/1/1
29	SQD	D	408	-	-	0/38/58/69	0/1/1/1
29	SQD	D	409	-	-	0/42/62/69	0/1/1/1
34	HEM	E	101	5,6	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	H	101	-	-	0/29/63/63	0/2/2/2
33	DGD	H	102	-	-	0/51/91/95	0/2/2/2
27	BCR	K	101	-	-	0/29/63/63	0/2/2/2
29	SQD	L	101	-	-	0/44/64/69	0/1/1/1
30	LHG	L	102	-	-	0/53/53/53	0/0/0/0
27	BCR	T	101	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	0/0/8/8
27	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
21	OEX	a	601	1,3,35	-	0/0/68/68	0/0/6/6
24	BCT	a	605	22	-	0/0/0/0	0/0/0/0
25	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	607	35	3/3/20/25	0/37/135/135	0/0/9/9
26	PHO	a	608	-	-	0/53/103/103	0/1/6/6
26	PHO	a	609	-	-	0/53/103/103	0/1/6/6
25	CLA	a	610	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	a	611	-	-	0/29/63/63	0/2/2/2
28	PL9	a	612	-	-	0/53/73/73	0/1/1/1
29	SQD	a	613	-	-	0/49/69/69	0/1/1/1
32	LMG	a	614	-	-	0/46/66/70	0/1/1/1
25	CLA	a	615	35	3/3/20/25	0/37/135/135	0/0/9/9
30	LHG	a	616	-	-	0/43/43/53	0/0/0/0
30	LHG	a	617	-	-	0/46/46/53	0/0/0/0
25	CLA	b	601	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	606[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	606[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	607	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	610	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	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
25	CLA	b	616	-	3/3/16/25	0/16/114/135	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
32	LMG	b	620	-	-	0/46/66/70	0/1/1/1
29	SQD	b	621	-	-	0/41/41/69	0/0/0/1
25	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	35	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	507	35	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	508	-	3/3/19/25	0/36/134/135	0/0/9/9
25	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	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
33	DGD	c	516	-	-	0/51/91/95	0/2/2/2
33	DGD	c	517	-	-	0/51/91/95	0/2/2/2
33	DGD	c	518	-	-	0/51/91/95	0/2/2/2
32	LMG	c	519	-	-	0/31/51/70	0/1/1/1
32	LMG	c	520	-	-	0/29/49/70	0/1/1/1
27	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	BCR	c	522	-	-	0/29/63/63	0/2/2/2
25	CLA	d	401	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	d	403	-	-	0/29/63/63	0/2/2/2
28	PL9	d	404	-	-	0/53/73/73	0/1/1/1
30	LHG	d	405	-	-	0/53/53/53	0/0/0/0
30	LHG	d	406	-	-	0/53/53/53	0/0/0/0
32	LMG	d	407	-	-	0/46/66/70	0/1/1/1
32	LMG	d	408	-	-	0/30/32/70	0/0/0/1
34	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
29	SQD	f	101	-	-	0/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
33	DGD	h	102	-	-	0/51/91/95	0/2/2/2
30	LHG	l	101	-	-	0/53/53/53	0/0/0/0
32	LMG	m	102	-	-	0/46/66/70	0/1/1/1
27	BCR	t	101	-	-	0/29/63/63	0/2/2/2
34	HEM	v	201	16	-	0/6/54/54	0/0/8/8

All (469) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	e	101	HEM	C3B-C2B	-5.17	1.33	1.40
34	e	101	HEM	C3C-C2C	-5.05	1.33	1.40
34	E	101	HEM	C3C-C2C	-5.04	1.34	1.40
34	E	101	HEM	C3B-C2B	-4.09	1.35	1.40
34	v	201	HEM	C3B-C2B	-4.01	1.35	1.40
34	V	201	HEM	C3B-C2B	-4.00	1.35	1.40
34	V	201	HEM	C3C-C2C	-3.99	1.35	1.40
34	v	201	HEM	C3C-C2C	-3.86	1.35	1.40
27	d	403	BCR	C1-C6	-3.48	1.49	1.53
27	Y	101	BCR	C1-C6	-3.47	1.49	1.53
27	C	516	BCR	C1-C6	-3.47	1.49	1.53
27	c	522	BCR	C1-C6	-3.46	1.49	1.53
27	t	101	BCR	C1-C6	-3.44	1.49	1.53
27	c	515	BCR	C1-C6	-3.43	1.49	1.53
27	b	617	BCR	C1-C6	-3.41	1.49	1.53
27	c	521	BCR	C1-C6	-3.40	1.49	1.53
27	K	101	BCR	C1-C6	-3.39	1.49	1.53
27	B	618	BCR	C1-C6	-3.39	1.49	1.53
27	b	618	BCR	C1-C6	-3.35	1.49	1.53
27	h	101	BCR	C1-C6	-3.30	1.49	1.53
27	A	610	BCR	C1-C6	-3.29	1.49	1.53
27	a	611	BCR	C1-C6	-3.26	1.49	1.53
27	Y	101	BCR	C30-C25	-3.24	1.49	1.53
27	H	101	BCR	C30-C25	-3.23	1.49	1.53
27	t	101	BCR	C30-C25	-3.15	1.49	1.53
27	c	514	BCR	C30-C25	-3.15	1.49	1.53
27	C	515	BCR	C1-C6	-3.11	1.49	1.53
27	b	619	BCR	C1-C6	-3.11	1.49	1.53
27	D	404	BCR	C30-C25	-3.11	1.49	1.53
27	H	101	BCR	C1-C6	-3.10	1.49	1.53
27	D	404	BCR	C1-C6	-3.08	1.49	1.53
27	T	101	BCR	C30-C25	-3.07	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	521	BCR	C30-C25	-3.07	1.49	1.53
27	b	617	BCR	C30-C25	-3.07	1.49	1.53
27	b	618	BCR	C30-C25	-3.06	1.49	1.53
27	C	515	BCR	C30-C25	-3.06	1.49	1.53
27	c	515	BCR	C30-C25	-3.05	1.49	1.53
27	c	514	BCR	C1-C6	-3.05	1.49	1.53
27	a	611	BCR	C30-C25	-3.04	1.49	1.53
27	A	610	BCR	C30-C25	-3.04	1.49	1.53
27	B	617	BCR	C1-C6	-3.01	1.49	1.53
27	B	619	BCR	C1-C6	-3.00	1.49	1.53
27	B	617	BCR	C30-C25	-2.99	1.49	1.53
27	T	101	BCR	C1-C6	-2.96	1.49	1.53
27	C	516	BCR	C30-C25	-2.94	1.49	1.53
27	B	618	BCR	C30-C25	-2.92	1.49	1.53
27	h	101	BCR	C30-C25	-2.89	1.49	1.53
27	B	619	BCR	C30-C25	-2.89	1.49	1.53
27	c	522	BCR	C30-C25	-2.88	1.49	1.53
27	b	619	BCR	C30-C25	-2.87	1.49	1.53
27	K	101	BCR	C30-C25	-2.87	1.49	1.53
27	d	403	BCR	C30-C25	-2.80	1.50	1.53
28	d	404	PL9	C3-C4	-2.63	1.45	1.49
25	B	611	CLA	CMB-C2B	-2.55	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.53	1.46	1.51
25	B	604	CLA	CMB-C2B	-2.52	1.46	1.51
25	c	506	CLA	CMB-C2B	-2.51	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.50	1.46	1.51
25	B	615	CLA	CMB-C2B	-2.49	1.46	1.51
25	A	607	CLA	CMB-C2B	-2.48	1.46	1.51
25	d	402	CLA	CMB-C2B	-2.47	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.47	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.47	1.46	1.51
25	a	607	CLA	CMB-C2B	-2.47	1.46	1.51
28	D	405	PL9	C3-C4	-2.47	1.45	1.49
25	c	504	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.47	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.46	1.46	1.51
25	A	609	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	609	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	601	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.46	1.46	1.51
25	b	606[B]	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	508	CLA	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	604	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	606[A]	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.45	1.46	1.51
25	d	401	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	603	CLA	CMB-C2B	-2.45	1.46	1.51
25	A	613	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.45	1.46	1.51
25	a	615	CLA	CMB-C2B	-2.44	1.46	1.51
28	a	612	PL9	C3-C4	-2.44	1.45	1.49
25	b	608	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.44	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	506	CLA	CMD-C2D	-2.43	1.46	1.51
25	B	601	CLA	CMB-C2B	-2.43	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	506	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	504	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.42	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.42	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.42	1.46	1.51
25	C	502	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	613	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	613	CLA	CMB-C2B	-2.41	1.46	1.51
25	C	507	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.41	1.46	1.51
25	C	514	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	614	CLA	CMB-C2B	-2.41	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	608	CLA	CMB-C2B	-2.40	1.46	1.51
25	D	402	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	501	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	602	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.39	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	611	PL9	C3-C4	-2.39	1.45	1.49
25	C	511	CLA	CMD-C2D	-2.39	1.46	1.51
25	b	605	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.38	1.46	1.51
33	C	519	DGD	O1G-C1G	-2.38	1.39	1.45
25	C	509	CLA	CMB-C2B	-2.38	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.38	1.46	1.51
25	a	610	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.37	1.46	1.51
25	c	505	CLA	CMD-C2D	-2.36	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.36	1.46	1.51
25	B	605	CLA	CMB-C2B	-2.36	1.46	1.51
25	A	606	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	510	CLA	CMD-C2D	-2.35	1.46	1.51
25	B	605	CLA	CMD-C2D	-2.34	1.46	1.51
25	B	604	CLA	CMD-C2D	-2.34	1.46	1.51
25	a	606	CLA	CMB-C2B	-2.33	1.46	1.51
25	c	503	CLA	CMD-C2D	-2.33	1.46	1.51
25	B	606	CLA	CMD-C2D	-2.33	1.46	1.51
25	C	513	CLA	CMD-C2D	-2.32	1.46	1.51
25	b	612	CLA	CMD-C2D	-2.32	1.46	1.51
25	B	612	CLA	CMB-C2B	-2.31	1.46	1.51
25	b	605	CLA	CMD-C2D	-2.31	1.46	1.51
25	C	502	CLA	CMD-C2D	-2.31	1.46	1.51
25	b	603	CLA	CMD-C2D	-2.31	1.46	1.51
25	b	615	CLA	CMD-C2D	-2.31	1.46	1.51
25	A	606	CLA	CMD-C2D	-2.31	1.46	1.51
25	b	607	CLA	CMD-C2D	-2.30	1.46	1.51
25	B	608	CLA	CMD-C2D	-2.30	1.46	1.51
25	B	603	CLA	CMD-C2D	-2.30	1.46	1.51
25	D	402	CLA	CMD-C2D	-2.30	1.46	1.51
25	B	612	CLA	CMD-C2D	-2.30	1.46	1.51
25	a	607	CLA	CMD-C2D	-2.30	1.46	1.51
25	c	502	CLA	CMD-C2D	-2.29	1.46	1.51
25	d	401	CLA	CMD-C2D	-2.29	1.46	1.51
25	c	509	CLA	CMD-C2D	-2.29	1.46	1.51
25	b	613	CLA	CMD-C2D	-2.29	1.46	1.51
25	a	610	CLA	CMD-C2D	-2.29	1.46	1.51
25	b	610	CLA	CMD-C2D	-2.29	1.46	1.51
25	a	606	CLA	CMD-C2D	-2.29	1.46	1.51
25	B	601	CLA	CMD-C2D	-2.29	1.46	1.51
25	C	510	CLA	CMD-C2D	-2.29	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	610	CLA	CMD-C2D	-2.28	1.46	1.51
25	B	611	CLA	CMD-C2D	-2.28	1.46	1.51
28	d	404	PL9	C6-C1	-2.28	1.44	1.48
33	c	516	DGD	O1G-C1G	-2.28	1.40	1.45
25	b	601	CLA	CMD-C2D	-2.28	1.46	1.51
25	A	607	CLA	CMD-C2D	-2.28	1.46	1.51
26	A	608	PHO	C1C-NC	-2.28	1.33	1.38
25	C	503	CLA	CMD-C2D	-2.27	1.46	1.51
25	c	501	CLA	CMD-C2D	-2.27	1.46	1.51
25	C	504	CLA	CMD-C2D	-2.27	1.46	1.51
25	c	504	CLA	CMD-C2D	-2.27	1.46	1.51
25	d	402	CLA	CMD-C2D	-2.27	1.46	1.51
25	B	602	CLA	CMD-C2D	-2.27	1.46	1.51
25	c	513	CLA	CMD-C2D	-2.27	1.46	1.51
25	B	613	CLA	CMD-C2D	-2.27	1.46	1.51
25	c	506	CLA	CMD-C2D	-2.26	1.46	1.51
25	D	403	CLA	CMD-C2D	-2.26	1.46	1.51
33	C	518	DGD	O1G-C1G	-2.26	1.40	1.45
25	C	507	CLA	CMD-C2D	-2.26	1.46	1.51
26	D	401	PHO	C1C-NC	-2.26	1.33	1.38
25	b	606[A]	CLA	CMD-C2D	-2.26	1.46	1.51
25	A	609	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	608	CLA	CMD-C2D	-2.25	1.46	1.51
25	C	505	CLA	CMD-C2D	-2.25	1.46	1.51
25	C	514	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	602	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	611	CLA	CMD-C2D	-2.25	1.46	1.51
25	b	606[B]	CLA	CMD-C2D	-2.25	1.46	1.51
25	c	507	CLA	CMD-C2D	-2.25	1.46	1.51
25	c	512	CLA	CMD-C2D	-2.25	1.46	1.51
25	c	508	CLA	CMD-C2D	-2.25	1.46	1.51
25	c	511	CLA	CMD-C2D	-2.25	1.46	1.51
25	B	615	CLA	CMD-C2D	-2.24	1.46	1.51
25	b	616	CLA	CMD-C2D	-2.24	1.46	1.51
26	a	608	PHO	C1C-NC	-2.24	1.33	1.38
25	C	512	CLA	CMD-C2D	-2.23	1.46	1.51
25	b	609	CLA	CMD-C2D	-2.23	1.46	1.51
25	B	609	CLA	CMD-C2D	-2.23	1.46	1.51
30	L	102	LHG	O7-C5	-2.23	1.40	1.46
26	a	609	PHO	C1C-NC	-2.21	1.33	1.38
25	C	509	CLA	CMD-C2D	-2.21	1.46	1.51
25	B	616	CLA	CMD-C2D	-2.21	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	604	CLA	CMD-C2D	-2.20	1.46	1.51
25	C	508	CLA	CMD-C2D	-2.20	1.46	1.51
25	B	607	CLA	CMD-C2D	-2.20	1.46	1.51
25	b	614	CLA	CMD-C2D	-2.19	1.46	1.51
25	a	615	CLA	CMD-C2D	-2.19	1.46	1.51
25	A	613	CLA	CMD-C2D	-2.19	1.46	1.51
25	B	614	CLA	CMD-C2D	-2.19	1.46	1.51
29	f	101	SQD	O2-C2	-2.18	1.37	1.43
29	A	612	SQD	O2-C2	-2.17	1.37	1.43
29	D	408	SQD	O2-C2	-2.17	1.37	1.43
29	a	613	SQD	O2-C2	-2.17	1.37	1.43
29	L	101	SQD	O2-C2	-2.16	1.37	1.43
29	B	625	SQD	O2-C2	-2.14	1.37	1.43
33	H	102	DGD	O1G-C1G	-2.12	1.40	1.45
29	B	624	SQD	O2-C2	-2.10	1.38	1.43
29	A	616	SQD	O2-C2	-2.09	1.38	1.43
28	A	611	PL9	C53-C6	-2.09	1.46	1.50
33	c	517	DGD	O1G-C1G	-2.09	1.40	1.45
29	D	409	SQD	O2-C2	-2.09	1.38	1.43
28	a	612	PL9	C53-C6	-2.07	1.46	1.50
29	f	101	SQD	O3-C3	-2.06	1.38	1.43
28	d	404	PL9	C53-C6	-2.06	1.46	1.50
29	f	101	SQD	O4-C4	-2.05	1.38	1.43
29	D	409	SQD	O3-C3	-2.05	1.38	1.43
25	b	616	CLA	CMC-C2C	-2.04	1.46	1.50
29	B	625	SQD	O4-C4	-2.04	1.38	1.43
29	B	624	SQD	O4-C4	-2.04	1.38	1.43
29	D	408	SQD	O4-C4	-2.03	1.38	1.43
29	D	409	SQD	O4-C4	-2.03	1.38	1.43
25	B	616	CLA	CMC-C2C	-2.03	1.46	1.50
29	A	616	SQD	O4-C4	-2.03	1.38	1.43
29	A	612	SQD	O3-C3	-2.02	1.38	1.43
29	B	625	SQD	O3-C3	-2.02	1.38	1.43
29	A	616	SQD	O3-C3	-2.02	1.38	1.43
29	A	612	SQD	O4-C4	-2.02	1.38	1.43
29	a	613	SQD	O4-C4	-2.02	1.38	1.43
29	D	408	SQD	O3-C3	-2.02	1.38	1.43
29	L	101	SQD	O3-C3	-2.01	1.38	1.43
29	a	613	SQD	O3-C3	-2.01	1.38	1.43
29	B	624	SQD	O3-C3	-2.01	1.38	1.43
25	B	606	CLA	CMC-C2C	-2.00	1.46	1.50
27	c	521	BCR	C33-C5	-2.00	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	C4C-NC	2.00	1.40	1.37
25	b	601	CLA	C4C-NC	2.01	1.40	1.37
25	D	402	CLA	C4C-NC	2.01	1.40	1.37
26	A	608	PHO	C1B-C2B	2.01	1.50	1.45
25	C	514	CLA	C4C-NC	2.01	1.40	1.37
25	C	509	CLA	C4C-NC	2.02	1.40	1.37
25	C	507	CLA	C4C-NC	2.02	1.40	1.37
30	a	616	LHG	P-O6	2.02	1.67	1.59
34	v	201	HEM	CAD-C3D	2.02	1.54	1.52
30	A	618	LHG	P-O6	2.02	1.67	1.59
25	C	502	CLA	C4C-NC	2.02	1.40	1.37
25	C	505	CLA	C4C-NC	2.03	1.40	1.37
26	A	608	PHO	C4B-NB	2.04	1.41	1.36
25	c	502	CLA	C4C-NC	2.04	1.40	1.37
25	d	402	CLA	C4C-NC	2.04	1.40	1.37
25	B	601	CLA	C4C-NC	2.04	1.40	1.37
25	b	608	CLA	C4C-NC	2.04	1.40	1.37
25	b	616	CLA	C4C-NC	2.04	1.40	1.37
25	A	609	CLA	C4C-NC	2.05	1.40	1.37
30	A	614	LHG	P-O6	2.05	1.67	1.59
25	c	512	CLA	C4C-NC	2.05	1.40	1.37
25	B	616	CLA	C4C-NC	2.06	1.40	1.37
25	c	508	CLA	C4C-NC	2.06	1.40	1.37
25	a	607	CLA	C4C-NC	2.07	1.40	1.37
34	E	101	HEM	CAD-C3D	2.07	1.54	1.52
25	c	513	CLA	C4C-NC	2.08	1.40	1.37
25	D	403	CLA	C4C-NC	2.10	1.40	1.37
25	c	510	CLA	C4C-NC	2.10	1.40	1.37
25	C	512	CLA	C4C-NC	2.10	1.40	1.37
25	A	607	CLA	C4C-NC	2.11	1.40	1.37
25	a	606	CLA	C4C-NC	2.13	1.40	1.37
32	B	626	LMG	C7-C8	2.15	1.56	1.50
26	A	608	PHO	CHD-C1D	2.18	1.43	1.38
26	D	401	PHO	CHD-C1D	2.23	1.43	1.38
26	a	608	PHO	CHD-C1D	2.24	1.43	1.38
26	a	609	PHO	CHD-C1D	2.26	1.43	1.38
26	a	608	PHO	C4C-C3C	2.28	1.49	1.45
26	A	608	PHO	C4C-C3C	2.28	1.49	1.45
26	a	609	PHO	C4C-C3C	2.31	1.49	1.45
26	D	401	PHO	C4C-C3C	2.38	1.49	1.45
32	C	521	LMG	C1-C2	2.39	1.59	1.52
26	a	608	PHO	C1A-NA	2.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	609	PHO	C1A-NA	2.52	1.42	1.37
26	D	401	PHO	C1A-NA	2.58	1.42	1.37
25	B	609	CLA	CHC-C1C	2.58	1.42	1.35
26	A	608	PHO	C1A-NA	2.58	1.43	1.37
25	c	507	CLA	CHC-C1C	2.58	1.42	1.35
25	b	615	CLA	CHC-C1C	2.59	1.42	1.35
25	B	613	CLA	CHC-C1C	2.60	1.42	1.35
26	a	608	PHO	C4C-NC	2.60	1.42	1.36
25	B	604	CLA	CHC-C1C	2.60	1.43	1.35
25	c	503	CLA	CHC-C1C	2.61	1.43	1.35
25	b	612	CLA	CHC-C1C	2.61	1.43	1.35
25	b	611	CLA	CHC-C1C	2.62	1.43	1.35
26	A	608	PHO	C4C-NC	2.63	1.42	1.36
25	A	609	CLA	CHC-C1C	2.63	1.43	1.35
25	b	610	CLA	CHC-C1C	2.63	1.43	1.35
25	C	503	CLA	CHC-C1C	2.63	1.43	1.35
25	b	607	CLA	CHC-C1C	2.63	1.43	1.35
25	C	508	CLA	CHC-C1C	2.64	1.43	1.35
25	C	509	CLA	CHC-C1C	2.64	1.43	1.35
25	B	615	CLA	CHC-C1C	2.64	1.43	1.35
25	b	609	CLA	CHC-C1C	2.65	1.43	1.35
25	B	608	CLA	CHC-C1C	2.65	1.43	1.35
25	D	402	CLA	CHC-C1C	2.65	1.43	1.35
25	c	506	CLA	CHC-C1C	2.65	1.43	1.35
25	C	510	CLA	CHC-C1C	2.65	1.43	1.35
25	c	510	CLA	CHC-C1C	2.65	1.43	1.35
25	B	611	CLA	CHC-C1C	2.65	1.43	1.35
25	c	502	CLA	CHC-C1C	2.65	1.43	1.35
25	d	401	CLA	CHC-C1C	2.65	1.43	1.35
25	C	502	CLA	CHC-C1C	2.66	1.43	1.35
25	c	504	CLA	CHC-C1C	2.66	1.43	1.35
25	b	601	CLA	CHC-C1C	2.66	1.43	1.35
25	B	606	CLA	CHC-C1C	2.66	1.43	1.35
25	B	616	CLA	CHC-C1C	2.66	1.43	1.35
25	c	501	CLA	CHC-C1C	2.67	1.43	1.35
25	D	403	CLA	CHC-C1C	2.67	1.43	1.35
25	a	610	CLA	CHC-C1C	2.67	1.43	1.35
25	B	603	CLA	CHC-C1C	2.67	1.43	1.35
25	C	512	CLA	CHC-C1C	2.67	1.43	1.35
26	a	609	PHO	C4C-NC	2.68	1.43	1.36
25	C	507	CLA	CHC-C1C	2.68	1.43	1.35
29	a	613	SQD	O47-C7	2.68	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	CHC-C1C	2.68	1.43	1.35
29	A	612	SQD	O47-C7	2.68	1.42	1.34
25	C	514	CLA	CHC-C1C	2.68	1.43	1.35
25	b	616	CLA	CHC-C1C	2.68	1.43	1.35
25	A	606	CLA	CHC-C1C	2.68	1.43	1.35
25	b	606[B]	CLA	CHC-C1C	2.68	1.43	1.35
25	C	513	CLA	CHC-C1C	2.69	1.43	1.35
25	b	603	CLA	CHC-C1C	2.69	1.43	1.35
25	c	508	CLA	CHC-C1C	2.69	1.43	1.35
25	b	606[A]	CLA	CHC-C1C	2.69	1.43	1.35
25	B	601	CLA	CHC-C1C	2.69	1.43	1.35
25	B	612	CLA	CHC-C1C	2.69	1.43	1.35
25	B	610	CLA	CHC-C1C	2.69	1.43	1.35
25	B	607	CLA	CHC-C1C	2.70	1.43	1.35
25	b	613	CLA	CHC-C1C	2.70	1.43	1.35
25	B	605	CLA	CHC-C1C	2.70	1.43	1.35
25	a	606	CLA	CHC-C1C	2.70	1.43	1.35
25	A	613	CLA	CHC-C1C	2.70	1.43	1.35
25	b	614	CLA	CHC-C1C	2.70	1.43	1.35
25	C	504	CLA	CHC-C1C	2.71	1.43	1.35
25	B	602	CLA	CHC-C1C	2.71	1.43	1.35
25	A	607	CLA	CHC-C1C	2.71	1.43	1.35
25	b	602	CLA	CHC-C1C	2.71	1.43	1.35
25	C	506	CLA	CHC-C1C	2.72	1.43	1.35
25	a	607	CLA	CHC-C1C	2.72	1.43	1.35
25	b	605	CLA	CHC-C1C	2.72	1.43	1.35
26	D	401	PHO	C4C-NC	2.72	1.43	1.36
29	L	101	SQD	O47-C7	2.72	1.42	1.34
25	a	615	CLA	CHC-C1C	2.73	1.43	1.35
29	f	101	SQD	O47-C7	2.73	1.42	1.34
25	b	604	CLA	CHC-C1C	2.73	1.43	1.35
25	c	511	CLA	CHC-C1C	2.73	1.43	1.35
25	c	512	CLA	CHC-C1C	2.73	1.43	1.35
25	C	505	CLA	CHC-C1C	2.74	1.43	1.35
25	B	614	CLA	CHC-C1C	2.74	1.43	1.35
25	d	402	CLA	CHC-C1C	2.75	1.43	1.35
25	c	505	CLA	CHC-C1C	2.75	1.43	1.35
25	C	511	CLA	CHC-C1C	2.75	1.43	1.35
25	c	513	CLA	CHC-C1C	2.76	1.43	1.35
29	A	616	SQD	O47-C7	2.78	1.42	1.34
29	B	625	SQD	O47-C7	2.78	1.42	1.34
29	D	409	SQD	O47-C7	2.78	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	408	SQD	O47-C7	2.79	1.42	1.34
29	B	624	SQD	O47-C7	2.79	1.42	1.34
29	b	621	SQD	O47-C7	2.79	1.42	1.34
25	b	608	CLA	CHC-C1C	2.80	1.43	1.35
26	a	608	PHO	CHC-C1C	2.82	1.44	1.38
26	D	401	PHO	CHC-C1C	2.88	1.44	1.38
26	a	609	PHO	CHC-C1C	2.98	1.44	1.38
26	A	608	PHO	CHC-C1C	2.99	1.44	1.38
29	B	624	SQD	O48-C23	3.00	1.42	1.33
29	a	613	SQD	O48-C23	3.04	1.42	1.33
29	A	612	SQD	O48-C23	3.06	1.42	1.33
29	D	409	SQD	O48-C23	3.09	1.42	1.33
29	L	101	SQD	O48-C23	3.09	1.42	1.33
29	D	408	SQD	O48-C23	3.09	1.42	1.33
29	f	101	SQD	O48-C23	3.09	1.42	1.33
29	B	625	SQD	O48-C23	3.10	1.42	1.33
29	A	616	SQD	O48-C23	3.10	1.42	1.33
29	b	621	SQD	O48-C23	3.13	1.42	1.33
34	e	101	HEM	C3B-CAB	3.47	1.55	1.47
26	D	401	PHO	C3B-C4B	3.49	1.50	1.43
26	a	608	PHO	C3B-C4B	3.52	1.50	1.43
26	A	608	PHO	C3B-C4B	3.56	1.50	1.43
25	D	403	CLA	CHB-C4A	3.56	1.38	1.33
26	a	609	PHO	C3B-C4B	3.61	1.50	1.43
34	E	101	HEM	C3C-CAC	3.65	1.55	1.47
34	e	101	HEM	C3C-CAC	3.66	1.55	1.47
34	E	101	HEM	C3B-CAB	3.68	1.55	1.47
34	V	201	HEM	C3B-CAB	3.70	1.55	1.47
25	b	608	CLA	CHB-C4A	3.72	1.38	1.33
34	v	201	HEM	C3B-CAB	3.73	1.55	1.47
25	c	505	CLA	CHB-C4A	3.76	1.38	1.33
25	c	513	CLA	CHB-C4A	3.77	1.38	1.33
25	b	611	CLA	CHB-C4A	3.79	1.38	1.33
25	B	610	CLA	CHB-C4A	3.80	1.38	1.33
34	v	201	HEM	C3C-CAC	3.82	1.55	1.47
25	b	603	CLA	CHB-C4A	3.82	1.38	1.33
25	a	607	CLA	CHB-C4A	3.85	1.38	1.33
25	b	616	CLA	CHB-C4A	3.87	1.38	1.33
25	A	607	CLA	CHB-C4A	3.88	1.38	1.33
25	C	510	CLA	CHB-C4A	3.88	1.38	1.33
25	a	610	CLA	CHB-C4A	3.89	1.38	1.33
34	V	201	HEM	C3C-CAC	3.89	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	CHB-C4A	3.89	1.38	1.33
25	B	607	CLA	CHB-C4A	3.90	1.38	1.33
25	C	505	CLA	CHB-C4A	3.90	1.38	1.33
25	C	506	CLA	CHB-C4A	3.90	1.38	1.33
25	b	613	CLA	CHB-C4A	3.91	1.38	1.33
25	a	615	CLA	CHB-C4A	3.91	1.38	1.33
25	b	609	CLA	CHB-C4A	3.91	1.38	1.33
25	c	502	CLA	CHB-C4A	3.92	1.38	1.33
25	B	616	CLA	CHB-C4A	3.92	1.38	1.33
25	C	503	CLA	CHB-C4A	3.92	1.38	1.33
25	b	607	CLA	CHB-C4A	3.93	1.38	1.33
25	C	508	CLA	CHB-C4A	3.93	1.38	1.33
25	c	501	CLA	CHB-C4A	3.94	1.38	1.33
25	C	509	CLA	CHB-C4A	3.94	1.38	1.33
25	B	602	CLA	CHB-C4A	3.94	1.38	1.33
25	d	402	CLA	CHB-C4A	3.95	1.38	1.33
25	b	610	CLA	CHB-C4A	3.95	1.38	1.33
25	B	605	CLA	CHB-C4A	3.95	1.38	1.33
25	A	609	CLA	CHB-C4A	3.95	1.38	1.33
25	A	613	CLA	CHB-C4A	3.96	1.38	1.33
25	B	613	CLA	CHB-C4A	3.96	1.38	1.33
25	B	612	CLA	CHB-C4A	3.96	1.38	1.33
25	B	614	CLA	CHB-C4A	3.97	1.38	1.33
25	C	502	CLA	CHB-C4A	3.97	1.38	1.33
25	c	511	CLA	CHB-C4A	3.97	1.38	1.33
25	b	614	CLA	CHB-C4A	3.98	1.38	1.33
25	C	507	CLA	CHB-C4A	3.99	1.38	1.33
25	B	609	CLA	CHB-C4A	4.01	1.38	1.33
25	b	605	CLA	CHB-C4A	4.01	1.38	1.33
25	C	514	CLA	CHB-C4A	4.02	1.38	1.33
25	c	506	CLA	CHB-C4A	4.02	1.38	1.33
25	B	608	CLA	CHB-C4A	4.03	1.38	1.33
25	B	603	CLA	CHB-C4A	4.03	1.38	1.33
25	c	512	CLA	CHB-C4A	4.03	1.38	1.33
25	C	504	CLA	CHB-C4A	4.04	1.38	1.33
25	b	606[A]	CLA	CHB-C4A	4.04	1.38	1.33
25	B	601	CLA	CHB-C4A	4.04	1.38	1.33
25	C	512	CLA	CHB-C4A	4.04	1.38	1.33
25	C	513	CLA	CHB-C4A	4.05	1.39	1.33
25	c	509	CLA	CHB-C4A	4.05	1.39	1.33
25	b	602	CLA	CHB-C4A	4.05	1.39	1.33
25	c	503	CLA	CHB-C4A	4.07	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	508	CLA	CHB-C4A	4.07	1.39	1.33
25	d	401	CLA	CHB-C4A	4.07	1.39	1.33
25	b	612	CLA	CHB-C4A	4.07	1.39	1.33
25	b	606[B]	CLA	CHB-C4A	4.07	1.39	1.33
25	B	611	CLA	CHB-C4A	4.08	1.39	1.33
25	c	504	CLA	CHB-C4A	4.09	1.39	1.33
25	D	402	CLA	CHB-C4A	4.10	1.39	1.33
25	c	507	CLA	CHB-C4A	4.11	1.39	1.33
25	b	604	CLA	CHB-C4A	4.12	1.39	1.33
25	B	615	CLA	CHB-C4A	4.13	1.39	1.33
25	b	601	CLA	CHB-C4A	4.14	1.39	1.33
25	c	510	CLA	CHB-C4A	4.14	1.39	1.33
25	A	606	CLA	CHB-C4A	4.15	1.39	1.33
25	b	615	CLA	CHB-C4A	4.19	1.39	1.33
25	B	606	CLA	CHB-C4A	4.20	1.39	1.33
25	a	606	CLA	CHB-C4A	4.22	1.39	1.33
25	B	604	CLA	CHB-C4A	4.26	1.39	1.33

All (893) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	516	DGD	O3G-C3G-C2G	-4.62	100.00	110.99
33	C	518	DGD	O3G-C3G-C2G	-4.56	100.15	110.99
29	D	408	SQD	O9-S-O7	-4.54	101.13	113.96
29	B	625	SQD	O9-S-O7	-4.54	101.15	113.96
29	L	101	SQD	O9-S-O7	-4.53	101.16	113.96
29	B	624	SQD	O9-S-O7	-4.50	101.24	113.96
29	A	616	SQD	O9-S-O7	-4.50	101.25	113.96
29	D	409	SQD	O9-S-O7	-4.47	101.32	113.96
29	a	613	SQD	O9-S-O7	-4.47	101.34	113.96
29	f	101	SQD	O9-S-O7	-4.43	101.45	113.96
29	A	612	SQD	O9-S-O7	-4.41	101.50	113.96
33	c	517	DGD	O3G-C3G-C2G	-4.39	100.55	110.99
33	C	519	DGD	O3G-C3G-C2G	-4.11	101.21	110.99
33	c	518	DGD	O3G-C3G-C2G	-4.01	101.46	110.99
33	H	102	DGD	O3G-C3G-C2G	-3.94	101.62	110.99
33	h	102	DGD	O3G-C3G-C2G	-3.86	101.81	110.99
33	C	517	DGD	O3G-C3G-C2G	-3.79	101.96	110.99
25	B	613	CLA	CMB-C2B-C1B	-3.73	121.96	128.31
25	D	403	CLA	CMB-C2B-C1B	-3.60	122.20	128.31
32	C	521	LMG	O6-C1-O1	-3.55	101.47	109.99
25	C	510	CLA	CMB-C2B-C1B	-3.51	122.33	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	613	CLA	CMB-C2B-C1B	-3.48	122.39	128.31
25	c	509	CLA	CMB-C2B-C1B	-3.47	122.41	128.31
25	b	611	CLA	CMB-C2B-C1B	-3.44	122.46	128.31
25	c	508	CLA	CMB-C2B-C1B	-3.43	122.48	128.31
25	B	612	CLA	CMB-C2B-C1B	-3.42	122.50	128.31
25	B	607	CLA	CMB-C2B-C1B	-3.38	122.57	128.31
25	b	603	CLA	CMB-C2B-C1B	-3.35	122.62	128.31
25	B	611	CLA	CMB-C2B-C1B	-3.34	122.63	128.31
25	A	606	CLA	CMB-C2B-C1B	-3.33	122.64	128.31
25	b	612	CLA	CMB-C2B-C1B	-3.32	122.66	128.31
25	c	510	CLA	CMB-C2B-C1B	-3.28	122.73	128.31
25	C	509	CLA	CMB-C2B-C1B	-3.28	122.74	128.31
25	C	506	CLA	CMB-C2B-C1B	-3.26	122.76	128.31
25	A	609	CLA	CMB-C2B-C1B	-3.26	122.77	128.31
25	C	511	CLA	CMB-C2B-C1B	-3.26	122.78	128.31
33	c	517	DGD	O6D-C1D-O3G	-3.22	102.27	109.99
25	B	614	CLA	CMB-C2B-C1B	-3.21	122.85	128.31
25	b	602	CLA	CMB-C2B-C1B	-3.21	122.86	128.31
25	B	602	CLA	CMB-C2B-C1B	-3.21	122.86	128.31
27	b	618	BCR	C15-C14-C13	-3.19	122.58	127.22
25	C	514	CLA	CMB-C2B-C1B	-3.19	122.89	128.31
25	a	606	CLA	CMB-C2B-C1B	-3.18	122.90	128.31
25	b	608	CLA	CMB-C2B-C1B	-3.18	122.91	128.31
25	b	614	CLA	CMB-C2B-C1B	-3.17	122.91	128.31
25	c	505	CLA	CMB-C2B-C1B	-3.17	122.91	128.31
25	c	511	CLA	CMB-C2B-C1B	-3.17	122.92	128.31
32	c	520	LMG	O6-C1-O1	-3.17	102.39	109.99
25	C	508	CLA	CMB-C2B-C1B	-3.16	122.93	128.31
25	c	513	CLA	CMB-C2B-C1B	-3.16	122.94	128.31
33	C	519	DGD	O6D-C1D-O3G	-3.15	102.43	109.99
25	C	507	CLA	CMB-C2B-C1B	-3.15	122.95	128.31
33	c	518	DGD	O6D-C1D-O3G	-3.15	102.44	109.99
25	C	512	CLA	CMB-C2B-C1B	-3.14	122.98	128.31
25	a	610	CLA	CMB-C2B-C1B	-3.11	123.02	128.31
25	B	605	CLA	CMB-C2B-C1B	-3.11	123.03	128.31
27	t	101	BCR	C33-C5-C6	-3.10	121.32	124.62
25	C	505	CLA	CMB-C2B-C1B	-3.10	123.04	128.31
33	C	518	DGD	O6D-C1D-O3G	-3.10	102.56	109.99
25	B	608	CLA	CMB-C2B-C1B	-3.09	123.06	128.31
33	C	517	DGD	O6D-C1D-O3G	-3.09	102.59	109.99
25	b	607	CLA	CMB-C2B-C1B	-3.09	123.06	128.31
25	b	616	CLA	CMB-C2B-C1B	-3.08	123.07	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	CMB-C2B-C1B	-3.08	123.07	128.31
33	c	516	DGD	O6D-C1D-O3G	-3.06	102.65	109.99
25	c	501	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
25	D	402	CLA	CMB-C2B-C1B	-3.05	123.13	128.31
25	B	610	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
25	b	609	CLA	CMB-C2B-C1B	-3.02	123.17	128.31
25	B	616	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
25	A	607	CLA	CMB-C2B-C1B	-3.01	123.20	128.31
25	B	603	CLA	CMB-C2B-C1B	-3.00	123.20	128.31
25	B	601	CLA	CMB-C2B-C1B	-3.00	123.21	128.31
25	d	402	CLA	CMB-C2B-C1B	-3.00	123.21	128.31
25	c	504	CLA	CMB-C2B-C1B	-2.97	123.27	128.31
33	H	102	DGD	O6D-C1D-O3G	-2.94	102.94	109.99
25	C	504	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
25	b	606[A]	CLA	CMB-C2B-C1B	-2.93	123.33	128.31
25	b	606[B]	CLA	O2D-CGD-O1D	-2.93	117.61	123.77
27	b	617	BCR	C33-C5-C6	-2.93	121.50	124.62
25	C	502	CLA	CMB-C2B-C1B	-2.92	123.35	128.31
25	c	502	CLA	CMB-C2B-C1B	-2.91	123.36	128.31
28	A	611	PL9	C22-C23-C24	-2.91	121.33	127.75
25	b	606[B]	CLA	CMB-C2B-C1B	-2.91	123.37	128.31
25	C	513	CLA	CMB-C2B-C1B	-2.90	123.38	128.31
25	a	607	CLA	CMB-C2B-C1B	-2.90	123.38	128.31
25	b	610	CLA	CMB-C2B-C1B	-2.90	123.39	128.31
28	a	612	PL9	C7-C3-C2	-2.90	118.45	122.66
25	b	601	CLA	CMB-C2B-C1B	-2.89	123.40	128.31
25	C	513	CLA	O2D-CGD-O1D	-2.88	117.70	123.77
25	B	602	CLA	O2D-CGD-O1D	-2.87	117.73	123.77
25	A	613	CLA	CMB-C2B-C1B	-2.86	123.44	128.31
25	B	604	CLA	CMB-C2B-C1B	-2.86	123.44	128.31
28	d	404	PL9	C27-C28-C29	-2.85	121.45	127.75
27	c	521	BCR	C33-C5-C6	-2.85	121.58	124.62
25	C	514	CLA	O2D-CGD-O1D	-2.85	117.77	123.77
25	B	609	CLA	CMB-C2B-C1B	-2.85	123.46	128.31
25	c	508	CLA	O2D-CGD-O1D	-2.85	117.77	123.77
25	c	507	CLA	CMB-C2B-C1B	-2.85	123.47	128.31
25	c	503	CLA	CMB-C2B-C1B	-2.85	123.47	128.31
25	a	615	CLA	CMB-C2B-C1B	-2.84	123.47	128.31
25	b	606[A]	CLA	O2D-CGD-O1D	-2.84	117.79	123.77
27	Y	101	BCR	C33-C5-C6	-2.84	121.60	124.62
26	D	401	PHO	CBD-CHA-C4D	-2.83	105.35	108.54
32	C	501	LMG	O6-C1-O1	-2.83	103.20	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	610	CLA	O2D-CGD-O1D	-2.83	117.82	123.77
25	C	503	CLA	CMB-C2B-C1B	-2.82	123.51	128.31
25	b	602	CLA	O2D-CGD-O1D	-2.82	117.83	123.77
25	c	501	CLA	O2D-CGD-O1D	-2.82	117.83	123.77
32	b	620	LMG	O1-C1-C2	-2.82	104.53	108.00
33	h	102	DGD	O6D-C1D-O3G	-2.82	103.23	109.99
27	b	618	BCR	C15-C16-C17	-2.82	117.16	123.23
27	h	101	BCR	C24-C23-C22	-2.81	121.96	126.21
25	C	502	CLA	O2D-CGD-O1D	-2.81	117.85	123.77
25	c	512	CLA	CMB-C2B-C1B	-2.80	123.54	128.31
25	c	505	CLA	O2D-CGD-O1D	-2.80	117.88	123.77
25	C	509	CLA	O2D-CGD-O1D	-2.80	117.88	123.77
25	B	606	CLA	CMB-C2B-C1B	-2.79	123.57	128.31
25	b	603	CLA	O2D-CGD-O1D	-2.77	117.93	123.77
25	B	614	CLA	O2D-CGD-O1D	-2.77	117.94	123.77
25	D	403	CLA	O2D-CGD-O1D	-2.77	117.94	123.77
25	C	508	CLA	O2D-CGD-O1D	-2.77	117.94	123.77
25	A	609	CLA	O2D-CGD-O1D	-2.76	117.95	123.77
25	b	605	CLA	CMB-C2B-C1B	-2.75	123.63	128.31
27	d	403	BCR	C33-C5-C6	-2.75	121.69	124.62
32	m	102	LMG	O6-C1-O1	-2.74	103.41	109.99
25	d	401	CLA	CMB-C2B-C1B	-2.74	123.65	128.31
25	B	601	CLA	O2D-CGD-O1D	-2.74	118.01	123.77
25	B	616	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
33	C	519	DGD	CDB-CCB-CBB	-2.73	100.37	114.54
33	C	517	DGD	CDB-CCB-CBB	-2.72	100.43	114.54
25	A	607	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
32	b	620	LMG	O6-C1-O1	-2.71	103.49	109.99
32	B	620	LMG	O6-C1-O1	-2.71	103.50	109.99
27	h	101	BCR	C33-C5-C6	-2.70	121.74	124.62
33	c	517	DGD	O5D-C6D-C5D	-2.70	104.34	109.14
28	a	612	PL9	C27-C28-C29	-2.70	121.80	127.75
25	c	507	CLA	O2D-CGD-O1D	-2.70	118.09	123.77
32	C	520	LMG	O6-C1-O1	-2.70	103.52	109.99
25	b	611	CLA	O2D-CGD-O1D	-2.70	118.10	123.77
33	C	518	DGD	CDB-CCB-CBB	-2.69	100.55	114.54
33	h	102	DGD	CDB-CCB-CBB	-2.69	100.57	114.54
25	b	604	CLA	CMB-C2B-C1B	-2.69	123.74	128.31
25	b	612	CLA	O2D-CGD-O1D	-2.69	118.11	123.77
25	c	512	CLA	O2D-CGD-O1D	-2.69	118.11	123.77
25	B	615	CLA	CMB-C2B-C1B	-2.69	123.74	128.31
32	B	626	LMG	O6-C1-O1	-2.68	103.55	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	522	BCR	C33-C5-C6	-2.68	121.76	124.62
27	K	101	BCR	C33-C5-C6	-2.68	121.76	124.62
28	A	611	PL9	C27-C28-C29	-2.68	121.83	127.75
25	b	601	CLA	O2D-CGD-O1D	-2.68	118.12	123.77
25	c	513	CLA	O2D-CGD-O1D	-2.68	118.13	123.77
28	a	612	PL9	C22-C23-C24	-2.68	121.85	127.75
33	c	516	DGD	O5D-C6D-C5D	-2.67	104.39	109.14
33	c	517	DGD	CDB-CCB-CBB	-2.67	100.67	114.54
26	a	609	PHO	O2D-CGD-O1D	-2.67	118.15	123.77
25	a	607	CLA	O2D-CGD-O1D	-2.67	118.16	123.77
28	A	611	PL9	C7-C3-C2	-2.67	118.78	122.66
25	C	505	CLA	O2D-CGD-O1D	-2.66	118.17	123.77
34	e	101	HEM	CBD-CAD-C3D	-2.66	107.80	112.47
33	H	102	DGD	CDB-CCB-CBB	-2.66	100.73	114.54
25	a	615	CLA	O2D-CGD-O1D	-2.66	118.18	123.77
25	c	504	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
25	B	611	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
25	b	607	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
25	C	506	CLA	O2D-CGD-O1D	-2.65	118.19	123.77
25	b	608	CLA	O2D-CGD-O1D	-2.65	118.19	123.77
25	c	511	CLA	O2D-CGD-O1D	-2.65	118.20	123.77
32	B	621	LMG	O6-C1-O1	-2.64	103.65	109.99
25	B	612	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
25	c	510	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
28	D	405	PL9	C27-C28-C29	-2.64	121.92	127.75
25	d	401	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
25	C	503	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
33	c	516	DGD	CDB-CCB-CBB	-2.64	100.85	114.54
27	C	516	BCR	C15-C16-C17	-2.64	117.55	123.23
25	B	604	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
33	c	516	DGD	C3G-C2G-C1G	-2.64	105.94	112.08
26	A	608	PHO	CBD-CHA-C4D	-2.63	105.57	108.54
32	c	519	LMG	O6-C1-O1	-2.63	103.67	109.99
25	B	610	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
27	c	515	BCR	C15-C16-C17	-2.63	117.57	123.23
25	C	507	CLA	O2D-CGD-O1D	-2.62	118.24	123.77
27	C	516	BCR	C33-C5-C6	-2.62	121.83	124.62
28	D	405	PL9	C7-C3-C2	-2.62	118.85	122.66
32	d	407	LMG	O6-C1-O1	-2.62	103.70	109.99
25	B	603	CLA	O2D-CGD-O1D	-2.62	118.26	123.77
25	b	604	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
25	A	613	CLA	O2D-CGD-O1D	-2.61	118.28	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	515	BCR	C33-C5-C6	-2.61	121.85	124.62
25	B	615	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
33	C	517	DGD	O5D-C6D-C5D	-2.60	104.51	109.14
25	b	616	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
26	a	608	PHO	CBD-CHA-C4D	-2.60	105.61	108.54
33	C	518	DGD	O5D-C6D-C5D	-2.60	104.52	109.14
28	D	405	PL9	C31-C32-C33	-2.59	104.81	111.61
25	C	512	CLA	O2D-CGD-O1D	-2.59	118.32	123.77
25	B	605	CLA	O2D-CGD-O1D	-2.58	118.33	123.77
34	E	101	HEM	CBD-CAD-C3D	-2.58	107.94	112.47
27	A	610	BCR	C33-C5-C6	-2.58	121.87	124.62
28	d	404	PL9	C22-C23-C24	-2.58	122.07	127.75
27	B	618	BCR	C33-C5-C6	-2.57	121.88	124.62
25	b	605	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
30	B	623	LHG	C11-C10-C9	-2.57	101.19	114.54
25	B	608	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
25	b	613	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
25	C	510	CLA	O2D-CGD-O1D	-2.56	118.38	123.77
25	C	504	CLA	O2D-CGD-O1D	-2.56	118.39	123.77
26	D	401	PHO	O2D-CGD-O1D	-2.54	118.41	123.77
28	A	611	PL9	C7-C8-C9	-2.54	122.38	126.70
33	c	516	DGD	O3G-C1D-C2D	-2.53	104.88	108.00
34	e	101	HEM	CBA-CAA-C2A	-2.53	108.04	112.49
27	b	618	BCR	C33-C5-C6	-2.53	121.93	124.62
30	d	405	LHG	C11-C10-C9	-2.53	101.40	114.54
27	b	617	BCR	C15-C14-C13	-2.52	123.55	127.22
25	c	502	CLA	O2D-CGD-O1D	-2.52	118.46	123.77
33	H	102	DGD	C3G-C2G-C1G	-2.52	106.21	112.08
27	a	611	BCR	C33-C5-C6	-2.52	121.94	124.62
33	c	518	DGD	CDB-CCB-CBB	-2.52	101.48	114.54
30	a	617	LHG	C20-C19-C18	-2.51	101.50	114.54
28	D	405	PL9	C7-C8-C9	-2.51	122.43	126.70
25	b	610	CLA	O2D-CGD-O1D	-2.51	118.49	123.77
25	b	614	CLA	O2D-CGD-O1D	-2.51	118.49	123.77
28	D	405	PL9	C22-C23-C24	-2.51	122.22	127.75
25	b	615	CLA	CMB-C2B-C1B	-2.50	124.07	128.31
33	C	519	DGD	O5D-C6D-C5D	-2.49	104.70	109.14
25	B	606	CLA	O2D-CGD-O1D	-2.49	118.52	123.77
25	C	511	CLA	O2D-CGD-O1D	-2.49	118.53	123.77
32	B	620	LMG	O1-C7-C8	-2.49	105.07	110.99
25	B	613	CLA	O2D-CGD-O1D	-2.48	118.54	123.77
25	d	402	CLA	O2D-CGD-O1D	-2.48	118.55	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	t	101	BCR	C15-C14-C13	-2.48	123.62	127.22
33	C	519	DGD	C1D-C2D-C3D	-2.48	105.07	109.98
32	m	102	LMG	O1-C1-C2	-2.48	104.95	108.00
28	D	405	PL9	C37-C38-C39	-2.48	122.29	127.75
27	T	101	BCR	C15-C14-C13	-2.47	123.62	127.22
32	d	407	LMG	O2-C2-C1	-2.47	104.52	110.01
25	D	402	CLA	O2D-CGD-O1D	-2.47	118.57	123.77
28	d	404	PL9	C7-C3-C2	-2.47	119.07	122.66
25	c	503	CLA	O2D-CGD-O1D	-2.47	118.58	123.77
28	D	405	PL9	C12-C13-C14	-2.46	122.31	127.75
27	h	101	BCR	C11-C10-C9	-2.45	123.65	127.22
27	T	101	BCR	C33-C5-C6	-2.45	122.01	124.62
32	D	407	LMG	O6-C1-O1	-2.45	104.11	109.99
25	b	615	CLA	O2D-CGD-O1D	-2.45	118.61	123.77
27	B	617	BCR	C33-C5-C6	-2.45	122.01	124.62
28	d	404	PL9	C7-C8-C9	-2.45	122.53	126.70
32	c	519	LMG	C38-C37-C36	-2.45	101.83	114.54
32	a	614	LMG	O1-C7-C8	-2.44	105.18	110.99
33	C	519	DGD	C3G-C2G-C1G	-2.44	106.40	112.08
30	d	405	LHG	C20-C19-C18	-2.44	101.88	114.54
25	B	609	CLA	O2D-CGD-O1D	-2.44	118.64	123.77
25	b	609	CLA	O2D-CGD-O1D	-2.44	118.64	123.77
27	t	101	BCR	C15-C16-C17	-2.44	117.98	123.23
25	c	506	CLA	O2D-CGD-O1D	-2.43	118.64	123.77
32	m	102	LMG	C40-C39-C38	-2.43	101.90	114.54
27	c	522	BCR	C24-C23-C22	-2.43	122.54	126.21
27	c	514	BCR	C33-C5-C6	-2.43	122.03	124.62
26	a	609	PHO	CBD-CHA-C4D	-2.43	105.80	108.54
33	c	517	DGD	C3G-C2G-C1G	-2.43	106.43	112.08
26	a	609	PHO	CMB-C2B-C1B	-2.42	121.19	125.06
30	A	618	LHG	C11-C10-C9	-2.42	101.95	114.54
30	l	101	LHG	C11-C10-C9	-2.42	101.95	114.54
27	B	618	BCR	C15-C14-C13	-2.42	123.70	127.22
28	A	611	PL9	C32-C33-C34	-2.42	122.42	127.75
33	h	102	DGD	C3G-C2G-C1G	-2.41	106.47	112.08
27	b	617	BCR	C15-C16-C17	-2.41	118.04	123.23
30	D	406	LHG	C20-C19-C18	-2.41	102.04	114.54
27	d	403	BCR	C28-C27-C26	-2.41	109.88	113.87
30	A	614	LHG	C11-C10-C9	-2.41	102.05	114.54
32	m	102	LMG	O1-C7-C8	-2.40	105.28	110.99
30	L	102	LHG	C11-C10-C9	-2.40	102.07	114.54
33	h	102	DGD	C1D-C2D-C3D	-2.40	105.22	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	608	PHO	O2D-CGD-O1D	-2.40	118.72	123.77
32	b	620	LMG	O1-C7-C8	-2.40	105.29	110.99
32	a	614	LMG	O1-C1-C2	-2.39	105.06	108.00
32	b	620	LMG	C40-C39-C38	-2.39	102.12	114.54
32	C	520	LMG	C40-C39-C38	-2.39	102.12	114.54
32	B	620	LMG	C40-C39-C38	-2.39	102.13	114.54
32	d	408	LMG	C40-C39-C38	-2.38	102.15	114.54
32	c	519	LMG	C40-C39-C38	-2.38	102.17	114.54
28	d	404	PL9	C37-C38-C39	-2.38	122.49	127.75
32	C	501	LMG	C40-C39-C38	-2.38	102.18	114.54
27	b	619	BCR	C33-C5-C6	-2.38	122.09	124.62
25	a	606	CLA	O2D-CGD-O1D	-2.38	118.76	123.77
32	C	521	LMG	C40-C39-C38	-2.38	102.20	114.54
34	V	201	HEM	CBA-CAA-C2A	-2.37	108.32	112.49
27	C	515	BCR	C33-C5-C6	-2.37	122.10	124.62
28	d	404	PL9	C31-C32-C33	-2.37	105.40	111.61
28	d	404	PL9	C36-C34-C33	-2.36	116.58	120.98
27	C	516	BCR	C7-C8-C9	-2.36	122.64	126.21
30	B	623	LHG	C20-C19-C18	-2.36	102.29	114.54
32	b	620	LMG	O2-C2-C1	-2.36	104.78	110.01
27	K	101	BCR	C15-C16-C17	-2.36	118.15	123.23
32	a	614	LMG	O3-C3-C2	-2.35	105.05	110.36
33	C	517	DGD	C3G-C2G-C1G	-2.35	106.60	112.08
32	B	626	LMG	C38-C37-C36	-2.35	102.33	114.54
27	T	101	BCR	C15-C16-C17	-2.35	118.17	123.23
32	a	614	LMG	C40-C39-C38	-2.35	102.35	114.54
32	D	407	LMG	C40-C39-C38	-2.34	102.37	114.54
32	d	407	LMG	C40-C39-C38	-2.34	102.37	114.54
28	D	405	PL9	C36-C34-C33	-2.34	116.62	120.98
30	d	406	LHG	C11-C10-C9	-2.34	102.39	114.54
32	B	626	LMG	C40-C39-C38	-2.34	102.39	114.54
32	m	102	LMG	C38-C37-C36	-2.34	102.40	114.54
30	l	101	LHG	C20-C19-C18	-2.34	102.40	114.54
33	c	518	DGD	C3G-C2G-C1G	-2.34	106.64	112.08
32	m	102	LMG	O2-C2-C1	-2.34	104.83	110.01
32	C	521	LMG	C38-C37-C36	-2.34	102.41	114.54
25	c	509	CLA	O2D-CGD-O1D	-2.33	118.86	123.77
26	A	608	PHO	O2D-CGD-O1D	-2.33	118.86	123.77
28	a	612	PL9	C32-C33-C34	-2.33	122.61	127.75
30	d	406	LHG	C20-C19-C18	-2.33	102.46	114.54
32	C	520	LMG	C38-C37-C36	-2.32	102.47	114.54
28	a	612	PL9	C37-C38-C39	-2.32	122.62	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	407	LMG	O2-C2-C1	-2.32	104.85	110.01
32	b	620	LMG	O3-C3-C2	-2.32	105.12	110.36
30	L	102	LHG	C20-C19-C18	-2.32	102.49	114.54
25	c	507	CLA	O2A-CGA-O1A	-2.31	117.44	123.51
32	a	614	LMG	C38-C37-C36	-2.31	102.53	114.54
27	C	516	BCR	C11-C10-C9	-2.31	123.86	127.22
25	B	607	CLA	O2D-CGD-O1D	-2.31	118.91	123.77
32	B	621	LMG	O2-C2-C1	-2.31	104.88	110.01
25	B	614	CLA	O2A-CGA-O1A	-2.31	117.46	123.51
27	C	516	BCR	C15-C14-C13	-2.31	123.87	127.22
32	b	620	LMG	C38-C37-C36	-2.31	102.55	114.54
32	d	408	LMG	C38-C37-C36	-2.31	102.56	114.54
32	C	521	LMG	O3-C3-C2	-2.31	105.16	110.36
30	D	406	LHG	C11-C10-C9	-2.30	102.57	114.54
30	a	617	LHG	C11-C10-C9	-2.30	102.57	114.54
32	d	407	LMG	C38-C37-C36	-2.30	102.58	114.54
32	C	520	LMG	O3-C3-C2	-2.30	105.17	110.36
32	c	519	LMG	O2-C2-C1	-2.30	104.90	110.01
32	C	501	LMG	C38-C37-C36	-2.30	102.59	114.54
32	B	621	LMG	C40-C39-C38	-2.30	102.59	114.54
30	A	618	LHG	C20-C19-C18	-2.30	102.61	114.54
32	c	519	LMG	O3-C3-C2	-2.30	105.18	110.36
28	A	611	PL9	C12-C13-C14	-2.30	122.69	127.75
33	C	518	DGD	C3G-C2G-C1G	-2.29	106.74	112.08
27	B	619	BCR	C33-C5-C6	-2.29	122.18	124.62
27	c	514	BCR	C24-C23-C22	-2.29	122.75	126.21
32	m	102	LMG	O3-C3-C2	-2.29	105.20	110.36
32	d	407	LMG	O1-C1-C2	-2.28	105.19	108.00
28	A	611	PL9	C37-C38-C39	-2.28	122.72	127.75
28	a	612	PL9	C31-C32-C33	-2.28	105.63	111.61
33	c	517	DGD	CBB-CAB-C9B	-2.28	102.70	114.54
28	d	404	PL9	C36-C37-C38	-2.28	105.63	111.61
32	B	621	LMG	C38-C37-C36	-2.28	102.71	114.54
27	B	619	BCR	C24-C23-C22	-2.27	122.77	126.21
32	C	520	LMG	O2-C2-C1	-2.27	104.96	110.01
27	c	514	BCR	C15-C14-C13	-2.27	123.92	127.22
32	B	621	LMG	O1-C1-C2	-2.27	105.20	108.00
32	d	407	LMG	O1-C7-C8	-2.27	105.58	110.99
26	a	608	PHO	CMB-C2B-C1B	-2.27	121.43	125.06
32	B	626	LMG	O3-C3-C2	-2.27	105.25	110.36
27	c	514	BCR	C15-C16-C17	-2.26	118.35	123.23
32	a	614	LMG	O2-C2-C1	-2.26	104.99	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	612	CLA	O2A-CGA-O1A	-2.26	117.58	123.51
32	B	621	LMG	O3-C3-C2	-2.26	105.26	110.36
32	c	520	LMG	O3-C3-C2	-2.26	105.27	110.36
27	A	610	BCR	C11-C10-C9	-2.26	123.94	127.22
30	d	405	LHG	C18-C17-C16	-2.26	102.83	114.54
28	A	611	PL9	C31-C32-C33	-2.25	105.70	111.61
33	c	518	DGD	O5D-C6D-C5D	-2.25	105.14	109.14
28	D	405	PL9	C36-C37-C38	-2.24	105.72	111.61
32	B	620	LMG	C38-C37-C36	-2.24	102.90	114.54
25	c	509	CLA	O2A-CGA-O1A	-2.23	117.66	123.51
27	D	404	BCR	C33-C5-C6	-2.23	122.25	124.62
27	K	101	BCR	C24-C23-C22	-2.22	122.85	126.21
27	D	404	BCR	C7-C8-C9	-2.22	122.86	126.21
32	B	620	LMG	O2-C2-C1	-2.21	105.10	110.01
33	C	519	DGD	O3E-C3E-C2E	-2.21	105.37	110.36
32	C	520	LMG	O1-C7-C8	-2.21	105.72	110.99
32	C	520	LMG	O1-C1-C2	-2.21	105.28	108.00
27	K	101	BCR	C15-C14-C13	-2.21	124.01	127.22
32	d	407	LMG	O3-C3-C2	-2.21	105.38	110.36
25	c	511	CLA	O2A-CGA-O1A	-2.21	117.72	123.51
27	C	515	BCR	C15-C14-C13	-2.21	124.01	127.22
32	C	521	LMG	O2-C2-C3	-2.21	105.38	110.36
27	B	618	BCR	C15-C16-C17	-2.21	118.47	123.23
30	B	623	LHG	C27-C26-C25	-2.20	103.09	114.54
32	D	407	LMG	C38-C37-C36	-2.20	103.10	114.54
32	c	519	LMG	O1-C7-C8	-2.20	105.75	110.99
27	H	101	BCR	C33-C5-C6	-2.20	122.28	124.62
30	A	614	LHG	C18-C17-C16	-2.20	103.14	114.54
28	A	611	PL9	C36-C37-C38	-2.19	105.85	111.61
30	L	102	LHG	C27-C26-C25	-2.19	103.16	114.54
28	a	612	PL9	C7-C8-C9	-2.19	122.97	126.70
27	B	617	BCR	C15-C16-C17	-2.19	118.52	123.23
27	b	617	BCR	C11-C10-C9	-2.19	124.04	127.22
26	D	401	PHO	CMB-C2B-C1B	-2.19	121.57	125.06
32	B	620	LMG	O3-C3-C2	-2.18	105.43	110.36
25	B	604	CLA	O2A-CGA-O1A	-2.18	117.78	123.51
30	L	102	LHG	C18-C17-C16	-2.18	103.21	114.54
27	d	403	BCR	C11-C10-C9	-2.18	124.05	127.22
27	C	515	BCR	C15-C16-C17	-2.18	118.54	123.23
30	l	101	LHG	C18-C17-C16	-2.18	103.23	114.54
30	A	618	LHG	C18-C17-C16	-2.18	103.24	114.54
27	c	515	BCR	C15-C14-C13	-2.17	124.06	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	518	DGD	C1D-C2D-C3D	-2.17	105.68	109.98
32	B	621	LMG	O1-C7-C8	-2.17	105.83	110.99
33	H	102	DGD	C1D-C2D-C3D	-2.17	105.69	109.98
28	a	612	PL9	O2-C1-C2	-2.16	116.90	121.78
25	B	611	CLA	O2A-CGA-O1A	-2.16	117.84	123.51
27	c	522	BCR	C15-C16-C17	-2.16	118.57	123.23
30	D	406	LHG	C27-C26-C25	-2.16	103.32	114.54
30	a	617	LHG	C27-C26-C25	-2.16	103.33	114.54
27	B	617	BCR	C15-C14-C13	-2.16	124.09	127.22
33	H	102	DGD	CBB-CAB-C9B	-2.16	103.34	114.54
30	d	405	LHG	C27-C26-C25	-2.15	103.35	114.54
33	c	516	DGD	CBB-CAB-C9B	-2.15	103.35	114.54
30	A	618	LHG	C27-C26-C25	-2.15	103.36	114.54
30	l	101	LHG	C27-C26-C25	-2.15	103.36	114.54
30	a	617	LHG	C18-C17-C16	-2.15	103.36	114.54
32	C	501	LMG	O3-C3-C2	-2.15	105.51	110.36
32	d	408	LMG	C42-C41-C40	-2.15	103.37	114.54
27	H	101	BCR	C7-C8-C9	-2.15	122.96	126.21
27	c	521	BCR	C24-C23-C22	-2.15	122.97	126.21
32	C	521	LMG	C3-C4-C5	-2.14	106.40	110.23
30	D	406	LHG	C18-C17-C16	-2.14	103.42	114.54
30	d	406	LHG	C18-C17-C16	-2.14	103.42	114.54
26	A	608	PHO	CMB-C2B-C1B	-2.14	121.64	125.06
30	A	614	LHG	C27-C26-C25	-2.14	103.45	114.54
27	a	611	BCR	C11-C10-C9	-2.14	124.12	127.22
32	a	614	LMG	O6-C1-O1	-2.14	104.87	109.99
33	h	102	DGD	CBB-CAB-C9B	-2.13	103.46	114.54
33	C	519	DGD	CBB-CAB-C9B	-2.13	103.47	114.54
25	B	610	CLA	O2A-CGA-O1A	-2.13	117.92	123.51
27	a	611	BCR	C7-C8-C9	-2.13	122.99	126.21
27	b	618	BCR	C35-C13-C14	-2.13	119.79	122.89
28	A	611	PL9	C46-C47-C48	-2.13	106.03	111.61
28	A	611	PL9	O2-C1-C2	-2.12	116.99	121.78
33	C	518	DGD	O3E-C3E-C2E	-2.12	105.58	110.36
27	h	101	BCR	C15-C14-C13	-2.12	124.14	127.22
30	B	623	LHG	C18-C17-C16	-2.11	103.56	114.54
25	b	603	CLA	O2A-CGA-O1A	-2.11	117.97	123.51
33	h	102	DGD	CAB-C9B-C8B	-2.11	103.58	114.54
27	B	618	BCR	C11-C10-C9	-2.11	124.15	127.22
33	C	517	DGD	CBB-CAB-C9B	-2.11	103.59	114.54
25	A	606	CLA	O2D-CGD-O1D	-2.11	119.33	123.77
32	c	519	LMG	O1-C1-C2	-2.11	105.41	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	517	DGD	O2D-C2D-C1D	-2.11	105.34	110.01
33	c	518	DGD	CBB-CAB-C9B	-2.10	103.61	114.54
28	a	612	PL9	C12-C13-C14	-2.10	123.13	127.75
28	d	404	PL9	C11-C12-C13	-2.10	106.11	111.61
28	D	405	PL9	O2-C1-C2	-2.09	117.06	121.78
25	D	403	CLA	O2A-CGA-O1A	-2.09	118.02	123.51
27	t	101	BCR	C11-C10-C9	-2.09	124.18	127.22
33	c	518	DGD	CAB-C9B-C8B	-2.09	103.67	114.54
33	C	518	DGD	CBB-CAB-C9B	-2.09	103.68	114.54
27	A	610	BCR	C24-C23-C22	-2.09	123.05	126.21
30	a	616	LHG	C27-C26-C25	-2.08	103.72	114.54
32	D	407	LMG	O3-C3-C2	-2.08	105.66	110.36
33	H	102	DGD	CAB-C9B-C8B	-2.08	103.72	114.54
27	a	611	BCR	C15-C14-C13	-2.08	124.19	127.22
25	B	609	CLA	O2A-CGA-O1A	-2.08	118.06	123.51
33	C	517	DGD	CAB-C9B-C8B	-2.08	103.75	114.54
33	h	102	DGD	O3E-C3E-C2E	-2.08	105.68	110.36
27	D	404	BCR	C15-C16-C17	-2.08	118.76	123.23
25	B	613	CLA	O2A-CGA-O1A	-2.07	118.08	123.51
33	c	517	DGD	C5B-C4B-C3B	-2.07	103.80	114.54
25	B	615	CLA	O2A-CGA-O1A	-2.07	118.09	123.51
32	C	501	LMG	O2-C2-C1	-2.07	105.42	110.01
32	c	520	LMG	C3-C4-C5	-2.07	106.54	110.23
33	C	518	DGD	O2D-C2D-C1D	-2.06	105.44	110.01
28	a	612	PL9	C42-C43-C44	-2.06	123.22	127.75
27	Y	101	BCR	C15-C16-C17	-2.05	118.80	123.23
28	d	404	PL9	C42-C43-C44	-2.05	123.22	127.75
27	T	101	BCR	C3-C4-C5	-2.05	110.47	113.87
25	A	609	CLA	O2A-CGA-O1A	-2.05	118.13	123.51
25	a	606	CLA	O2A-CGA-O1A	-2.05	118.14	123.51
25	C	507	CLA	O2A-CGA-O1A	-2.05	118.14	123.51
33	h	102	DGD	O2D-C2D-C1D	-2.05	105.47	110.01
32	D	407	LMG	C1-C2-C3	-2.04	105.93	109.98
33	C	519	DGD	O2D-C2D-C1D	-2.04	105.48	110.01
28	d	404	PL9	C32-C33-C34	-2.04	123.24	127.75
33	c	516	DGD	CAB-C9B-C8B	-2.04	103.96	114.54
25	B	603	CLA	O2A-CGA-O1A	-2.04	118.17	123.51
34	v	201	HEM	CBA-CAA-C2A	-2.03	108.92	112.49
25	C	512	CLA	O2A-CGA-O1A	-2.03	118.18	123.51
25	b	604	CLA	O2A-CGA-O1A	-2.03	118.18	123.51
26	a	608	PHO	O2A-CGA-O1A	-2.03	118.18	123.51
33	C	519	DGD	CAB-C9B-C8B	-2.03	103.99	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	CLA	O2A-CGA-O1A	-2.02	118.21	123.51
33	c	518	DGD	O3E-C3E-C2E	-2.02	105.80	110.36
30	d	406	LHG	C27-C26-C25	-2.02	104.05	114.54
25	A	607	CLA	O2A-CGA-O1A	-2.02	118.21	123.51
27	b	619	BCR	C15-C16-C17	-2.02	118.88	123.23
27	A	610	BCR	C15-C14-C13	-2.02	124.28	127.22
25	b	608	CLA	OBD-CAD-CBD	-2.02	122.89	125.94
25	b	613	CLA	O2A-CGA-O1A	-2.02	118.22	123.51
33	C	519	DGD	C5B-C4B-C3B	-2.01	104.08	114.54
34	E	101	HEM	CBA-CAA-C2A	-2.01	108.95	112.49
27	h	101	BCR	C38-C26-C25	-2.01	122.48	124.62
26	A	608	PHO	C2B-C1B-NB	-2.01	106.82	109.81
33	C	518	DGD	CAB-C9B-C8B	-2.01	104.12	114.54
33	c	516	DGD	C5B-C4B-C3B	-2.01	104.12	114.54
28	d	404	PL9	C12-C13-C14	-2.01	123.32	127.75
28	d	404	PL9	O2-C1-C2	-2.01	117.26	121.78
25	B	607	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
32	c	520	LMG	O2-C2-C1	-2.00	105.56	110.01
33	C	517	DGD	C5B-C4B-C3B	-2.00	104.15	114.54
25	b	616	CLA	O2D-CGD-CBD	2.00	114.10	111.22
34	v	201	HEM	CMB-C2B-C3B	2.00	129.01	125.09
25	C	506	CLA	O2D-CGD-CBD	2.00	114.11	111.22
25	C	511	CLA	CMD-C2D-C3D	2.01	129.01	125.09
29	D	409	SQD	O5-C1-C2	2.01	114.45	110.28
25	C	502	CLA	O1D-CGD-CBD	2.01	127.77	124.64
25	D	402	CLA	C4A-NA-C1A	2.02	108.94	106.38
25	c	510	CLA	CMD-C2D-C3D	2.02	129.03	125.09
25	B	614	CLA	O1D-CGD-CBD	2.02	127.78	124.64
25	B	610	CLA	C4A-NA-C1A	2.02	108.94	106.38
25	A	613	CLA	CMD-C2D-C3D	2.04	129.07	125.09
25	B	615	CLA	O2D-CGD-CBD	2.04	114.16	111.22
25	c	503	CLA	O1D-CGD-CBD	2.04	127.81	124.64
25	C	512	CLA	O2D-CGD-CBD	2.04	114.16	111.22
25	D	403	CLA	CMD-C2D-C3D	2.04	129.08	125.09
25	C	512	CLA	CMD-C2D-C3D	2.04	129.08	125.09
25	b	602	CLA	C4A-NA-C1A	2.04	108.97	106.38
25	c	508	CLA	C4A-NA-C1A	2.05	108.97	106.38
25	A	609	CLA	C4A-NA-C1A	2.05	108.97	106.38
25	B	605	CLA	CMD-C2D-C3D	2.05	129.09	125.09
25	b	603	CLA	CMD-C2D-C3D	2.05	129.09	125.09
25	B	616	CLA	CMD-C2D-C3D	2.05	129.09	125.09
25	C	504	CLA	CMD-C2D-C3D	2.05	129.09	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402	CLA	O2D-CGD-CBD	2.05	114.17	111.22
25	D	403	CLA	C4A-NA-C1A	2.05	108.98	106.38
25	C	505	CLA	CMD-C2D-C3D	2.05	129.10	125.09
25	b	606[A]	CLA	C4A-NA-C1A	2.05	108.98	106.38
27	H	101	BCR	C2-C1-C6	2.06	113.54	110.48
25	D	402	CLA	CMD-C2D-C3D	2.06	129.12	125.09
25	B	610	CLA	CMD-C2D-C3D	2.06	129.12	125.09
25	b	608	CLA	O2D-CGD-CBD	2.06	114.19	111.22
25	b	601	CLA	O2D-CGD-CBD	2.06	114.19	111.22
34	V	201	HEM	CMB-C2B-C3B	2.06	129.13	125.09
26	a	608	PHO	C1B-NB-C4B	2.08	110.45	106.50
25	b	615	CLA	CMB-C2B-C3B	2.08	129.15	125.09
25	b	606[B]	CLA	C4A-NA-C1A	2.08	109.02	106.38
25	B	611	CLA	CMD-C2D-C3D	2.08	129.16	125.09
25	d	401	CLA	C4A-NA-C1A	2.08	109.02	106.38
25	B	608	CLA	C4A-NA-C1A	2.08	109.02	106.38
25	C	508	CLA	CMD-C2D-C3D	2.09	129.17	125.09
25	b	607	CLA	CMD-C2D-C3D	2.09	129.17	125.09
25	c	504	CLA	O1D-CGD-CBD	2.10	127.90	124.64
25	B	603	CLA	O2D-CGD-CBD	2.10	114.24	111.22
25	c	512	CLA	CMD-C2D-C3D	2.10	129.19	125.09
25	d	401	CLA	CMD-C2D-C3D	2.10	129.19	125.09
25	c	512	CLA	O2D-CGD-CBD	2.10	114.25	111.22
25	b	605	CLA	C4A-NA-C1A	2.10	109.04	106.38
25	B	601	CLA	O1D-CGD-CBD	2.10	127.91	124.64
28	A	611	PL9	C20-C19-C21	2.10	118.57	115.37
25	c	511	CLA	CMD-C2D-C3D	2.10	129.20	125.09
29	A	612	SQD	C44-O6-C1	2.11	118.21	113.81
25	C	510	CLA	CMD-C2D-C3D	2.11	129.21	125.09
25	C	514	CLA	C4A-NA-C1A	2.11	109.06	106.38
25	B	607	CLA	CMD-C2D-C3D	2.12	129.23	125.09
25	B	605	CLA	C4A-NA-C1A	2.12	109.06	106.38
27	t	101	BCR	C4-C5-C6	2.12	125.06	122.73
25	B	614	CLA	O2D-CGD-CBD	2.12	114.28	111.22
25	b	608	CLA	CMD-C2D-C3D	2.12	129.24	125.09
34	E	101	HEM	CMB-C2B-C3B	2.12	129.24	125.09
25	b	612	CLA	O1D-CGD-CBD	2.12	127.94	124.64
25	c	506	CLA	C4A-NA-C1A	2.12	109.07	106.38
25	C	509	CLA	C4A-NA-C1A	2.13	109.08	106.38
25	c	513	CLA	O1D-CGD-CBD	2.13	127.95	124.64
25	C	514	CLA	CMD-C2D-C3D	2.14	129.27	125.09
34	v	201	HEM	CMC-C2C-C3C	2.14	129.27	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	CMD-C2D-C3D	2.14	129.27	125.09
25	B	608	CLA	CMD-C2D-C3D	2.14	129.28	125.09
25	d	402	CLA	C4A-NA-C1A	2.15	109.10	106.38
25	b	604	CLA	CMB-C2B-C3B	2.15	129.29	125.09
25	b	601	CLA	C4A-NA-C1A	2.15	109.11	106.38
25	c	509	CLA	CMD-C2D-C3D	2.15	129.30	125.09
25	c	505	CLA	C4A-NA-C1A	2.15	109.11	106.38
25	A	609	CLA	CMD-C2D-C3D	2.16	129.31	125.09
25	b	609	CLA	CMD-C2D-C3D	2.16	129.31	125.09
25	B	610	CLA	O1D-CGD-CBD	2.16	128.00	124.64
26	D	401	PHO	C1B-NB-C4B	2.16	110.61	106.50
25	b	606[A]	CLA	CMD-C2D-C3D	2.16	129.32	125.09
25	B	606	CLA	O2D-CGD-CBD	2.16	114.34	111.22
25	B	607	CLA	O1D-CGD-CBD	2.17	128.01	124.64
25	b	610	CLA	C4A-NA-C1A	2.17	109.13	106.38
25	C	513	CLA	CMD-C2D-C3D	2.17	129.34	125.09
25	B	616	CLA	O2D-CGD-CBD	2.17	114.35	111.22
29	B	624	SQD	O48-C23-C24	2.17	118.54	111.85
25	a	610	CLA	C4A-NA-C1A	2.18	109.14	106.38
25	b	611	CLA	C4A-NA-C1A	2.18	109.14	106.38
25	c	504	CLA	C4A-NA-C1A	2.18	109.14	106.38
25	B	611	CLA	C4A-NA-C1A	2.18	109.14	106.38
26	A	608	PHO	C1B-NB-C4B	2.18	110.64	106.50
25	B	612	CLA	O1D-CGD-CBD	2.18	128.03	124.64
25	C	507	CLA	CMD-C2D-C3D	2.18	129.36	125.09
25	C	509	CLA	CMD-C2D-C3D	2.19	129.37	125.09
25	b	614	CLA	C4A-NA-C1A	2.19	109.16	106.38
25	a	610	CLA	CMD-C2D-C3D	2.19	129.37	125.09
26	a	609	PHO	C1B-NB-C4B	2.19	110.67	106.50
25	C	502	CLA	O2D-CGD-CBD	2.19	114.38	111.22
25	c	506	CLA	CMD-C2D-C3D	2.19	129.38	125.09
25	b	603	CLA	O1D-CGD-CBD	2.20	128.06	124.64
25	C	504	CLA	O1D-CGD-CBD	2.20	128.06	124.64
25	b	606[B]	CLA	CMD-C2D-C3D	2.20	129.39	125.09
25	C	511	CLA	C4A-NA-C1A	2.20	109.17	106.38
25	c	505	CLA	O2D-CGD-CBD	2.20	114.40	111.22
25	C	506	CLA	CMD-C2D-C3D	2.21	129.41	125.09
25	C	502	CLA	C4A-NA-C1A	2.21	109.18	106.38
25	B	615	CLA	CMD-C2D-C3D	2.21	129.41	125.09
25	c	508	CLA	CMD-C2D-C3D	2.21	129.41	125.09
25	B	615	CLA	CMB-C2B-C3B	2.22	129.42	125.09
25	c	504	CLA	CMD-C2D-C3D	2.22	129.43	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	502	CLA	CMD-C2D-C3D	2.23	129.44	125.09
25	c	507	CLA	CMD-C2D-C3D	2.23	129.45	125.09
25	c	501	CLA	C4A-NA-C1A	2.23	109.21	106.38
25	c	502	CLA	O1D-CGD-CBD	2.24	128.13	124.64
25	b	604	CLA	O2D-CGD-CBD	2.25	114.46	111.22
25	b	614	CLA	CMD-C2D-C3D	2.25	129.48	125.09
25	B	614	CLA	CMD-C2D-C3D	2.25	129.48	125.09
27	d	403	BCR	C29-C30-C25	2.25	113.83	110.48
25	C	505	CLA	O1D-CGD-CBD	2.25	128.14	124.64
25	b	612	CLA	C4A-NA-C1A	2.25	109.24	106.38
25	b	610	CLA	CMD-C2D-C3D	2.26	129.51	125.09
25	B	609	CLA	CMD-C2D-C3D	2.26	129.51	125.09
25	B	601	CLA	C4A-NA-C1A	2.26	109.25	106.38
25	B	604	CLA	CMB-C2B-C3B	2.26	129.51	125.09
25	b	609	CLA	C4A-NA-C1A	2.26	109.25	106.38
25	c	502	CLA	C4A-NA-C1A	2.27	109.25	106.38
25	C	503	CLA	O1D-CGD-CBD	2.27	128.16	124.64
25	B	613	CLA	O1D-CGD-CBD	2.27	128.17	124.64
25	C	503	CLA	C4A-NA-C1A	2.27	109.26	106.38
25	c	511	CLA	O2D-CGD-CBD	2.27	114.49	111.22
25	C	503	CLA	CMD-C2D-C3D	2.27	129.53	125.09
29	L	101	SQD	C3-C4-C5	2.27	114.28	110.23
25	b	616	CLA	C4A-NA-C1A	2.28	109.27	106.38
25	B	612	CLA	C4A-NA-C1A	2.28	109.27	106.38
25	b	613	CLA	CMD-C2D-C3D	2.28	129.54	125.09
25	C	506	CLA	C4A-NA-C1A	2.28	109.27	106.38
25	B	604	CLA	O2D-CGD-CBD	2.28	114.51	111.22
25	B	609	CLA	O1D-CGD-CBD	2.28	128.19	124.64
25	b	610	CLA	O1D-CGD-CBD	2.28	128.19	124.64
25	d	401	CLA	O2D-CGD-CBD	2.29	114.51	111.22
25	b	615	CLA	CMD-C2D-C3D	2.29	129.56	125.09
25	b	605	CLA	CMB-C2B-C3B	2.29	129.57	125.09
29	D	408	SQD	C3-C4-C5	2.29	114.32	110.23
27	B	619	BCR	C2-C1-C6	2.29	113.89	110.48
25	B	606	CLA	CMB-C2B-C3B	2.30	129.58	125.09
25	c	509	CLA	O1D-CGD-CBD	2.30	128.21	124.64
27	d	403	BCR	C27-C26-C25	2.30	125.26	122.73
25	C	513	CLA	C4A-NA-C1A	2.30	109.30	106.38
25	B	616	CLA	C4A-NA-C1A	2.30	109.30	106.38
25	b	609	CLA	O1D-CGD-CBD	2.30	128.22	124.64
25	B	613	CLA	C4A-NA-C1A	2.31	109.30	106.38
25	C	507	CLA	C4A-NA-C1A	2.31	109.31	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	514	CLA	O2D-CGD-CBD	2.31	114.55	111.22
25	b	607	CLA	O1D-CGD-CBD	2.31	128.23	124.64
25	b	613	CLA	O1D-CGD-CBD	2.31	128.23	124.64
25	C	513	CLA	O2D-CGD-CBD	2.31	114.55	111.22
27	T	101	BCR	C2-C1-C6	2.32	113.93	110.48
25	c	510	CLA	C4A-NA-C1A	2.33	109.33	106.38
29	f	101	SQD	C44-O6-C1	2.33	118.68	113.81
25	b	613	CLA	C4A-NA-C1A	2.33	109.33	106.38
25	B	605	CLA	O1D-CGD-CBD	2.33	128.27	124.64
25	d	401	CLA	CMB-C2B-C3B	2.33	129.66	125.09
29	L	101	SQD	C44-O6-C1	2.34	118.69	113.81
25	b	612	CLA	CMD-C2D-C3D	2.34	129.66	125.09
26	a	608	PHO	C3D-C4D-CHA	2.34	112.83	107.14
25	B	603	CLA	CMD-C2D-C3D	2.34	129.66	125.09
29	B	625	SQD	O5-C5-C4	2.34	114.13	109.67
25	C	510	CLA	C4A-NA-C1A	2.34	109.35	106.38
25	B	609	CLA	CMB-C2B-C3B	2.34	129.67	125.09
25	b	606[A]	CLA	O2D-CGD-CBD	2.34	114.60	111.22
29	f	101	SQD	O47-C7-C8	2.35	119.19	110.82
29	A	616	SQD	O5-C5-C4	2.35	114.15	109.67
25	c	507	CLA	O2D-CGD-CBD	2.36	114.62	111.22
25	A	613	CLA	CMB-C2B-C3B	2.36	129.70	125.09
25	b	605	CLA	O1D-CGD-CBD	2.36	128.31	124.64
26	A	608	PHO	C3D-C4D-CHA	2.36	112.88	107.14
25	c	512	CLA	CMB-C2B-C3B	2.36	129.71	125.09
26	a	609	PHO	C3D-C4D-CHA	2.37	112.89	107.14
25	B	606	CLA	C4A-NA-C1A	2.37	109.38	106.38
25	b	606[B]	CLA	CMB-C2B-C3B	2.37	129.72	125.09
25	c	503	CLA	CMB-C2B-C3B	2.37	129.72	125.09
29	D	409	SQD	O5-C5-C4	2.37	114.19	109.67
29	D	409	SQD	O8-S-C6	2.37	109.92	104.99
25	b	610	CLA	CMB-C2B-C3B	2.38	129.73	125.09
25	a	615	CLA	CMB-C2B-C3B	2.38	129.74	125.09
29	A	616	SQD	O48-C23-C24	2.38	119.17	111.85
25	b	602	CLA	O2D-CGD-CBD	2.38	114.65	111.22
25	b	606[B]	CLA	O2D-CGD-CBD	2.38	114.65	111.22
25	B	615	CLA	C4A-NA-C1A	2.38	109.40	106.38
25	B	609	CLA	C4A-NA-C1A	2.38	109.40	106.38
26	a	609	PHO	CBD-CHA-C1A	2.39	130.92	126.70
25	C	507	CLA	O1D-CGD-CBD	2.39	128.36	124.64
29	B	625	SQD	O6-C1-C2	2.40	110.95	108.00
25	b	606[A]	CLA	CMB-C2B-C3B	2.40	129.78	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	C4A-NA-C1A	2.40	109.43	106.38
25	b	601	CLA	CMB-C2B-C3B	2.41	129.80	125.09
25	C	504	CLA	CMB-C2B-C3B	2.42	129.83	125.09
25	C	513	CLA	CMB-C2B-C3B	2.43	129.84	125.09
29	A	616	SQD	C44-O6-C1	2.43	118.89	113.81
25	C	503	CLA	CMB-C2B-C3B	2.43	129.84	125.09
29	b	621	SQD	O48-C23-C24	2.43	119.33	111.85
26	A	608	PHO	CBD-CHA-C1A	2.43	130.99	126.70
25	C	504	CLA	C4A-NA-C1A	2.44	109.47	106.38
25	C	508	CLA	O2D-CGD-CBD	2.44	114.74	111.22
25	c	506	CLA	O1D-CGD-CBD	2.44	128.43	124.64
26	D	401	PHO	C3D-C4D-CHA	2.44	113.08	107.14
25	c	507	CLA	CMB-C2B-C3B	2.44	129.87	125.09
25	c	509	CLA	C4A-NA-C1A	2.45	109.48	106.38
25	a	615	CLA	O2D-CGD-CBD	2.45	114.75	111.22
25	b	615	CLA	C4A-NA-C1A	2.45	109.48	106.38
29	f	101	SQD	O48-C23-C24	2.45	119.40	111.85
25	c	502	CLA	CMB-C2B-C3B	2.45	129.89	125.09
25	C	502	CLA	CMB-C2B-C3B	2.45	129.89	125.09
25	a	607	CLA	CMB-C2B-C3B	2.46	129.89	125.09
29	D	409	SQD	O48-C23-C24	2.46	119.41	111.85
29	A	612	SQD	O8-S-C6	2.46	110.09	104.99
25	B	601	CLA	CMB-C2B-C3B	2.48	129.93	125.09
25	c	504	CLA	CMB-C2B-C3B	2.48	129.93	125.09
25	a	607	CLA	O2D-CGD-CBD	2.48	114.79	111.22
29	A	616	SQD	O8-S-C6	2.48	110.15	104.99
29	D	408	SQD	O8-S-C6	2.48	110.15	104.99
29	B	625	SQD	O8-S-C6	2.49	110.16	104.99
25	d	402	CLA	CMB-C2B-C3B	2.49	129.95	125.09
25	B	610	CLA	CMB-C2B-C3B	2.49	129.96	125.09
25	a	610	CLA	O2D-CGD-CBD	2.49	114.81	111.22
25	c	507	CLA	C4A-NA-C1A	2.49	109.54	106.38
25	C	508	CLA	C4A-NA-C1A	2.50	109.55	106.38
26	D	401	PHO	CBD-CHA-C1A	2.51	131.12	126.70
26	a	608	PHO	CBD-CHA-C1A	2.51	131.12	126.70
25	c	501	CLA	CMB-C2B-C3B	2.52	130.01	125.09
25	B	603	CLA	CMB-C2B-C3B	2.52	130.01	125.09
25	c	503	CLA	C4A-NA-C1A	2.52	109.58	106.38
25	b	611	CLA	O2D-CGD-CBD	2.53	114.86	111.22
25	A	607	CLA	CMB-C2B-C3B	2.53	130.03	125.09
25	b	609	CLA	CMB-C2B-C3B	2.53	130.03	125.09
29	L	101	SQD	O48-C23-C24	2.53	119.63	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	C4A-NA-C1A	2.53	109.59	106.38
25	a	606	CLA	O1D-CGD-CBD	2.53	128.58	124.64
25	c	501	CLA	O2D-CGD-CBD	2.53	114.87	111.22
29	a	613	SQD	O48-C23-C24	2.54	119.66	111.85
29	A	612	SQD	O48-C23-C24	2.54	119.67	111.85
25	C	505	CLA	CMB-C2B-C3B	2.54	130.06	125.09
25	c	506	CLA	CMB-C2B-C3B	2.55	130.07	125.09
25	D	403	CLA	O2D-CGD-CBD	2.55	114.89	111.22
25	D	402	CLA	CMB-C2B-C3B	2.56	130.09	125.09
28	d	404	PL9	C20-C19-C21	2.56	119.27	115.37
29	B	625	SQD	O48-C23-C24	2.56	119.73	111.85
25	B	611	CLA	O2D-CGD-CBD	2.57	114.92	111.22
25	B	608	CLA	CMB-C2B-C3B	2.57	130.12	125.09
30	B	623	LHG	O8-C23-C24	2.57	119.77	111.85
29	L	101	SQD	O8-S-C6	2.58	110.34	104.99
30	L	102	LHG	O8-C23-C24	2.58	119.80	111.85
25	b	616	CLA	CMB-C2B-C3B	2.59	130.15	125.09
25	B	616	CLA	CMB-C2B-C3B	2.60	130.17	125.09
30	d	405	LHG	O8-C23-C24	2.60	119.85	111.85
25	C	512	CLA	CMB-C2B-C3B	2.60	130.18	125.09
30	a	617	LHG	O8-C23-C24	2.60	119.86	111.85
25	B	612	CLA	CMD-C2D-C3D	2.62	130.21	125.09
25	b	607	CLA	CMB-C2B-C3B	2.62	130.21	125.09
30	A	618	LHG	O8-C23-C24	2.63	119.95	111.85
29	D	409	SQD	C44-O6-C1	2.63	119.32	113.81
25	B	611	CLA	CMB-C2B-C3B	2.64	130.25	125.09
25	B	605	CLA	CMB-C2B-C3B	2.64	130.26	125.09
25	C	507	CLA	CMB-C2B-C3B	2.65	130.28	125.09
29	D	408	SQD	O48-C23-C24	2.65	120.02	111.85
25	B	614	CLA	CMB-C2B-C3B	2.66	130.29	125.09
25	a	610	CLA	CMB-C2B-C3B	2.66	130.30	125.09
30	A	614	LHG	O8-C23-C24	2.66	120.05	111.85
26	D	401	PHO	O1D-CGD-CBD	2.67	128.79	124.64
28	D	405	PL9	C20-C19-C21	2.68	119.45	115.37
25	c	511	CLA	CMB-C2B-C3B	2.68	130.32	125.09
25	A	613	CLA	O2D-CGD-CBD	2.68	115.08	111.22
25	C	509	CLA	O2D-CGD-CBD	2.68	115.08	111.22
25	b	604	CLA	C4A-NA-C1A	2.68	109.78	106.38
25	C	514	CLA	CMB-C2B-C3B	2.68	130.33	125.09
25	b	608	CLA	CMB-C2B-C3B	2.69	130.34	125.09
29	A	612	SQD	O5-C5-C4	2.69	114.80	109.67
29	f	101	SQD	O8-S-C6	2.69	110.58	104.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	614	CLA	CMB-C2B-C3B	2.69	130.35	125.09
25	C	508	CLA	CMB-C2B-C3B	2.69	130.36	125.09
30	l	101	LHG	O8-C23-C24	2.70	120.17	111.85
25	a	606	CLA	CMB-C2B-C3B	2.71	130.39	125.09
25	c	505	CLA	CMB-C2B-C3B	2.72	130.40	125.09
29	a	613	SQD	O8-S-C6	2.72	110.64	104.99
25	A	609	CLA	CMB-C2B-C3B	2.72	130.41	125.09
25	B	602	CLA	CMB-C2B-C3B	2.73	130.42	125.09
25	b	602	CLA	CMB-C2B-C3B	2.73	130.43	125.09
25	c	513	CLA	CMB-C2B-C3B	2.73	130.43	125.09
30	d	406	LHG	O8-C23-C24	2.73	120.26	111.85
28	a	612	PL9	C20-C19-C21	2.74	119.54	115.37
29	B	625	SQD	C44-O6-C1	2.75	119.55	113.81
25	B	602	CLA	O2D-CGD-CBD	2.76	115.20	111.22
25	c	510	CLA	CMB-C2B-C3B	2.76	130.50	125.09
25	A	607	CLA	O2D-CGD-CBD	2.77	115.22	111.22
25	c	508	CLA	O2D-CGD-CBD	2.77	115.22	111.22
29	B	624	SQD	C1-O5-C5	2.78	119.19	113.74
25	C	509	CLA	CMB-C2B-C3B	2.78	130.53	125.09
30	D	406	LHG	O8-C23-C24	2.78	120.42	111.85
25	C	511	CLA	CMB-C2B-C3B	2.78	130.53	125.09
25	b	611	CLA	CMB-C2B-C3B	2.79	130.54	125.09
29	a	613	SQD	O5-C5-C4	2.79	114.98	109.67
29	B	624	SQD	O8-S-C6	2.80	110.80	104.99
25	C	506	CLA	CMB-C2B-C3B	2.80	130.57	125.09
25	A	609	CLA	O2D-CGD-CBD	2.80	115.26	111.22
25	b	612	CLA	CMB-C2B-C3B	2.81	130.58	125.09
26	a	608	PHO	O1D-CGD-CBD	2.82	129.02	124.64
25	A	606	CLA	CMB-C2B-C3B	2.83	130.62	125.09
25	b	603	CLA	CMB-C2B-C3B	2.83	130.63	125.09
25	B	607	CLA	CMB-C2B-C3B	2.85	130.67	125.09
25	c	508	CLA	CMB-C2B-C3B	2.87	130.71	125.09
29	f	101	SQD	O5-C5-C4	2.91	115.22	109.67
29	B	624	SQD	O5-C5-C4	2.94	115.27	109.67
29	A	616	SQD	O6-C1-C2	2.96	111.65	108.00
25	b	613	CLA	CMB-C2B-C3B	2.98	130.91	125.09
25	c	509	CLA	CMB-C2B-C3B	2.98	130.92	125.09
30	a	616	LHG	O8-C23-C24	2.99	121.06	111.85
29	D	408	SQD	O5-C5-C4	3.01	115.41	109.67
25	B	612	CLA	CMB-C2B-C3B	3.02	131.00	125.09
29	D	409	SQD	C1-O5-C5	3.03	119.69	113.74
25	C	510	CLA	CMB-C2B-C3B	3.04	131.03	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	404	PL9	C40-C39-C41	3.04	120.00	115.37
27	C	516	BCR	C27-C26-C25	3.05	126.09	122.73
27	c	522	BCR	C27-C26-C25	3.06	126.10	122.73
27	B	619	BCR	C27-C26-C25	3.07	126.11	122.73
26	A	608	PHO	O1D-CGD-CBD	3.07	129.41	124.64
27	h	101	BCR	C27-C26-C25	3.11	126.15	122.73
27	D	404	BCR	C27-C26-C25	3.12	126.16	122.73
25	D	403	CLA	CMB-C2B-C3B	3.12	131.20	125.09
27	B	617	BCR	C27-C26-C25	3.15	126.19	122.73
27	B	618	BCR	C27-C26-C25	3.15	126.20	122.73
26	a	609	PHO	O1D-CGD-CBD	3.16	129.55	124.64
25	B	613	CLA	CMB-C2B-C3B	3.17	131.29	125.09
28	A	611	PL9	C40-C39-C41	3.17	120.20	115.37
27	K	101	BCR	C27-C26-C25	3.18	126.22	122.73
27	c	521	BCR	C27-C26-C25	3.18	126.23	122.73
27	b	619	BCR	C27-C26-C25	3.20	126.25	122.73
29	L	101	SQD	O5-C5-C4	3.22	115.81	109.67
27	a	611	BCR	C27-C26-C25	3.22	126.28	122.73
27	T	101	BCR	C27-C26-C25	3.24	126.30	122.73
27	C	515	BCR	C27-C26-C25	3.25	126.31	122.73
27	A	610	BCR	C27-C26-C25	3.27	126.33	122.73
27	c	514	BCR	C27-C26-C25	3.27	126.33	122.73
28	a	612	PL9	C40-C39-C41	3.28	120.36	115.37
27	t	101	BCR	C27-C26-C25	3.28	126.34	122.73
27	b	617	BCR	C27-C26-C25	3.30	126.36	122.73
27	c	515	BCR	C27-C26-C25	3.31	126.37	122.73
27	Y	101	BCR	C27-C26-C25	3.33	126.39	122.73
29	B	624	SQD	C44-O6-C1	3.33	120.77	113.81
27	b	618	BCR	C27-C26-C25	3.37	126.44	122.73
28	D	405	PL9	C40-C39-C41	3.41	120.56	115.37
29	a	613	SQD	O47-C7-C8	3.45	118.79	111.53
27	H	101	BCR	C27-C26-C25	3.50	126.58	122.73
29	D	409	SQD	O47-C7-C8	3.53	118.97	111.53
29	D	408	SQD	O47-C7-C8	3.53	118.97	111.53
29	L	101	SQD	O47-C7-C8	3.57	119.05	111.53
29	B	624	SQD	O47-C7-C8	3.63	119.18	111.53
29	A	616	SQD	O47-C7-C8	3.78	119.49	111.53
29	B	625	SQD	O47-C7-C8	3.83	119.61	111.53
30	a	616	LHG	O4-P-O5	3.87	132.71	112.56
30	D	406	LHG	O4-P-O5	3.88	132.75	112.56
30	l	101	LHG	O4-P-O5	3.88	132.76	112.56
30	A	614	LHG	O4-P-O5	3.89	132.79	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	618	LHG	O4-P-O5	3.89	132.79	112.56
30	B	623	LHG	O4-P-O5	3.89	132.82	112.56
30	L	102	LHG	O4-P-O5	3.91	132.90	112.56
30	a	617	LHG	O4-P-O5	3.92	132.95	112.56
30	d	406	LHG	O4-P-O5	3.93	132.99	112.56
30	d	405	LHG	O4-P-O5	3.94	133.07	112.56
29	f	101	SQD	O6-C1-C2	3.98	112.90	108.00
29	A	612	SQD	O47-C7-C8	4.01	119.97	111.53
29	L	101	SQD	O6-C1-C2	4.04	112.97	108.00
29	b	621	SQD	O47-C7-C8	4.04	120.04	111.53
29	a	613	SQD	O6-C1-C2	4.51	113.55	108.00
29	D	408	SQD	O6-C1-C2	4.53	113.58	108.00
29	A	612	SQD	O6-C1-C2	4.76	113.86	108.00
29	B	624	SQD	O6-C1-C2	5.15	114.34	108.00
29	B	624	SQD	O7-S-C6	5.69	110.93	106.92
29	a	613	SQD	O9-S-C6	5.91	111.09	106.92
29	f	101	SQD	O7-S-C6	5.93	111.09	106.92
29	L	101	SQD	O9-S-C6	5.93	111.10	106.92
29	B	625	SQD	O9-S-C6	6.04	111.17	106.92
29	A	616	SQD	O9-S-C6	6.36	111.40	106.92
29	A	612	SQD	O9-S-C6	6.39	111.42	106.92
29	f	101	SQD	O9-S-C6	6.41	111.44	106.92
29	D	408	SQD	O7-S-C6	6.42	111.44	106.92
29	B	624	SQD	O9-S-C6	6.45	111.47	106.92
29	A	616	SQD	O7-S-C6	6.53	111.52	106.92
29	a	613	SQD	O7-S-C6	6.57	111.55	106.92
29	B	625	SQD	O7-S-C6	6.60	111.57	106.92
29	A	612	SQD	O7-S-C6	6.85	111.75	106.92
29	D	409	SQD	O7-S-C6	7.05	111.89	106.92
29	L	101	SQD	O7-S-C6	7.08	111.91	106.92
29	D	408	SQD	O9-S-C6	7.14	111.95	106.92
29	D	409	SQD	O9-S-C6	7.25	112.03	106.92

All (213) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	C	508	CLA	NC
25	C	508	CLA	ND
25	C	508	CLA	NA
25	b	613	CLA	NC
25	b	613	CLA	ND
25	b	613	CLA	NA

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Mol	Chain	Res	Type	Atom
25	C	510	CLA	NC
25	C	510	CLA	ND
25	C	510	CLA	NA
25	a	615	CLA	NA
25	a	615	CLA	NC
25	a	615	CLA	ND
25	A	613	CLA	NA
25	A	613	CLA	NC
25	A	613	CLA	ND
25	b	606[B]	CLA	NC
25	b	606[B]	CLA	ND
25	b	606[B]	CLA	NA
25	b	605	CLA	NC
25	b	605	CLA	ND
25	b	605	CLA	NA
25	c	506	CLA	NC
25	c	506	CLA	ND
25	c	506	CLA	NA
25	c	501	CLA	NC
25	c	501	CLA	ND
25	c	501	CLA	NA
25	C	502	CLA	NC
25	C	502	CLA	ND
25	C	502	CLA	NA
25	D	402	CLA	NC
25	D	402	CLA	ND
25	D	402	CLA	NA
25	B	604	CLA	NC
25	B	604	CLA	ND
25	B	604	CLA	NA
25	C	504	CLA	NC
25	C	504	CLA	ND
25	C	504	CLA	NA
25	B	606	CLA	NC
25	B	606	CLA	ND
25	B	606	CLA	NA
25	b	601	CLA	NC
25	b	601	CLA	ND
25	b	601	CLA	NA
25	A	607	CLA	NA
25	A	607	CLA	NC
25	A	607	CLA	ND

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Mol	Chain	Res	Type	Atom
25	C	511	CLA	NC
25	C	511	CLA	ND
25	C	511	CLA	NA
25	b	608	CLA	NC
25	b	608	CLA	ND
25	b	608	CLA	NA
25	C	509	CLA	NC
25	C	509	CLA	ND
25	C	509	CLA	NA
25	C	512	CLA	NA
25	C	512	CLA	NC
25	C	512	CLA	ND
25	c	502	CLA	NC
25	c	502	CLA	ND
25	c	502	CLA	NA
25	B	602	CLA	NC
25	B	602	CLA	ND
25	B	602	CLA	NA
25	B	603	CLA	NC
25	B	603	CLA	ND
25	B	603	CLA	NA
25	d	402	CLA	NC
25	d	402	CLA	ND
25	d	402	CLA	NA
25	C	507	CLA	NC
25	C	507	CLA	ND
25	C	507	CLA	NA
25	b	612	CLA	NC
25	b	612	CLA	ND
25	b	612	CLA	NA
25	d	401	CLA	NC
25	d	401	CLA	ND
25	d	401	CLA	NA
25	b	602	CLA	NC
25	b	602	CLA	ND
25	b	602	CLA	NA
25	C	506	CLA	NC
25	C	506	CLA	ND
25	C	506	CLA	NA
25	A	606	CLA	NC
25	A	606	CLA	ND
25	A	606	CLA	NA

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Mol	Chain	Res	Type	Atom
25	c	508	CLA	NC
25	c	508	CLA	ND
25	c	508	CLA	NA
25	B	607	CLA	NC
25	B	607	CLA	ND
25	B	607	CLA	NA
25	c	513	CLA	NC
25	c	513	CLA	ND
25	c	513	CLA	NA
25	b	614	CLA	NC
25	b	614	CLA	ND
25	b	614	CLA	NA
25	C	503	CLA	NC
25	C	503	CLA	ND
25	C	503	CLA	NA
25	B	609	CLA	NC
25	B	609	CLA	ND
25	B	609	CLA	NA
25	b	606[A]	CLA	NC
25	b	606[A]	CLA	ND
25	b	606[A]	CLA	NA
25	a	607	CLA	NA
25	a	607	CLA	NC
25	a	607	CLA	ND
25	c	505	CLA	NC
25	c	505	CLA	ND
25	c	505	CLA	NA
25	B	615	CLA	NC
25	B	615	CLA	ND
25	B	615	CLA	NA
25	B	610	CLA	NC
25	B	610	CLA	ND
25	B	610	CLA	NA
25	C	514	CLA	NC
25	C	514	CLA	ND
25	C	514	CLA	NA
25	A	609	CLA	NC
25	A	609	CLA	ND
25	A	609	CLA	NA
25	C	505	CLA	NA
25	C	505	CLA	NC
25	C	505	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	601	CLA	NC
25	B	601	CLA	ND
25	B	601	CLA	NA
25	b	611	CLA	NC
25	b	611	CLA	ND
25	b	611	CLA	NA
25	c	511	CLA	NA
25	c	511	CLA	NC
25	c	511	CLA	ND
25	a	606	CLA	NA
25	a	606	CLA	NC
25	a	606	CLA	ND
25	c	503	CLA	NC
25	c	503	CLA	ND
25	c	503	CLA	NA
25	c	509	CLA	NC
25	c	509	CLA	ND
25	c	509	CLA	NA
25	b	616	CLA	NC
25	b	616	CLA	ND
25	b	616	CLA	NA
25	b	604	CLA	NC
25	b	604	CLA	ND
25	b	604	CLA	NA
25	c	512	CLA	NC
25	c	512	CLA	ND
25	c	512	CLA	NA
25	B	605	CLA	NC
25	B	605	CLA	ND
25	B	605	CLA	NA
25	b	607	CLA	NA
25	b	607	CLA	NC
25	b	607	CLA	ND
25	c	507	CLA	NC
25	c	507	CLA	ND
25	c	507	CLA	NA
25	C	513	CLA	NC
25	C	513	CLA	ND
25	C	513	CLA	NA
25	B	612	CLA	NC
25	B	612	CLA	ND
25	B	612	CLA	NA

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Mol	Chain	Res	Type	Atom
25	a	610	CLA	NC
25	a	610	CLA	ND
25	a	610	CLA	NA
25	b	609	CLA	NC
25	b	609	CLA	ND
25	b	609	CLA	NA
25	c	504	CLA	NC
25	c	504	CLA	ND
25	c	504	CLA	NA
25	B	611	CLA	NC
25	B	611	CLA	ND
25	B	611	CLA	NA
25	b	603	CLA	NC
25	b	603	CLA	ND
25	b	603	CLA	NA
25	D	403	CLA	NC
25	D	403	CLA	ND
25	D	403	CLA	NA
25	B	613	CLA	NC
25	B	613	CLA	ND
25	B	613	CLA	NA
25	c	510	CLA	NC
25	c	510	CLA	ND
25	c	510	CLA	NA
25	B	616	CLA	NC
25	B	616	CLA	ND
25	B	616	CLA	NA
25	b	615	CLA	NC
25	b	615	CLA	ND
25	b	615	CLA	NA
25	B	614	CLA	NA
25	B	614	CLA	NC
25	B	614	CLA	ND
25	b	610	CLA	NC
25	b	610	CLA	ND
25	b	610	CLA	NA
25	B	608	CLA	NC
25	B	608	CLA	ND
25	B	608	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	C	521	LMG	C7-O1-C1-O6

There are no ring outliers.

70 monomers are involved in 216 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	606	CLA	7	0
25	A	607	CLA	9	0
26	A	608	PHO	4	0
25	A	609	CLA	1	0
27	A	610	BCR	2	0
28	A	611	PL9	3	0
25	A	613	CLA	1	0
29	A	616	SQD	2	0
30	A	618	LHG	3	0
25	B	601	CLA	7	0
25	B	602	CLA	5	0
25	B	603	CLA	4	0
25	B	604	CLA	6	0
25	B	605	CLA	6	0
25	B	606	CLA	3	0
25	B	607	CLA	2	0
25	B	608	CLA	4	0
25	B	609	CLA	7	0
25	B	610	CLA	4	0
25	B	611	CLA	4	0
25	B	612	CLA	2	0
25	B	613	CLA	3	0
25	B	614	CLA	8	0
25	B	615	CLA	8	0
25	B	616	CLA	1	0
27	B	617	BCR	4	0
27	B	618	BCR	4	0
27	B	619	BCR	4	0
32	B	620	LMG	1	0
32	B	621	LMG	1	0
30	B	623	LHG	4	0
29	B	624	SQD	4	0
29	B	625	SQD	2	0
32	B	626	LMG	1	0
32	C	501	LMG	1	0
25	C	502	CLA	4	0
25	C	503	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	504	CLA	6	0
25	C	505	CLA	6	0
25	C	506	CLA	5	0
25	C	507	CLA	4	0
25	C	508	CLA	7	0
25	C	509	CLA	8	0
25	C	510	CLA	5	0
25	C	511	CLA	7	0
25	C	512	CLA	4	0
25	C	513	CLA	5	0
25	C	514	CLA	3	0
27	C	515	BCR	6	0
27	C	516	BCR	2	0
33	C	517	DGD	3	0
33	C	518	DGD	3	0
33	C	519	DGD	1	0
32	C	521	LMG	1	0
25	D	402	CLA	6	0
25	D	403	CLA	3	0
27	D	404	BCR	4	0
30	D	406	LHG	4	0
32	D	407	LMG	2	0
29	D	408	SQD	2	0
29	D	409	SQD	1	0
34	E	101	HEM	5	0
27	H	101	BCR	4	0
33	H	102	DGD	2	0
27	K	101	BCR	2	0
29	L	101	SQD	3	0
30	L	102	LHG	1	0
27	T	101	BCR	5	0
34	V	201	HEM	2	0
27	Y	101	BCR	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	334/344 (97%)	-0.36	3 (0%) 85 87	28, 34, 52, 81	0
1	a	334/344 (97%)	-0.21	4 (1%) 81 83	28, 36, 63, 83	0
2	B	504/510 (98%)	-0.31	15 (2%) 54 58	28, 38, 65, 97	0
2	b	504/510 (98%)	-0.10	25 (4%) 32 36	29, 41, 76, 102	0
3	C	451/461 (97%)	-0.20	9 (1%) 68 72	30, 41, 61, 101	0
3	c	451/461 (97%)	-0.15	7 (1%) 74 77	31, 44, 65, 97	0
4	D	341/352 (96%)	-0.35	3 (0%) 85 87	28, 35, 52, 92	0
4	d	341/352 (96%)	-0.18	6 (1%) 71 75	28, 39, 61, 98	0
5	E	81/84 (96%)	0.12	6 (7%) 17 18	37, 55, 75, 97	0
5	e	82/84 (97%)	0.54	6 (7%) 18 19	42, 61, 83, 99	0
6	F	34/45 (75%)	-0.45	1 (2%) 55 60	41, 48, 70, 82	0
6	f	34/45 (75%)	-0.08	3 (8%) 12 14	44, 55, 83, 91	0
7	H	65/66 (98%)	-0.32	1 (1%) 76 79	36, 44, 61, 93	0
7	h	63/66 (95%)	0.14	4 (6%) 23 25	42, 51, 66, 70	0
8	I	36/38 (94%)	0.38	4 (11%) 7 7	36, 44, 78, 90	0
8	i	35/38 (92%)	-0.23	1 (2%) 55 60	36, 45, 72, 94	0
9	J	36/40 (90%)	-0.18	3 (8%) 14 15	39, 54, 81, 88	0
9	j	36/40 (90%)	0.14	3 (8%) 14 15	41, 57, 87, 96	0
10	K	37/46 (80%)	-0.02	1 (2%) 58 62	47, 56, 76, 83	0
10	k	37/46 (80%)	-0.22	0 100 100	52, 58, 74, 89	0
11	L	37/37 (100%)	-0.15	0 100 100	31, 34, 67, 72	0
11	l	37/37 (100%)	-0.18	4 (10%) 8 7	30, 37, 80, 104	0
12	M	32/36 (88%)	-0.37	1 (3%) 52 57	34, 39, 69, 93	0
12	m	32/36 (88%)	-0.46	1 (3%) 52 57	34, 40, 60, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.13	14 (5%) 27 30	28, 46, 84, 131	0
13	o	244/272 (89%)	-0.06	11 (4%) 37 41	30, 46, 85, 133	0
14	T	29/32 (90%)	0.30	2 (6%) 20 22	33, 37, 58, 84	0
14	t	29/32 (90%)	-0.13	1 (3%) 49 53	32, 37, 71, 88	0
15	U	97/134 (72%)	0.11	3 (3%) 52 57	36, 47, 74, 103	0
15	u	97/134 (72%)	-0.24	2 (2%) 67 71	34, 44, 62, 102	0
16	V	137/163 (84%)	-0.43	0 100 100	35, 44, 60, 85	0
16	v	137/163 (84%)	0.08	4 (2%) 55 60	37, 50, 71, 92	0
17	Y	27/46 (58%)	1.63	10 (37%) 0 0	57, 75, 102, 112	0
17	y	30/46 (65%)	0.42	5 (16%) 2 2	59, 74, 88, 97	0
18	X	38/41 (92%)	0.00	2 (5%) 30 33	43, 51, 76, 83	0
18	x	38/41 (92%)	0.51	3 (7%) 15 17	48, 60, 81, 100	0
19	Z	62/62 (100%)	1.15	13 (20%) 1 1	57, 72, 113, 123	0
19	z	62/62 (100%)	1.48	18 (29%) 1 0	59, 74, 111, 124	0
20	R	34/41 (82%)	1.79	17 (50%) 0 0	64, 76, 94, 102	0
20	r	34/41 (82%)	3.50	24 (70%) 0 0	75, 91, 109, 110	0
All	All	5313/5700 (93%)	-0.08	240 (4%) 37 41	28, 42, 78, 133	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	30	PRO	11.3
8	I	37	LEU	10.6
13	o	61	GLN	9.5
2	b	127	ARG	8.6
20	r	35	LEU	8.1
19	z	33	TRP	7.9
19	z	34	ASP	7.2
19	Z	62	VAL	7.1
3	c	23	ALA	7.0
20	r	26	TYR	6.9
3	C	24	THR	6.6
17	Y	20	ALA	6.5
20	r	25	PRO	6.5
3	C	23	ALA	6.4
2	b	128	THR	6.3

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Mol	Chain	Res	Type	RSRZ
17	Y	22	LEU	6.3
13	o	3	GLN	6.3
19	z	3	ILE	6.2
13	O	60	ARG	6.1
19	Z	32	ASP	6.0
17	Y	40	ALA	6.0
13	O	62	GLU	5.9
19	z	36	SER	5.9
20	r	9	LEU	5.7
14	T	29	ILE	5.5
18	x	38	GLN	5.5
6	f	12	SER	5.4
4	D	12	ARG	5.4
13	O	61	GLN	5.4
13	o	60	ARG	5.3
20	r	28	VAL	5.3
19	z	1	MET	5.2
20	r	23	ILE	5.2
1	A	13	LEU	5.2
11	l	1	MET	5.1
20	r	27	ALA	5.0
5	e	4	THR	5.0
5	e	79	PHE	4.9
2	b	85	GLY	4.9
13	O	56	PRO	4.8
20	r	13	LEU	4.8
20	r	34	LEU	4.8
8	i	36	ASP	4.7
8	I	36	ASP	4.7
18	X	2	THR	4.7
19	Z	42	LEU	4.6
3	C	29	GLU	4.6
13	o	62	GLU	4.6
12	m	33	GLN	4.5
20	R	35	LEU	4.5
20	r	31	VAL	4.5
20	r	20	VAL	4.4
13	O	4	THR	4.4
19	Z	33	TRP	4.4
13	o	56	PRO	4.4
1	a	11	ALA	4.4
13	O	3	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
20	r	10	LEU	4.3
20	r	29	LYS	4.3
9	J	5	GLY	4.2
2	b	86	ILE	4.2
20	R	27	ALA	4.2
2	b	487	SER	4.2
20	r	18	TRP	4.1
20	R	3	TRP	4.0
20	r	14	LEU	4.0
17	Y	42	ARG	3.9
9	j	7	ARG	3.9
20	R	6	LEU	3.8
13	o	57	LYS	3.8
20	r	30	GLN	3.8
3	c	143	TYR	3.8
20	r	2	ASP	3.7
2	B	494	GLY	3.7
4	d	12	ARG	3.6
20	r	24	LEU	3.6
5	E	84	LYS	3.6
2	b	298	LEU	3.6
9	j	6	GLY	3.6
13	o	58	ASN	3.6
2	b	495	PHE	3.6
9	J	6	GLY	3.6
17	Y	41	VAL	3.6
5	e	74	GLN	3.6
20	r	32	GLN	3.5
19	Z	1	MET	3.5
2	B	295	GLY	3.4
12	M	33	GLN	3.4
3	c	24	THR	3.4
13	O	63	ALA	3.4
2	B	289	GLN	3.3
5	e	81[A]	GLU	3.3
20	r	33	LYS	3.3
20	r	21	ARG	3.3
19	z	39	LEU	3.3
6	F	12	SER	3.3
13	o	5	LEU	3.2
17	Y	21	GLN	3.2
19	Z	34	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	b	503	THR	3.2
2	B	488	PRO	3.2
20	R	21	ARG	3.2
11	l	2	GLU	3.1
20	R	18	TRP	3.1
14	T	30	THR	3.1
1	a	13	LEU	3.1
5	E	79	PHE	3.1
19	z	35	ARG	3.1
4	d	238	THR	3.0
20	R	28	VAL	3.0
16	v	12	LEU	3.0
16	v	21	LEU	3.0
2	B	489	GLU	3.0
13	O	59	LYS	3.0
2	B	293	ALA	2.9
7	h	21	VAL	2.9
1	a	15	GLU	2.9
8	I	2	GLU	2.9
9	j	5	GLY	2.9
13	O	246	ALA	2.9
2	b	289	GLN	2.9
2	B	496	TYR	2.9
19	z	10	ALA	2.8
2	B	487	SER	2.8
1	A	11	ALA	2.8
17	y	40	ALA	2.8
2	B	490	GLN	2.8
20	R	20	VAL	2.8
7	h	55	LEU	2.8
7	h	56	ASP	2.8
19	z	40	ILE	2.8
11	l	3	PRO	2.7
4	D	13	GLY	2.7
3	c	29	GLU	2.7
2	B	294	SER	2.7
19	z	42	LEU	2.7
19	z	32	ASP	2.7
19	z	60	PHE	2.7
6	f	13	TYR	2.7
19	z	41	PHE	2.7
13	o	207	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
15	u	86	GLU	2.7
19	Z	38	GLN	2.7
20	r	3	TRP	2.6
3	C	27	ASP	2.6
2	b	295	GLY	2.6
20	r	22	ASN	2.6
2	B	127	ARG	2.6
13	o	63	ALA	2.6
19	z	7	LEU	2.6
2	b	126	PRO	2.6
13	O	55	GLU	2.6
2	b	496	TYR	2.6
15	u	8	GLU	2.6
7	h	6	TRP	2.5
20	R	26	TYR	2.5
2	B	493	TRP	2.5
17	Y	37	PHE	2.5
3	C	30	SER	2.5
19	Z	4	LEU	2.5
3	C	25	ASN	2.4
19	Z	31	GLN	2.4
18	x	39	ARG	2.4
15	U	75	LEU	2.4
13	o	4	THR	2.4
20	R	2	ASP	2.4
19	z	37	LYS	2.4
13	O	207	ARG	2.4
3	C	28	GLN	2.4
2	b	293	ALA	2.4
2	b	463	PHE	2.4
17	y	45	ASN	2.4
4	d	123	ILE	2.4
20	R	25	PRO	2.4
3	c	191	PRO	2.3
19	Z	7	LEU	2.3
17	Y	43	ARG	2.3
1	A	12	ASN	2.3
2	b	243	ALA	2.3
7	H	65	LEU	2.3
17	y	42	ARG	2.3
16	v	15	GLU	2.3
19	Z	61	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
17	Y	44	GLY	2.3
4	d	150	ILE	2.3
11	l	7	ARG	2.2
18	X	3	ILE	2.2
4	d	124	GLY	2.2
2	b	252	VAL	2.2
3	c	279	LEU	2.2
2	b	247	PHE	2.2
2	b	297	THR	2.2
20	R	24	LEU	2.2
13	O	58	ASN	2.2
17	y	19	ILE	2.2
4	d	36	LEU	2.2
20	R	30	GLN	2.2
2	b	249	ALA	2.2
15	U	67	LEU	2.2
2	B	485	GLU	2.2
17	y	41	VAL	2.1
20	r	4	ARG	2.1
2	b	406	LEU	2.1
20	R	14	LEU	2.1
20	R	31	VAL	2.1
2	B	495	PHE	2.1
17	Y	25	ILE	2.1
5	e	77	GLU	2.1
2	b	246	PHE	2.1
2	b	248	ALA	2.1
19	z	6	GLN	2.1
20	R	32	GLN	2.1
5	E	82	GLN	2.1
2	b	296	ALA	2.1
9	J	7	ARG	2.1
15	U	8	GLU	2.1
5	E	17	VAL	2.1
8	I	35	LYS	2.1
5	E	83	LEU	2.1
10	K	17	ILE	2.1
19	Z	35	ARG	2.1
14	t	30	THR	2.1
16	v	110	LYS	2.1
13	O	64	GLU	2.0
19	z	2	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	2.0
6	f	14	PRO	2.0
19	z	38	GLN	2.0
2	b	347	ARG	2.0
3	C	146	PHE	2.0
13	O	57	LYS	2.0
1	a	248	ILE	2.0
20	R	34	LEU	2.0
5	e	60	GLN	2.0
5	E	21	VAL	2.0
3	C	437	PHE	2.0
3	c	262	ARG	2.0
18	x	2	THR	2.0
2	B	459	ALA	2.0
4	D	351	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
8	FME	I	1	10/11	0.96	0.17	-	45,49,54,55	0
8	FME	i	1	10/11	0.93	0.18	-	45,53,58,58	0
14	FME	T	1	10/11	0.95	0.10	-	32,40,59,74	0
12	FME	m	1	10/11	0.96	0.14	-	39,51,70,77	0
14	FME	t	1	10/11	0.96	0.10	-	31,38,58,64	0
12	FME	M	1	10/11	0.94	0.15	-	41,53,62,63	0

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
32	LMG	B	626	51/55	0.61	0.31	6.97	55,76,89,91	0
31	UNL	c	525	12/-	0.79	0.25	6.66	50,62,73,73	0
31	UNL	a	619	12/-	0.78	0.26	5.78	60,65,71,76	0
32	LMG	C	521	51/55	0.82	0.27	5.74	45,65,116,118	0
31	UNL	A	617	20/-	0.65	0.23	5.63	58,66,76,77	0
32	LMG	c	520	34/55	0.87	0.26	4.35	58,66,78,88	0
32	LMG	b	620	51/55	0.83	0.27	4.12	55,72,98,110	0
31	UNL	D	410	18/-	0.66	0.20	4.04	41,53,74,74	0
28	PL9	A	611	55/55	0.80	0.27	3.75	42,60,82,88	55
32	LMG	d	408	38/55	0.69	0.27	3.74	58,68,101,106	0
28	PL9	a	612	55/55	0.77	0.28	3.69	51,67,89,96	0
31	UNL	B	627	15/-	0.86	0.18	3.51	48,55,65,68	0
31	UNL	j	801	15/-	0.88	0.18	3.46	50,60,77,77	0
29	SQD	B	625	54/54	0.74	0.26	3.46	52,72,92,105	0
30	LHG	A	618	49/49	0.80	0.27	3.44	56,90,112,115	0
31	UNL	C	522	17/-	0.82	0.21	3.14	42,56,67,75	0
29	SQD	D	409	47/54	0.74	0.21	3.13	41,59,109,125	0
32	LMG	B	621	51/55	0.88	0.23	3.05	54,71,102,110	0
31	UNL	M	102	17/-	0.81	0.21	2.93	52,61,73,74	0
30	LHG	a	617	42/49	0.83	0.30	2.66	67,88,102,111	0
25	CLA	C	514	65/65	0.91	0.23	2.55	49,60,136,139	0
31	UNL	m	103	16/-	0.85	0.16	2.55	39,51,73,76	0
31	UNL	M	101	15/-	0.88	0.15	2.37	42,52,63,75	0
31	UNL	d	409	17/-	0.87	0.28	2.35	51,58,67,70	0
31	UNL	t	102	18/-	0.87	0.17	2.31	43,56,65,66	0
30	LHG	d	406	49/49	0.95	0.17	2.28	31,44,55,64	0
31	UNL	A	615	9/-	0.91	0.17	2.20	41,52,68,70	0
25	CLA	B	616	65/65	0.94	0.15	2.00	29,39,96,102	0
32	LMG	C	501	48/55	0.79	0.20	1.99	46,61,76,89	0
25	CLA	D	403	65/65	0.91	0.19	1.96	31,37,89,99	0
29	SQD	b	621	40/54	0.75	0.20	1.91	48,58,68,70	0
32	LMG	D	407	51/55	0.94	0.14	1.90	32,52,72,82	0
29	SQD	B	624	54/54	0.81	0.20	1.88	43,62,96,106	0
31	UNL	c	524	20/-	0.81	0.18	1.83	45,67,82,83	0
32	LMG	c	519	37/55	0.88	0.15	1.75	48,67,76,77	0
31	UNL	T	102	14/-	0.90	0.16	1.73	36,53,63,67	0
31	UNL	x	101	16/-	0.79	0.22	1.73	41,51,65,68	0
31	UNL	J	102	12/-	0.63	0.39	1.63	61,79,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	CLA	A	607	65/65	0.94	0.16	1.56	25,35,123,129	0
29	SQD	A	616	54/54	0.80	0.21	1.54	50,70,96,103	0
27	BCR	d	403	40/40	0.88	0.15	1.49	41,54,79,82	0
25	CLA	c	506	65/65	0.91	0.15	1.48	33,48,82,95	0
31	UNL	T	103	12/-	0.86	0.14	1.45	42,54,59,61	0
32	LMG	a	614	51/55	0.84	0.19	1.45	41,60,74,80	0
32	LMG	B	620	51/55	0.84	0.18	1.35	32,57,73,77	0
25	CLA	B	601	65/65	0.91	0.15	1.32	39,54,81,87	0
30	LHG	D	406	49/49	0.94	0.18	1.31	32,40,56,74	0
33	DGD	c	516	62/66	0.95	0.17	1.29	28,44,67,72	0
25	CLA	B	606	65/65	0.92	0.13	1.22	28,37,63,74	0
25	CLA	a	610	65/65	0.91	0.15	1.21	24,32,77,81	0
25	CLA	b	601	65/65	0.87	0.21	1.20	40,61,83,94	0
27	BCR	B	618	40/40	0.94	0.16	1.18	30,44,55,60	0
27	BCR	D	404	40/40	0.90	0.16	1.15	31,44,82,86	0
24	BCT	a	605	4/4	0.95	0.14	1.13	37,45,46,53	2
30	LHG	B	623	49/49	0.94	0.17	1.10	36,47,63,70	0
33	DGD	C	518	62/66	0.93	0.15	1.09	40,50,89,97	0
25	CLA	b	605	65/65	0.95	0.14	1.08	25,37,46,52	0
27	BCR	B	617	40/40	0.94	0.13	1.08	29,45,53,57	0
31	UNL	b	623	11/-	0.84	0.18	1.08	59,66,68,71	0
27	BCR	T	101	40/40	0.91	0.17	1.06	35,46,57,68	0
30	LHG	L	102	49/49	0.95	0.15	0.99	35,42,50,58	0
31	UNL	H	103	7/-	0.89	0.15	0.97	48,53,60,61	0
25	CLA	B	613	65/65	0.95	0.20	0.97	26,33,63,76	0
33	DGD	c	517	62/66	0.93	0.13	0.96	39,52,81,86	0
29	SQD	D	408	43/54	0.91	0.22	0.96	54,76,105,108	0
25	CLA	b	606[B]	65/65	0.93	0.15	0.91	37,43,52,58	64
25	CLA	b	606[A]	65/65	0.93	0.15	0.90	37,43,52,55	64
25	CLA	C	510	65/65	0.94	0.17	0.88	32,42,66,70	0
25	CLA	C	508	65/65	0.89	0.18	0.88	30,42,59,78	0
25	CLA	B	607	65/65	0.94	0.16	0.87	27,36,63,71	0
33	DGD	h	102	62/66	0.88	0.21	0.87	38,51,60,64	0
31	UNL	a	618	17/-	0.80	0.16	0.86	46,57,71,72	0
32	LMG	d	407	51/55	0.94	0.15	0.86	38,58,88,93	0
25	CLA	B	603	65/65	0.96	0.15	0.85	25,36,56,63	0
25	CLA	d	402	65/65	0.89	0.17	0.84	36,43,83,90	0
25	CLA	C	502	65/65	0.94	0.17	0.84	31,37,50,59	0
28	PL9	d	404	55/55	0.94	0.14	0.82	27,39,50,54	0
25	CLA	B	605	65/65	0.96	0.14	0.80	26,33,48,53	0
27	BCR	C	516	40/40	0.93	0.14	0.80	34,44,55,57	0
33	DGD	C	517	62/66	0.95	0.16	0.80	29,42,72,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	PHO	D	401	64/64	0.96	0.14	0.77	23,33,38,44	0
25	CLA	C	505	65/65	0.95	0.17	0.76	34,42,80,85	0
32	LMG	m	102	51/55	0.89	0.16	0.75	43,56,69,77	0
25	CLA	B	614	65/65	0.94	0.13	0.73	25,37,75,81	0
27	BCR	t	101	40/40	0.94	0.15	0.73	33,43,53,62	0
25	CLA	C	504	65/65	0.91	0.17	0.73	36,44,50,59	0
27	BCR	b	618	40/40	0.91	0.17	0.71	33,44,56,59	0
25	CLA	C	503	65/65	0.93	0.18	0.71	28,39,53,65	0
27	BCR	b	617	40/40	0.91	0.14	0.67	33,44,52,52	0
29	SQD	L	101	49/54	0.84	0.18	0.61	41,66,96,109	0
30	LHG	A	614	47/49	0.95	0.13	0.61	33,44,73,76	0
26	PHO	a	608	64/64	0.94	0.14	0.61	28,34,42,49	0
25	CLA	B	612	65/65	0.95	0.15	0.59	25,33,42,45	0
25	CLA	b	602	65/65	0.92	0.17	0.59	33,41,59,66	0
25	CLA	b	610	65/65	0.94	0.15	0.58	31,40,51,66	0
25	CLA	C	513	65/65	0.89	0.17	0.56	41,54,81,86	0
25	CLA	c	502	65/65	0.93	0.18	0.55	31,41,55,63	0
25	CLA	c	501	65/65	0.94	0.15	0.54	29,38,53,56	0
27	BCR	c	515	40/40	0.94	0.13	0.54	30,46,51,63	0
28	PL9	D	405	55/55	0.95	0.14	0.54	25,35,47,49	0
25	CLA	c	509	65/65	0.93	0.15	0.52	37,45,61,64	0
25	CLA	a	615	65/65	0.95	0.13	0.51	24,34,52,62	0
30	LHG	d	405	49/49	0.93	0.15	0.50	43,53,68,72	0
25	CLA	b	608	65/65	0.95	0.22	0.50	32,41,56,60	0
33	DGD	H	102	62/66	0.91	0.17	0.50	39,47,63,65	0
25	CLA	B	611	65/65	0.94	0.15	0.49	25,34,48,52	0
25	CLA	b	609	65/65	0.91	0.14	0.49	35,46,60,66	0
30	LHG	l	101	49/49	0.94	0.12	0.48	37,49,62,76	0
33	DGD	C	519	62/66	0.94	0.12	0.48	33,50,79,84	0
25	CLA	c	512	65/65	0.89	0.15	0.47	45,57,89,94	0
29	SQD	A	612	52/54	0.92	0.16	0.46	48,63,85,91	0
25	CLA	A	609	54/65	0.96	0.12	0.44	25,32,72,78	0
30	LHG	a	616	39/49	0.94	0.13	0.42	39,48,66,71	0
29	SQD	a	613	54/54	0.89	0.14	0.40	40,62,72,76	0
25	CLA	b	603	65/65	0.96	0.16	0.38	29,38,57,62	0
25	CLA	b	613	65/65	0.95	0.18	0.38	29,38,74,89	0
25	CLA	B	610	65/65	0.95	0.13	0.37	26,37,47,55	0
26	PHO	a	609	64/64	0.94	0.17	0.34	34,40,49,52	0
25	CLA	c	513	65/65	0.90	0.18	0.33	48,63,86,90	0
25	CLA	C	511	65/65	0.95	0.18	0.32	30,43,58,70	0
25	CLA	B	608	65/65	0.95	0.18	0.32	30,38,57,60	0
25	CLA	a	607	65/65	0.95	0.13	0.31	28,43,84,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	CLA	A	606	65/65	0.93	0.12	0.27	23,32,50,59	0
25	CLA	b	612	65/65	0.95	0.14	0.26	26,38,49,56	0
25	CLA	B	609	65/65	0.91	0.12	0.26	28,39,58,69	0
27	BCR	h	101	40/40	0.83	0.17	0.26	40,48,64,68	0
27	BCR	K	101	40/40	0.93	0.14	0.24	37,52,63,66	0
25	CLA	b	607	65/65	0.95	0.12	0.24	29,37,62,68	0
27	BCR	c	522	40/40	0.91	0.14	0.24	42,54,63,69	0
33	DGD	c	518	62/66	0.94	0.12	0.23	34,48,73,77	0
26	PHO	A	608	64/64	0.95	0.15	0.22	29,37,43,46	0
34	HEM	v	201	43/43	0.97	0.11	0.22	31,40,47,54	0
25	CLA	B	615	65/65	0.95	0.11	0.14	28,40,58,66	0
25	CLA	C	506	65/65	0.94	0.12	0.14	27,40,65,70	0
25	CLA	A	613	65/65	0.95	0.13	0.13	25,33,44,53	0
25	CLA	B	604	65/65	0.93	0.16	0.12	27,33,72,81	0
25	CLA	c	503	65/65	0.93	0.15	0.12	36,45,50,57	0
25	CLA	b	604	65/65	0.94	0.18	0.11	25,35,69,82	0
25	CLA	b	614	65/65	0.94	0.13	0.11	31,39,75,79	0
27	BCR	C	515	40/40	0.92	0.13	0.10	44,53,65,67	0
25	CLA	B	602	65/65	0.95	0.12	0.10	26,36,57,66	0
25	CLA	c	507	65/65	0.92	0.14	0.09	36,46,62,72	0
25	CLA	a	606	65/65	0.94	0.12	0.09	26,33,42,58	0
27	BCR	H	101	40/40	0.87	0.15	0.07	36,50,64,65	0
27	BCR	c	521	40/40	0.91	0.12	0.07	49,59,72,73	0
29	SQD	f	101	41/54	0.89	0.20	0.06	59,84,105,109	0
27	BCR	Y	101	40/40	0.91	0.12	0.05	43,51,62,68	0
27	BCR	a	611	40/40	0.94	0.11	0.04	26,37,49,54	0
32	LMG	C	520	48/55	0.82	0.19	0.00	47,69,88,95	0
25	CLA	c	505	65/65	0.95	0.12	-0.08	32,41,69,76	0
27	BCR	B	619	40/40	0.92	0.10	-0.08	34,45,56,58	0
25	CLA	C	509	65/65	0.94	0.12	-0.10	31,41,86,89	0
25	CLA	c	510	65/65	0.92	0.16	-0.11	36,46,61,72	0
25	CLA	d	401	65/65	0.95	0.12	-0.15	25,34,55,69	0
21	OEX	A	601	10/10	0.99	0.11	-0.20	32,34,40,41	1
25	CLA	C	507	65/65	0.93	0.12	-0.22	34,46,77,89	0
25	CLA	C	512	65/65	0.93	0.13	-0.27	39,52,67,71	0
34	HEM	e	101	43/43	0.95	0.13	-0.30	47,58,73,80	0
34	HEM	V	201	43/43	0.97	0.09	-0.31	29,36,44,46	0
25	CLA	D	402	65/65	0.95	0.12	-0.32	21,31,54,78	0
25	CLA	c	508	64/65	0.95	0.11	-0.32	36,45,82,87	0
27	BCR	c	514	40/40	0.92	0.13	-0.40	49,58,62,64	0
25	CLA	b	615	65/65	0.93	0.11	-0.41	33,44,62,69	0
25	CLA	b	611	65/65	0.94	0.12	-0.42	29,36,55,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CL	A	604	1/1	0.99	0.13	-0.52	33,33,33,33	0
34	HEM	E	101	43/43	0.96	0.11	-0.56	43,49,57,65	0
25	CLA	c	504	60/65	0.95	0.12	-0.59	34,47,69,77	0
25	CLA	c	511	65/65	0.94	0.12	-0.60	40,54,66,73	0
24	BCT	A	605	4/4	0.98	0.07	-0.66	42,43,44,53	0
27	BCR	A	610	40/40	0.95	0.09	-0.69	31,37,41,41	0
27	BCR	b	619	40/40	0.93	0.10	-0.70	32,48,60,61	0
25	CLA	b	616	47/65	0.94	0.09	-0.70	31,42,53,57	0
21	OEX	a	601	10/10	0.99	0.10	-1.56	28,32,35,42	0
23	CL	a	603	1/1	0.98	0.07	-2.21	33,33,33,33	0
22	FE2	A	602	1/1	0.99	0.04	-2.55	36,36,36,36	0
23	CL	A	603	1/1	0.99	0.06	-3.19	32,32,32,32	0
22	FE2	a	602	1/1	0.99	0.05	-3.22	43,43,43,43	0
23	CL	a	604	1/1	0.99	0.08	-5.01	35,35,35,35	0
31	UNL	B	622	11/-	0.89	0.14	-	41,47,60,61	0
31	UNL	C	523	16/-	0.68	0.22	-	55,71,94,101	0
31	UNL	c	523	8/-	0.81	0.15	-	49,59,77,84	0
31	UNL	I	101	7/-	0.80	0.19	-	53,57,64,65	0
31	UNL	b	622	17/-	0.81	0.19	-	47,53,63,65	0
31	UNL	J	101	11/-	0.78	0.23	-	48,61,68,68	0
31	UNL	i	101	20/-	0.87	0.23	-	51,59,77,79	0
31	UNL	E	102	12/-	0.51	0.25	-	63,85,93,95	0
31	UNL	I	102	20/-	0.74	0.21	-	46,64,81,84	0
31	UNL	j	802	12/-	0.66	0.21	-	62,72,86,89	0
31	UNL	m	101	9/-	0.85	0.18	-	51,53,61,62	0
31	UNL	D	411	10/-	0.86	0.20	-	49,55,72,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.