



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:42 am GMT

PDB ID : 4PJ0  
Title : Structure of T.elongatus Photosystem II, rows of dimers crystal packing  
Authors : Hellmich, J.; Bommer, M.; Burkhardt, A.; Ibrahim, M.; Kern, J.; Meents, A.; Mueh, F.; Dobbek, H.; Zouni, A.  
Deposited on : 2014-05-10  
Resolution : 2.44 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

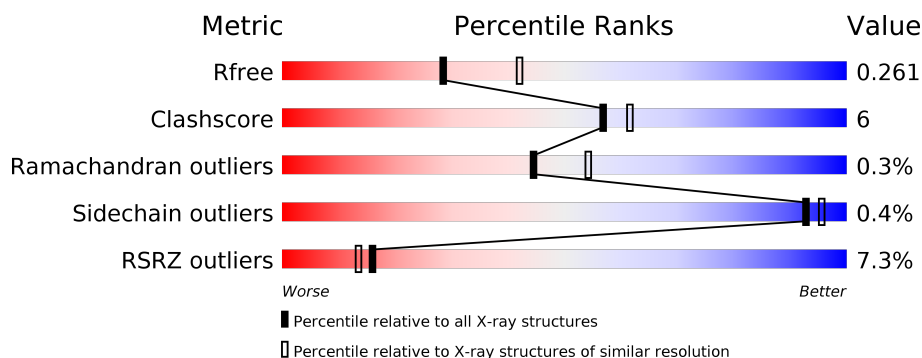
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1152 (2.46-2.42)
Clashscore	112137	1224 (2.46-2.42)
Ramachandran outliers	110173	1217 (2.46-2.42)
Sidechain outliers	110143	1217 (2.46-2.42)
RSRZ outliers	101464	1158 (2.46-2.42)

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  $\geq 3$ , 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>3%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div></div> </div> <div></div> </div>
1	a	344	<div> <div>%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div></div> </div>
2	B	510	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div></div> </div> <div></div> </div>
2	b	510	<div> <div>6%</div> <div> <div></div> <div>98%</div> <div></div> </div> <div></div> </div>
3	C	461	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div></div> </div> <div></div> </div>
3	c	461	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div></div> </div>

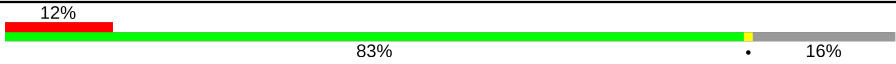
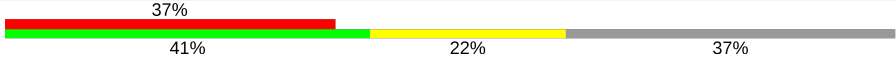


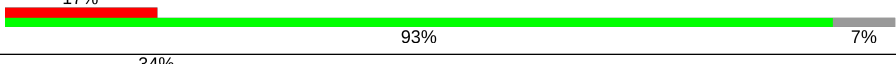

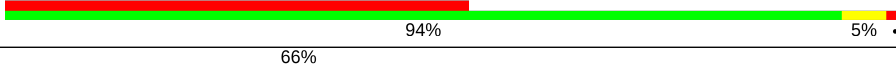

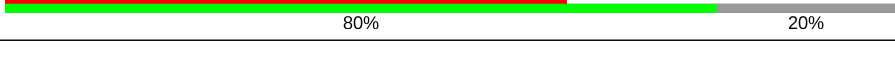
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Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	

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Mol	Chain	Length	Quality of chain
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
23	LMG	A	603	-	-	-	X
23	LMG	A	612	-	-	-	X
23	LMG	B	620	-	-	-	X
23	LMG	B	624	-	-	-	X
23	LMG	C	521	-	-	-	X
23	LMG	a	603	-	-	-	X
23	LMG	a	614	-	-	-	X
23	LMG	b	624	-	-	-	X
23	LMG	c	520	-	-	-	X
24	CL	a	604	-	-	-	X
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	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	-	-	-
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	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	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	-	-	-
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	403	X	-	-	-
26	BCR	D	406	-	-	-	X
26	BCR	b	617	-	-	-	X
26	BCR	d	404	-	-	-	X
26	BCR	t	102	-	-	-	X
27	PL9	A	610	-	-	-	X
27	PL9	D	407	-	-	-	X
27	PL9	a	612	-	-	-	X
27	PL9	d	405	-	-	-	X
28	SQD	L	101	-	-	-	X
28	SQD	L	103	-	-	-	X
29	LHG	a	616	-	-	-	X
29	LHG	d	407	-	-	-	X
30	SO4	V	202	-	-	-	X
32	UNL	B	621	-	-	-	X
32	UNL	B	622	-	-	-	X
32	UNL	B	623	-	-	-	X
32	UNL	D	410	-	-	-	X
32	UNL	J	101	-	-	-	X
32	UNL	T	102	-	-	-	X
32	UNL	T	103	-	-	-	X
32	UNL	X	101	-	-	-	X
32	UNL	b	621	-	-	-	X
32	UNL	b	622	-	-	-	X
32	UNL	d	409	-	-	-	X

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 50236 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	0	0
			3980	2611	665	691	13			
2	b	503	Total	C	N	O	S	0	0	0
			3958	2599	657	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			
3	c	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			661	431	107	123			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	0	0
			498	333	80	83	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	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	36	Total	C	N	O	0	0	0
			284	198	41	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			284	198	41	45			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			
12	m	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1859	1162	314	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			
14	t	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	96	Total	C	N	O	0	0	0
			765	486	128	151			

- 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	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

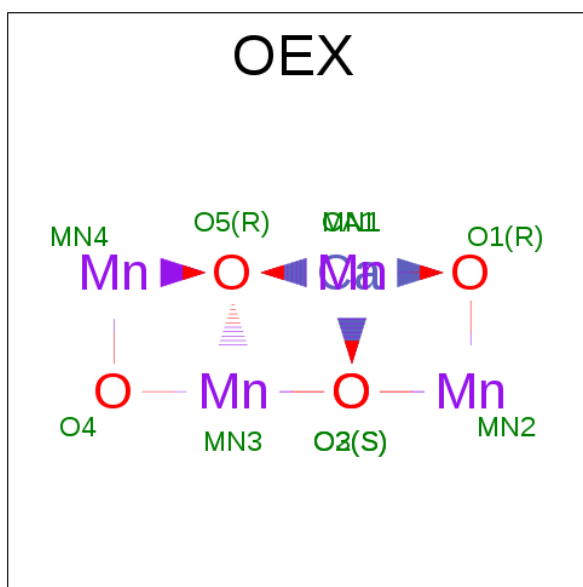
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			273	186	47	40				
20	r	33	Total	C	N	O		0	0	0
			265	182	46	37				

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).

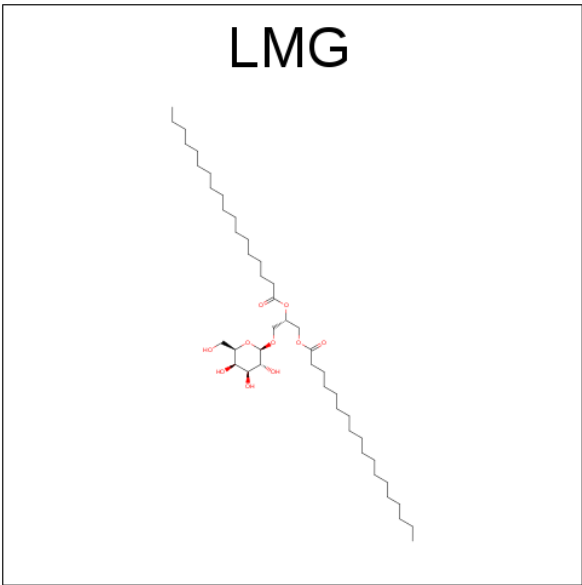


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 22 is FE (III) ION (three-letter code: FE) (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 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).

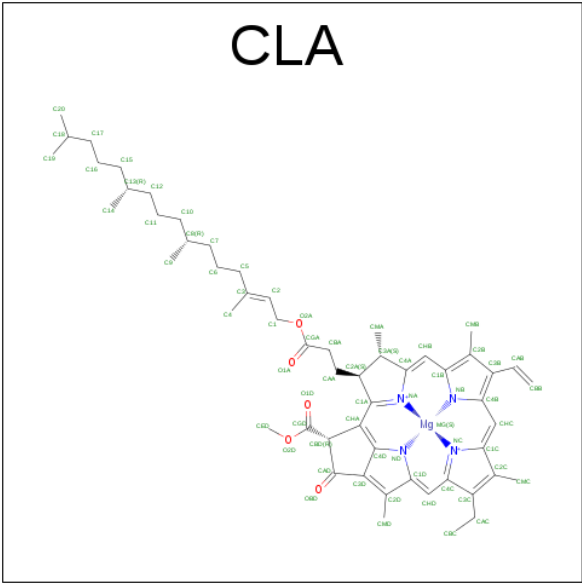


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			51	41	10		
23	A	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	B	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	C	1	Total	C	O	0	0
			51	41	10		
23	D	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	a	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		
23	b	1	Total	C	O	0	0
			51	41	10		
23	c	1	Total	C	O	0	0
			51	41	10		
23	c	1	Total	C	O	0	0
			51	41	10		
23	d	1	Total	C	O	0	0
			51	41	10		

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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
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 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 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	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 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	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
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

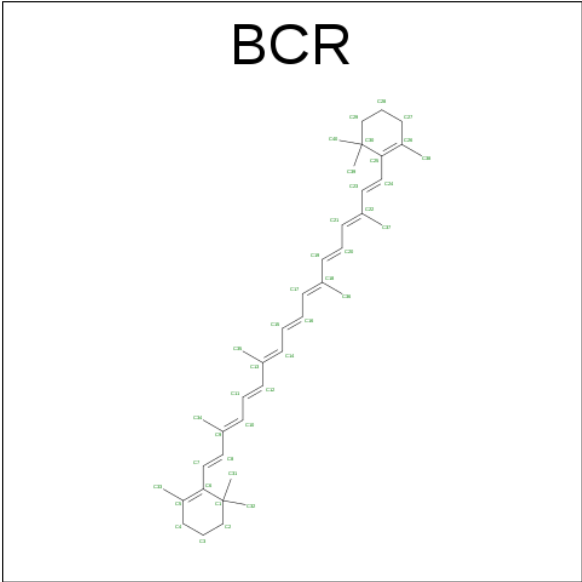
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	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		
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	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	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 BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).





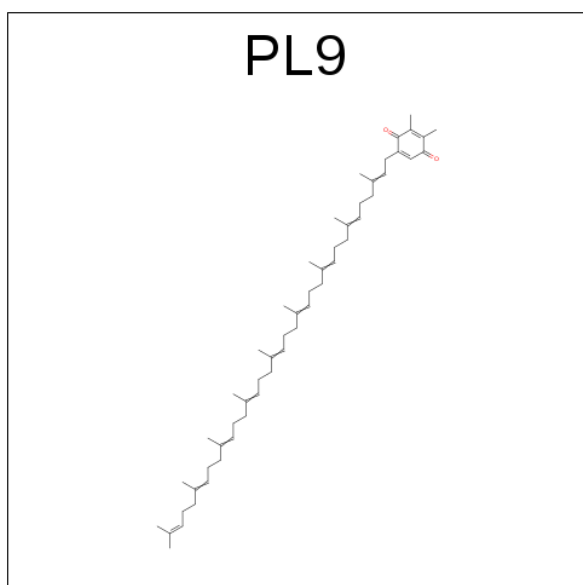
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

- Molecule 27 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:  $C_{53}H_{80}O_2$ ).



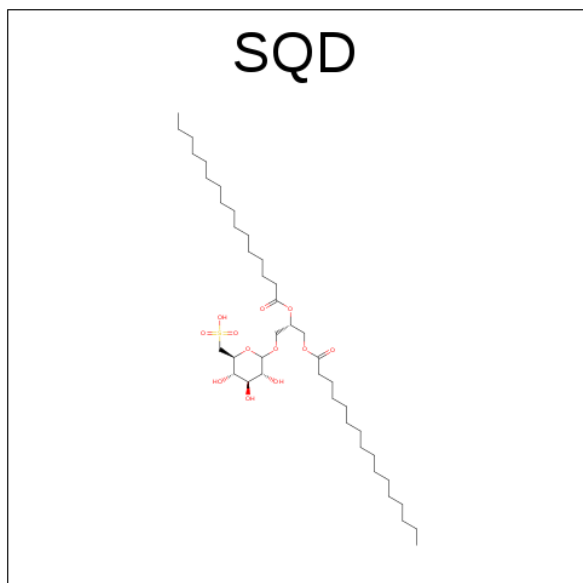
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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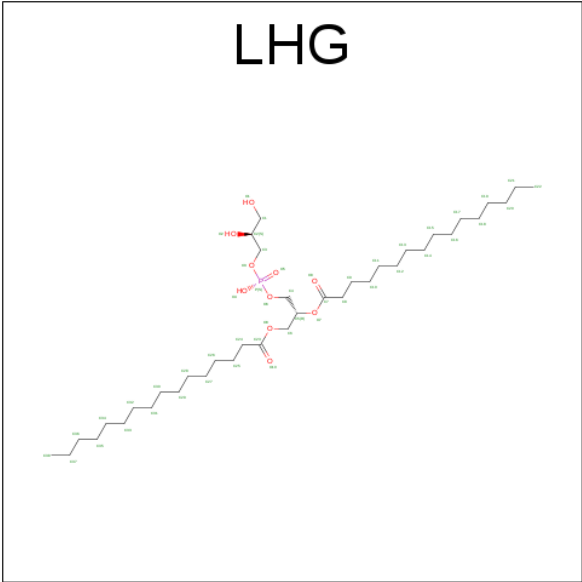
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			43	30	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	f	1	Total	C	O	S	0	0
			43	30	12	1		

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



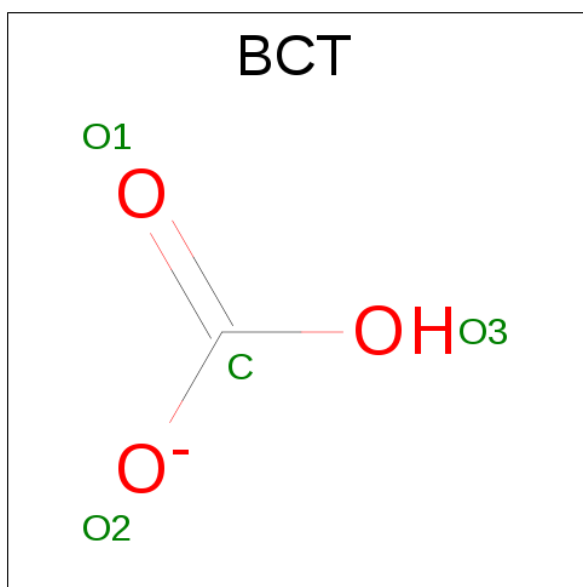
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			42	31	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 30 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	O	S	0	0
			5	4	1		
30	O	1	Total	O	S	0	0
			5	4	1		
30	O	1	Total	O	S	0	0
			5	4	1		
30	U	1	Total	O	S	0	0
			5	4	1		
30	V	1	Total	O	S	0	0
			5	4	1		
30	a	1	Total	O	S	0	0
			5	4	1		
30	d	1	Total	O	S	0	0
			5	4	1		
30	o	1	Total	O	S	0	0
			5	4	1		
30	u	1	Total	O	S	0	0
			5	4	1		
30	u	1	Total	O	S	0	0
			5	4	1		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

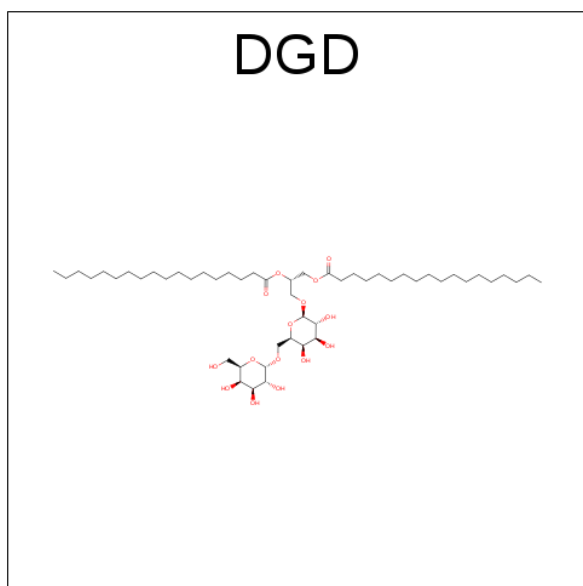
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	J	1	Total	C	0	0
			11	11		
32	i	1	Total	C	0	0
			16	16		
32	D	1	Total	C	0	0
			15	15		
32	k	1	Total	C	0	0
			9	9		
32	B	6	Total	C	0	0
			68	68		
32	I	1	Total	C	0	0
			14	14		
32	C	1	Total	C	0	0
			15	15		
32	j	1	Total	C	0	0
			15	15		
32	c	1	Total	C	0	0
			15	15		
32	x	1	Total	C	0	0
			16	16		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	T	2	Total C 27 27	0	0
32	X	1	Total C 10 10	0	0
32	d	1	Total C 15 15	0	0
32	t	1	Total C 15 15	0	0
32	m	2	Total C 25 25	0	0
32	b	5	Total C 60 60	0	0
32	M	2	Total C 26 26	0	0

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



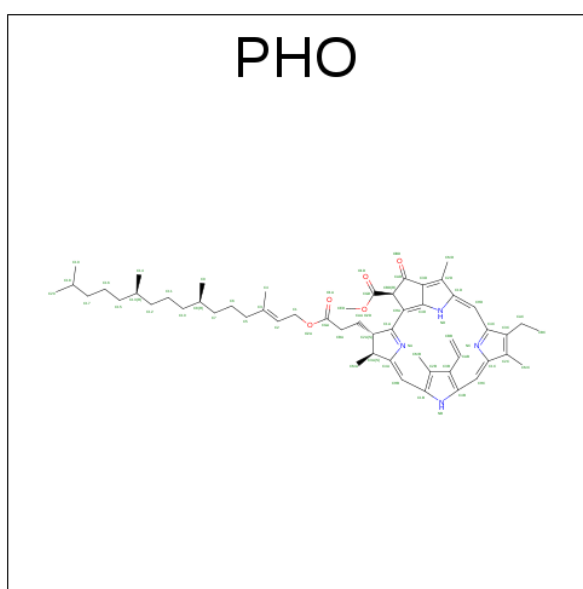
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	H	1	Total C O 62 47 15	0	0

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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		

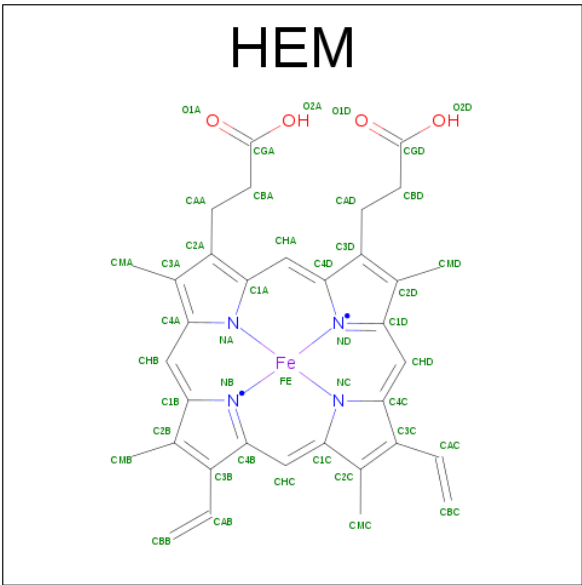
- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	33	Total	O	0	0
			33	33		
36	B	42	Total	O	0	0
			42	42		
36	C	24	Total	O	0	0
			24	24		
36	D	27	Total	O	0	0
			27	27		
36	E	2	Total	O	0	0
			2	2		
36	H	8	Total	O	0	0
			8	8		
36	L	1	Total	O	0	0
			1	1		
36	O	15	Total	O	0	0
			15	15		

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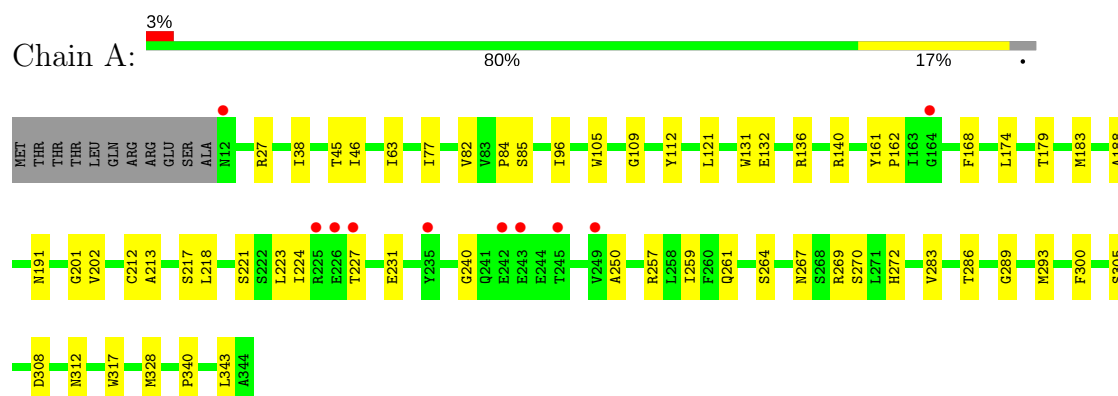
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	T	3	Total O 3 3	0	0
36	U	6	Total O 6 6	0	0
36	V	9	Total O 9 9	0	0
36	X	1	Total O 1 1	0	0
36	a	24	Total O 24 24	0	0
36	b	37	Total O 37 37	0	0
36	c	26	Total O 26 26	0	0
36	d	17	Total O 17 17	0	0
36	h	1	Total O 1 1	0	0
36	i	1	Total O 1 1	0	0
36	j	1	Total O 1 1	0	0
36	l	3	Total O 3 3	0	0
36	m	1	Total O 1 1	0	0
36	o	11	Total O 11 11	0	0
36	t	1	Total O 1 1	0	0
36	u	7	Total O 7 7	0	0
36	v	3	Total O 3 3	0	0

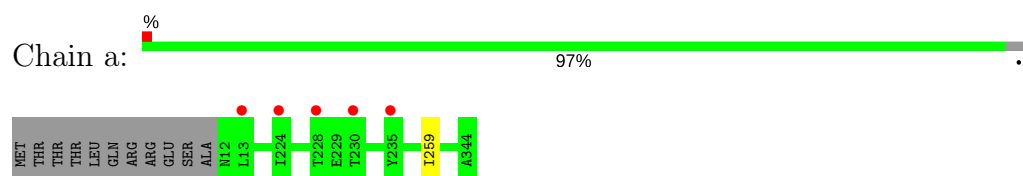
### 3 Residue-property plots [i](#)

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

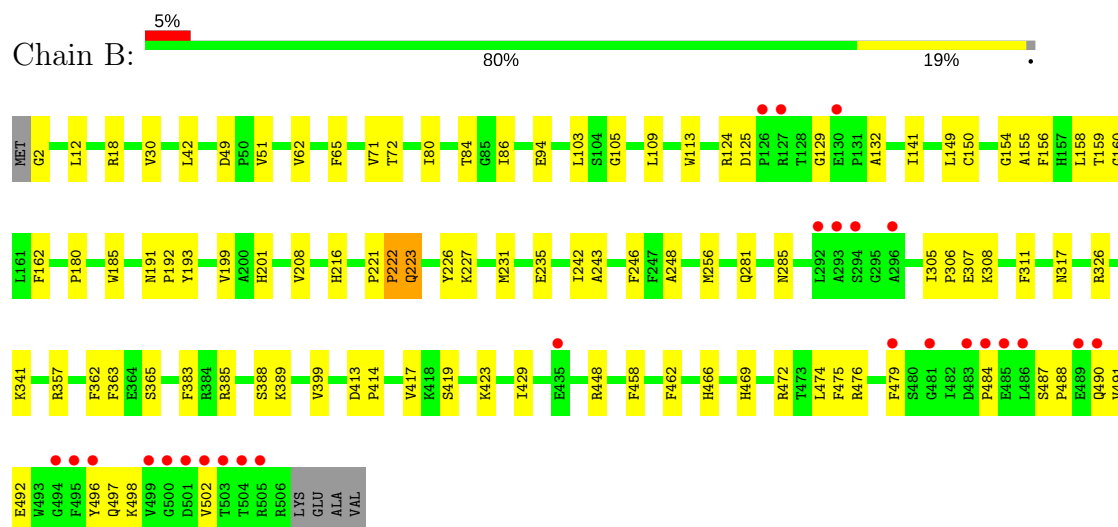
#### • Molecule 1: Photosystem Q(B) protein 1



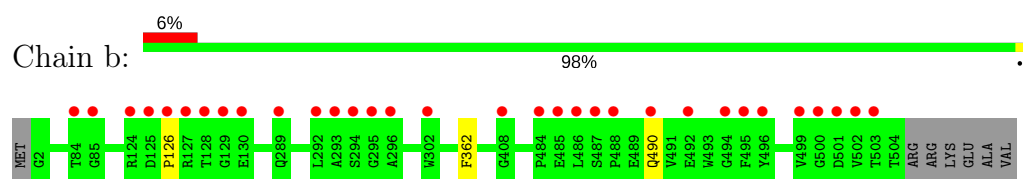
#### • Molecule 1: Photosystem Q(B) protein 1



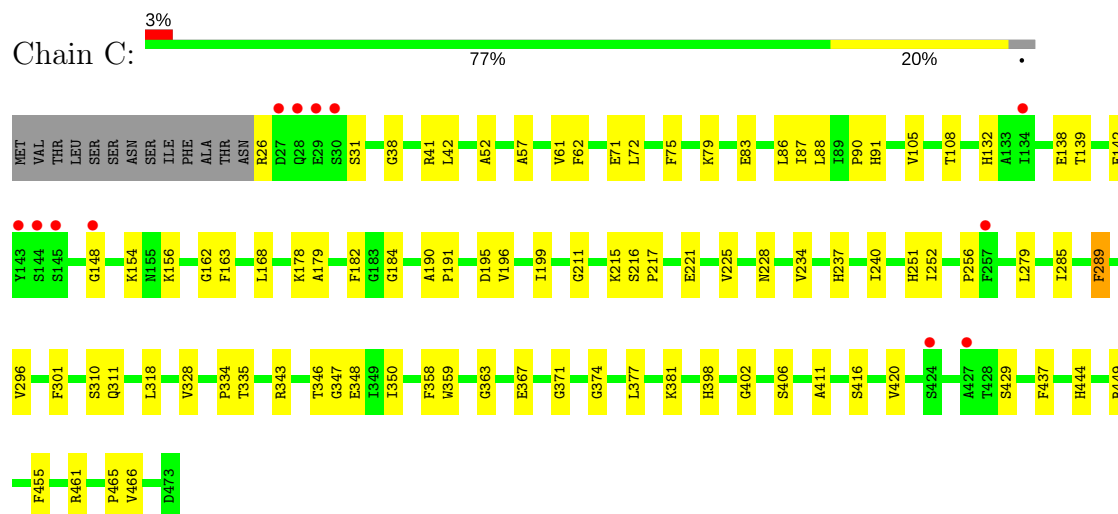
#### • Molecule 2: CP47 protein



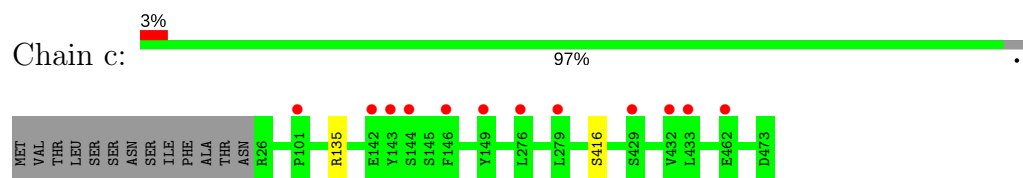
#### • Molecule 2: CP47 protein



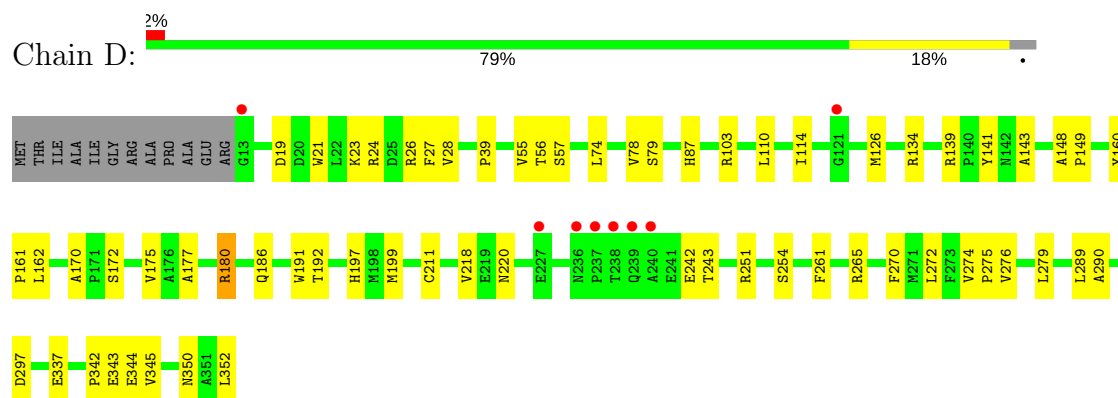
• Molecule 3: Photosystem II CP43 protein



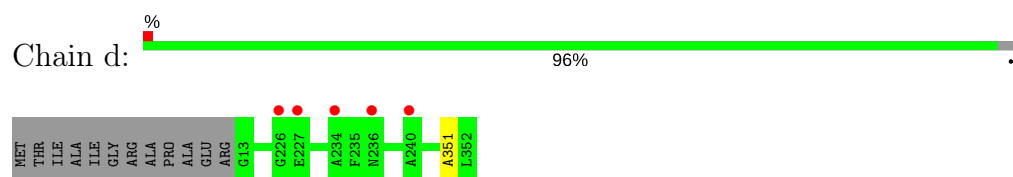
• Molecule 3: Photosystem II CP43 protein



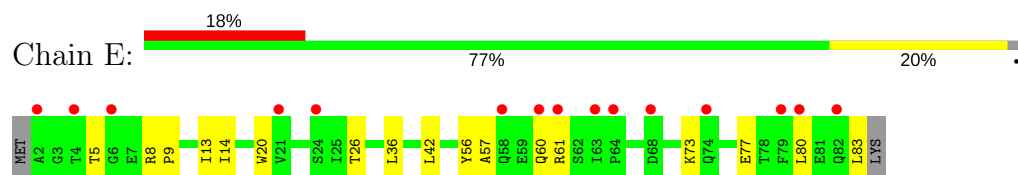
• Molecule 4: Photosystem II D2 protein



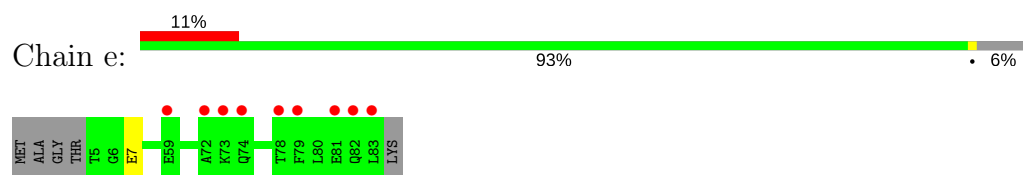
• Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



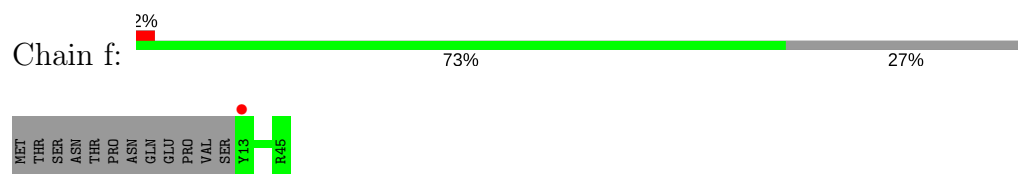
- Molecule 5: Cytochrome b559 subunit alpha



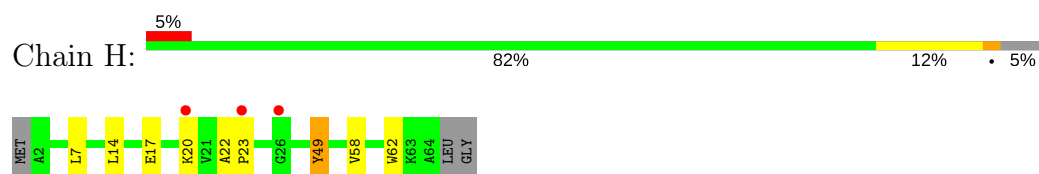
- Molecule 6: Cytochrome b559 subunit beta



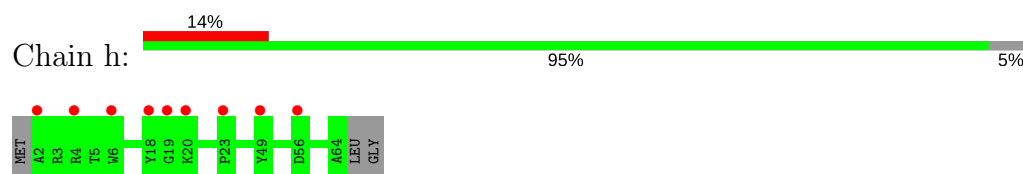
- Molecule 6: Cytochrome b559 subunit beta



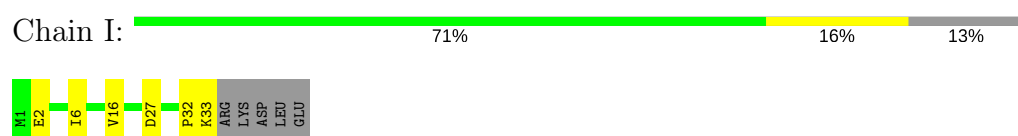
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

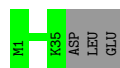


- Molecule 8: Photosystem II reaction center protein I




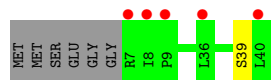
- Molecule 8: Photosystem II reaction center protein I

Chain i:  92% 8%




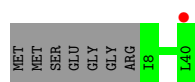
- Molecule 9: Photosystem II reaction center protein J

Chain J:  13% 83% 15%



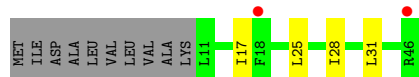
- Molecule 9: Photosystem II reaction center protein J

Chain j:  3% 83% 18%




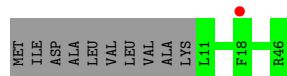
- Molecule 10: Photosystem II reaction center protein K

Chain K:  4% 70% 9% 22%




- Molecule 10: Photosystem II reaction center protein K

Chain k:  2% 78% 22%



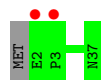
- Molecule 11: Photosystem II reaction center protein L

Chain L:  84% 14%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  5% 97%




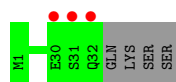
- Molecule 12: Photosystem II reaction center protein M

Chain M:  72% 17% 11%



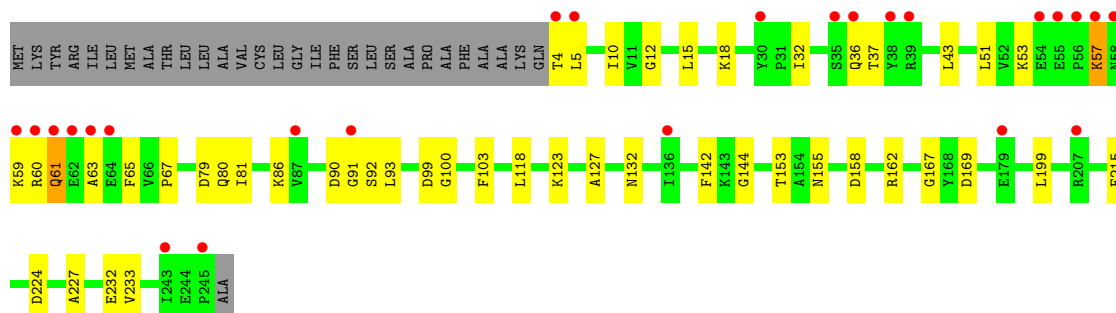
- Molecule 12: Photosystem II reaction center protein M

Chain m:  8% 89% 11%




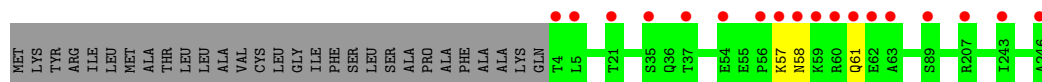
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  9% 71% 17% 11%



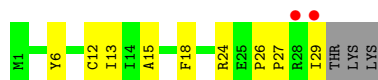
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  7% 88% 11%



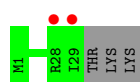
- Molecule 14: Photosystem II reaction center protein T

Chain T:  6% 63% 28% 9%



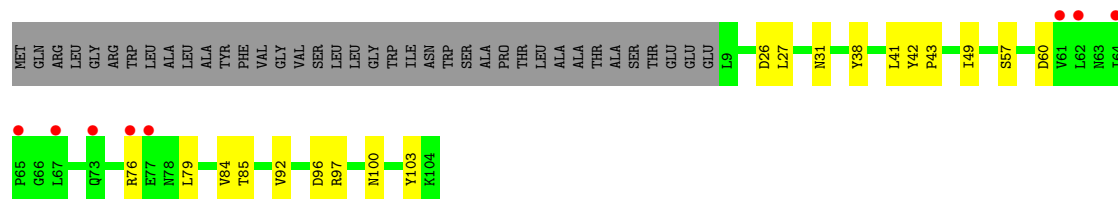
- Molecule 14: Photosystem II reaction center protein T

Chain t:  6% 91% 9%



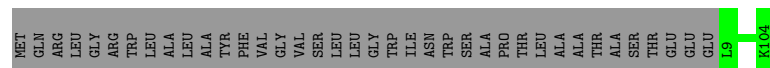
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  6% 57% 14% 28%



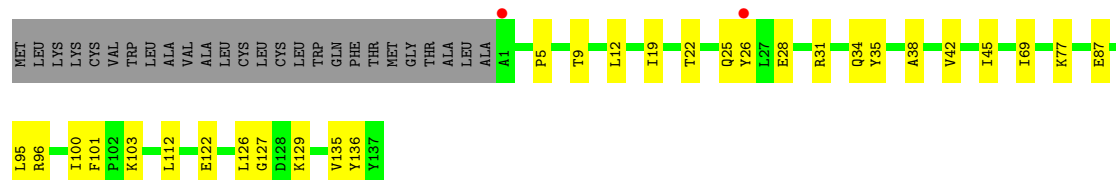
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 72% 28%



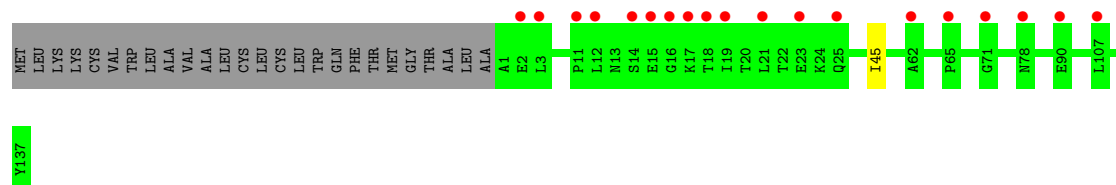
- Molecule 16: Cytochrome c-550

Chain V: 66% 18% 16%



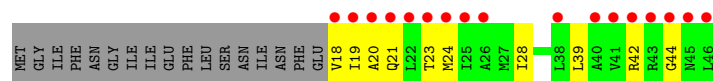
- Molecule 16: Cytochrome c-550

Chain v: 12% 83% 16%



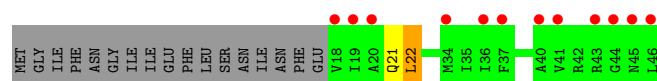
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 37% 41% 22% 37%



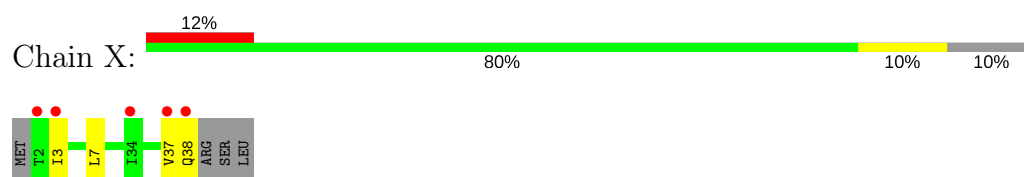
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 26% 59% 37%

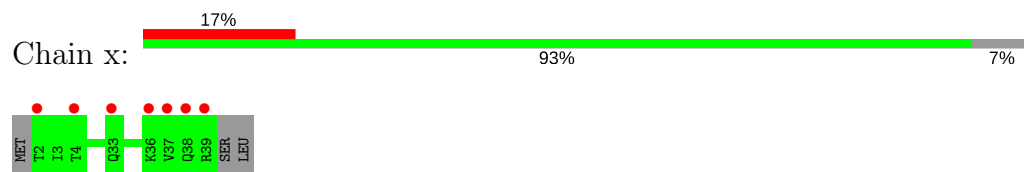


- Molecule 18: Photosystem II reaction center X protein

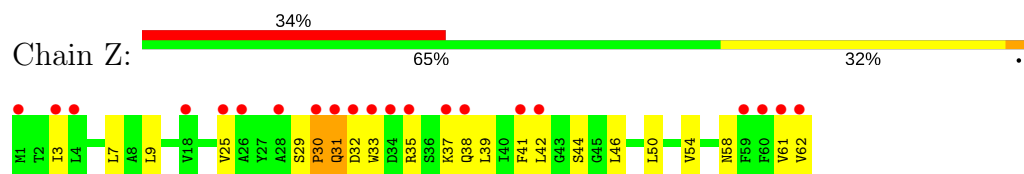




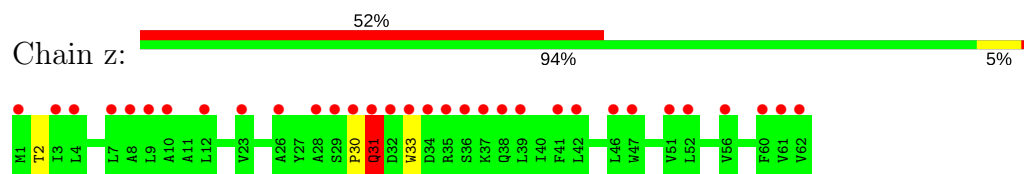
- Molecule 18: Photosystem II reaction center X protein



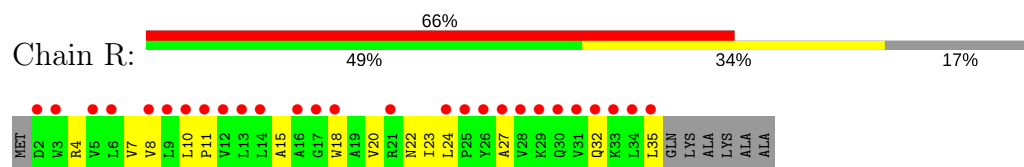
- Molecule 19: Photosystem II reaction center protein Z



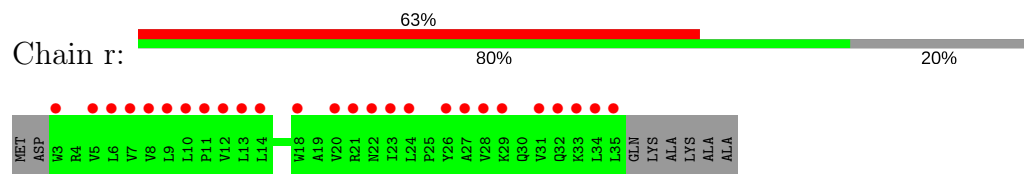
- Molecule 19: Photosystem II reaction center protein Z



- 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, $\alpha$ , $\beta$ , $\gamma$	116.45Å 218.89Å 302.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.44 49.12 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.12-2.44) 98.4 (49.12-2.44)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, $R_{free}$	0.216 , 0.256 0.223 , 0.261	Depositor DCC
$R_{free}$ test set	14111 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	50236	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, PHO, DGD, CL, SO4, CLA, PL9, FE, BCT, HEM, LMG, UNL, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.22	0/2702	0.39	0/3685
1	a	0.22	0/2702	0.37	0/3685
2	B	0.23	0/4120	0.38	1/5614 (0.0%)
2	b	0.22	0/4098	0.38	0/5586
3	C	0.21	0/3579	0.35	0/4872
3	c	0.21	0/3579	0.38	0/4872
4	D	0.22	0/2801	0.37	0/3818
4	d	0.22	0/2801	0.37	0/3818
5	E	0.21	0/680	0.39	0/929
5	e	0.21	0/664	0.38	0/907
6	F	0.22	0/278	0.38	0/379
6	f	0.22	0/278	0.39	0/379
7	H	0.22	0/511	0.37	0/697
7	h	0.22	0/511	0.38	0/697
8	I	0.23	0/273	0.37	0/370
8	i	0.23	0/293	0.39	0/395
9	J	0.20	0/255	0.33	0/346
9	j	0.21	0/244	0.36	0/332
10	K	0.30	0/294	0.55	0/405
10	k	0.23	0/294	0.40	0/405
11	L	0.22	0/303	0.34	0/412
11	l	0.22	0/303	0.35	0/412
12	M	0.22	0/252	0.40	0/344
12	m	0.22	0/252	0.39	0/344
13	O	0.21	0/1890	0.39	0/2564
13	o	0.22	0/1896	0.43	0/2571
14	T	0.24	0/258	0.37	0/349
14	t	0.24	0/258	0.37	0/349
15	U	0.20	0/776	0.36	0/1052
15	u	0.21	0/776	0.36	0/1052
16	V	0.20	0/1085	0.38	0/1473
16	v	0.20	0/1085	0.38	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Y	0.20	0/216	0.39	0/289
17	y	0.21	0/216	0.63	1/289 (0.3%)
18	X	0.21	0/273	0.34	0/370
18	x	0.21	0/284	0.35	0/384
19	Z	0.22	0/490	0.40	0/669
19	z	0.43	0/490	0.62	0/669
20	R	0.20	0/279	0.37	0/383
20	r	0.21	0/271	0.46	0/372
All	All	0.22	0/42610	0.39	2/58011 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
19	z	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	y	22	LEU	CA-CB-CG	5.69	128.38	115.30
2	B	223	GLN	N-CA-C	-5.33	96.61	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	PRO	Peptide
19	z	31	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2514	52	0
1	a	2617	0	2514	0	0
2	B	3980	0	3841	92	0
2	b	3958	0	3815	0	0
3	C	3466	0	3389	67	0
3	c	3466	0	3389	0	0
4	D	2706	0	2608	56	0
4	d	2706	0	2608	0	0
5	E	661	0	643	17	0
5	e	645	0	628	0	0
6	F	269	0	277	5	0
6	f	269	0	277	0	0
7	H	498	0	518	11	0
7	h	498	0	518	0	0
8	I	266	0	282	5	0
8	i	286	0	308	0	0
9	J	249	0	262	1	0
9	j	238	0	249	0	0
10	K	284	0	292	4	0
10	k	284	0	292	0	0
11	L	296	0	304	7	0
11	l	296	0	304	0	0
12	M	249	0	268	6	0
12	m	249	0	268	0	0
13	O	1859	0	1833	32	0
13	o	1865	0	1838	0	0
14	T	249	0	255	9	0
14	t	249	0	255	0	0
15	U	765	0	767	11	0
15	u	765	0	767	0	0
16	V	1064	0	1073	22	0
16	v	1064	0	1073	0	0
17	Y	215	0	246	9	0
17	y	215	0	246	0	0
18	X	270	0	299	4	0
18	x	281	0	312	0	0
19	Z	479	0	516	24	0
19	z	479	0	516	0	0
20	R	273	0	305	9	0
20	r	265	0	301	0	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	1	0	0	0	0
23	A	102	0	144	2	0
23	B	102	0	144	4	0
23	C	102	0	144	4	0
23	D	51	0	72	0	0
23	a	102	0	144	0	0
23	b	102	0	144	0	0
23	c	102	0	144	0	0
23	d	51	0	72	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	195	0	216	9	0
25	B	1040	0	1152	55	0
25	C	845	0	936	55	0
25	D	195	0	216	11	0
25	a	260	0	288	0	0
25	b	1040	0	1152	0	0
25	c	845	0	936	0	0
25	d	130	0	144	0	0
26	A	40	0	56	3	0
26	B	120	0	168	15	0
26	C	120	0	168	11	0
26	D	40	0	56	2	0
26	H	40	0	56	5	0
26	K	40	0	56	4	0
26	T	40	0	56	6	0
26	a	40	0	56	0	0
26	b	120	0	168	0	0
26	c	80	0	112	0	0
26	d	40	0	56	0	0
26	h	40	0	56	0	0
26	k	40	0	56	0	0
26	t	40	0	56	0	0
26	z	40	0	56	0	0
27	A	55	0	80	6	0
27	D	55	0	80	3	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	54	0	78	2	0
28	F	43	0	53	2	0
28	L	108	0	156	10	0
28	a	54	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	f	43	0	53	0	0
29	A	98	0	148	13	0
29	D	49	0	74	5	0
29	E	42	0	57	0	0
29	L	49	0	74	4	0
29	a	91	0	131	0	0
29	d	98	0	148	0	0
29	l	49	0	74	0	0
30	A	5	0	0	0	0
30	O	10	0	0	0	0
30	U	5	0	0	0	0
30	V	5	0	0	0	0
30	a	5	0	0	0	0
30	d	5	0	0	0	0
30	o	5	0	0	0	0
30	u	10	0	0	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0
32	B	68	0	0	0	0
32	C	15	0	0	0	0
32	D	15	0	0	0	0
32	I	14	0	0	0	0
32	J	11	0	0	0	0
32	M	26	0	0	0	0
32	T	27	0	0	0	0
32	X	10	0	0	0	0
32	b	60	0	0	0	0
32	c	15	0	0	0	0
32	d	15	0	0	0	0
32	i	16	0	0	0	0
32	j	15	0	0	0	0
32	k	9	0	0	0	0
32	m	25	0	0	0	0
32	t	15	0	0	0	0
32	x	16	0	0	0	0
33	C	186	0	246	12	0
33	H	62	0	82	3	0
33	c	186	0	246	0	0
33	h	62	0	82	0	0
34	D	128	0	148	6	0
34	a	64	0	74	0	0
34	d	64	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	E	43	0	30	3	0
35	V	43	0	30	0	0
35	e	43	0	30	0	0
35	v	43	0	30	0	0
36	A	33	0	0	0	0
36	B	42	0	0	3	0
36	C	24	0	0	0	0
36	D	27	0	0	0	0
36	E	2	0	0	0	0
36	H	8	0	0	0	0
36	L	1	0	0	0	0
36	O	15	0	0	0	0
36	T	3	0	0	1	0
36	U	6	0	0	0	0
36	V	9	0	0	0	0
36	X	1	0	0	0	0
36	a	24	0	0	0	0
36	b	37	0	0	0	0
36	c	26	0	0	0	0
36	d	17	0	0	0	0
36	h	1	0	0	0	0
36	i	1	0	0	0	0
36	j	1	0	0	0	0
36	l	3	0	0	0	0
36	m	1	0	0	0	0
36	o	11	0	0	0	0
36	t	1	0	0	0	0
36	u	7	0	0	0	0
36	v	3	0	0	0	0
All	All	50236	0	50766	498	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 6.

All (498) 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)
17:Y:18:VAL:HG23	17:Y:19:ILE:HD12	4.34	0.83
25:B:604:CLA:H93	25:B:605:CLA:HAB	1.66	0.77
3:C:79:LYS:HG3	16:V:103:LYS:HD3	4.60	0.75
25:C:503:CLA:H172	25:C:510:CLA:HBB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:607:CLA:HAB	25:D:404:CLA:H72	1.69	0.73
25:C:501:CLA:H71	25:C:501:CLA:HBB1	1.71	0.72
26:K:101:BCR:H10C	17:Y:28:ILE:HG23	1.70	0.71
19:Z:31:GLN:NE2	19:Z:31:GLN:HA	4.46	0.69
4:D:192:THR:HG23	25:D:404:CLA:HBC2	1.74	0.69
29:A:614:LHG:H352	29:A:614:LHG:H151	1.76	0.68
23:B:624:LMG:H402	23:B:624:LMG:H232	14.33	0.67
25:C:510:CLA:HED2	25:C:510:CLA:H2	2.05	0.67
4:D:279:LEU:HD22	34:D:402:PHO:HBC3	1.76	0.67
3:C:148:GLY:O	3:C:156:LYS:NZ	2.28	0.66
2:B:469:HIS:HE1	25:B:611:CLA:NA	1.95	0.65
25:C:502:CLA:HBB2	25:C:510:CLA:H151	2.16	0.65
19:Z:31:GLN:HE21	19:Z:31:GLN:HA	4.30	0.64
11:L:7:ARG:NH1	28:L:103:SQD:O7	30.75	0.64
1:A:183:MET:HA	25:A:606:CLA:HMD2	1.79	0.64
25:C:501:CLA:H203	25:C:507:CLA:H13	1.92	0.64
26:B:617:BCR:H383	28:L:101:SQD:H81	1.80	0.64
4:D:199:MET:HG2	27:D:407:PL9:H321	1.80	0.64
29:L:102:LHG:H271	12:M:22:LEU:HD21	1.78	0.64
2:B:216:HIS:HE1	25:B:609:CLA:C1A	2.11	0.63
25:C:511:CLA:HMB2	26:C:522:BCR:H382	1.79	0.63
2:B:71:VAL:HG23	25:B:606:CLA:HMA2	1.85	0.63
3:C:138:GLU:HG3	3:C:139:THR:HG23	5.75	0.63
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.84	0.63
25:A:608:CLA:H193	25:C:505:CLA:H13	1.79	0.63
23:B:620:LMG:H401	12:M:17:VAL:HG21	1.79	0.63
2:B:103:LEU:HD21	25:B:605:CLA:HMC3	1.80	0.63
17:Y:42:ARG:NH1	19:Z:32:ASP:OD2	4.09	0.63
28:A:611:SQD:H131	29:A:614:LHG:H142	1.81	0.62
13:O:91:GLY:HA3	13:O:132:ASN:HA	2.31	0.62
29:A:614:LHG:H112	29:A:614:LHG:H382	1.81	0.62
2:B:216:HIS:HE1	25:B:609:CLA:NA	1.91	0.62
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.81	0.62
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.45	0.62
2:B:357:ARG:NH2	4:D:337:GLU:O	2.55	0.62
19:Z:29:SER:OG	19:Z:32:ASP:OD2	2.27	0.62
25:C:505:CLA:HAB	25:C:505:CLA:H71	2.14	0.62
2:B:192:PRO:HG2	7:H:49:TYR:CD1	2.35	0.61
3:C:251:HIS:HE1	25:C:506:CLA:NA	1.97	0.61
20:R:18:TRP:O	20:R:22:ASN:ND2	2.35	0.61
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:PRO:HG3	7:H:49:TYR:CD1	3.63	0.61
11:L:7:ARG:NH1	28:L:103:SQD:S	32.03	0.61
13:O:10:ILE:HG23	13:O:15:LEU:HB2	1.86	0.61
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.47	0.61
1:A:38:ILE:HG23	23:A:603:LMG:H191	2.84	0.61
19:Z:39:LEU:HA	19:Z:42:LEU:HB2	2.25	0.60
4:D:343:GLU:HG2	16:V:135:VAL:HG11	1.84	0.60
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.89	0.60
25:B:602:CLA:H101	25:B:609:CLA:H18	1.83	0.60
2:B:2:GLY:N	11:L:11:GLU:OE2	2.43	0.60
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.84	0.60
6:F:21:VAL:HG21	28:F:101:SQD:H242	1.82	0.59
2:B:124:ARG:NH1	2:B:129:GLY:O	2.82	0.59
2:B:475:PHE:HB2	2:B:479:PHE:CE1	2.37	0.59
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.59
4:D:21:TRP:O	4:D:26:ARG:NH1	2.35	0.59
25:C:513:CLA:HAB	26:C:514:BCR:H24C	1.84	0.59
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.91	0.59
15:U:26:ASP:OD2	15:U:85:THR:OG1	2.21	0.59
2:B:383:PHE:N	4:D:344:GLU:O	2.33	0.58
25:C:505:CLA:H141	8:I:16:VAL:HG22	1.85	0.58
20:R:32:GLN:HA	20:R:35:LEU:HB3	4.97	0.58
19:Z:61:VAL:HG23	19:Z:62:VAL:HG13	7.49	0.58
25:B:614:CLA:H43	28:L:101:SQD:H112	1.84	0.58
25:A:606:CLA:HMB1	25:A:606:CLA:HBB1	1.87	0.58
2:B:488:PRO:O	2:B:492:GLU:HG2	2.03	0.57
25:B:613:CLA:HBB1	25:B:613:CLA:HMB1	2.23	0.57
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.86	0.57
3:C:26:ARG:NH1	25:C:511:CLA:O1A	2.37	0.57
4:D:186:GLN:HB2	25:D:404:CLA:HBC1	1.85	0.57
34:D:402:PHO:HBA2	25:D:404:CLA:H142	1.86	0.57
19:Z:41:PHE:HA	19:Z:44:SER:HB2	1.87	0.57
2:B:248:ALA:HA	25:B:603:CLA:H42	1.86	0.57
2:B:458:PHE:HB3	25:B:604:CLA:HBC2	1.92	0.57
25:C:503:CLA:H191	25:C:503:CLA:HMD2	1.86	0.57
26:B:617:BCR:H14C	29:L:102:LHG:H381	1.87	0.57
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.40	0.57
1:A:84:PRO:HA	1:A:112:TYR:CG	2.40	0.56
2:B:308:LYS:NZ	36:B:731:HOH:O	2.39	0.56
25:C:501:CLA:H151	25:C:507:CLA:HMB3	1.87	0.56
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:PRO:HB2	33:C:516:DGD:HA32	1.88	0.56
25:C:506:CLA:H43	26:C:514:BCR:HC8	44.68	0.56
5:E:26:THR:HB	35:E:102:HEM:HAB	1.88	0.56
16:V:77:LYS:HG2	16:V:95:LEU:HD12	1.87	0.56
4:D:274:VAL:HG22	27:D:407:PL9:H222	1.87	0.55
1:A:131:TRP:CH2	25:C:505:CLA:HAA2	2.45	0.55
33:C:517:DGD:HA81	33:C:517:DGD:HAH2	1.88	0.55
25:B:612:CLA:H171	25:B:613:CLA:HBB2	1.87	0.55
2:B:497:GLN:HE22	18:X:38:GLN:HB3	4.57	0.55
25:B:611:CLA:H71	29:L:102:LHG:H321	1.89	0.55
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.96	0.55
3:C:465:PRO:HB3	8:I:32:PRO:HB3	2.29	0.55
2:B:105:GLY:HA3	26:B:618:BCR:H282	1.89	0.54
13:O:155:ASN:ND2	15:U:100:ASN:O	2.38	0.54
19:Z:32:ASP:HB2	19:Z:35:ARG:CZ	3.83	0.54
2:B:12:LEU:HB2	25:B:612:CLA:HMC2	2.05	0.54
2:B:201:HIS:HE1	25:B:602:CLA:ND	2.02	0.54
13:O:53:LYS:NZ	13:O:63:ALA:O	2.41	0.54
13:O:57:LYS:HB2	13:O:61:GLN:HE22	13.00	0.54
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.88	0.54
10:K:17:ILE:H	10:K:17:ILE:HD12	1.71	0.53
25:B:607:CLA:HAC2	26:T:101:BCR:H272	32.84	0.53
14:T:15:ALA:HA	26:T:101:BCR:H12C	1.90	0.53
2:B:155:ALA:O	2:B:159:THR:OG1	2.30	0.53
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.90	0.53
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.89	0.53
29:A:614:LHG:H372	29:A:614:LHG:H132	1.90	0.53
7:H:17:GLU:OE1	7:H:20:LYS:NZ	2.29	0.53
2:B:18:ARG:NH2	28:L:103:SQD:O9	37.96	0.53
17:Y:42:ARG:HH22	19:Z:35:ARG:NH1	4.91	0.53
2:B:383:PHE:O	2:B:385:ARG:NH2	2.61	0.53
2:B:256:MET:O	2:B:448:ARG:NH1	2.54	0.53
25:B:608:CLA:H162	25:D:403:CLA:H3A	43.22	0.52
4:D:24:ARG:HD3	18:X:37:VAL:HG22	2.13	0.52
5:E:42:LEU:HA	20:R:4:ARG:HH21	1.74	0.52
28:L:103:SQD:H342	14:T:12:CYS:HB3	1.91	0.52
3:C:444:HIS:HE1	25:C:508:CLA:NA	2.05	0.52
11:L:7:ARG:NH2	28:L:101:SQD:O9	2.43	0.52
13:O:53:LYS:HB3	13:O:232:GLU:HB2	1.91	0.52
2:B:311:PHE:O	2:B:317:ASN:ND2	2.43	0.52
15:U:27:LEU:HD22	15:U:49:ILE:HG21	2.01	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:LEU:HD11	3:C:108:THR:HB	2.08	0.52
13:O:32:ILE:HG21	13:O:93:LEU:HD21	1.91	0.52
1:A:257:ARG:NH1	2:B:491:VAL:O	2.56	0.52
1:A:140:ARG:HH22	29:A:614:LHG:HC41	1.74	0.52
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.05	0.52
3:C:163:PHE:CD2	25:C:512:CLA:HAB	3.70	0.51
3:C:461:ARG:NH1	4:D:242:GLU:O	2.73	0.51
3:C:139:THR:OG1	3:C:142:GLU:OE1	2.23	0.51
16:V:28:GLU:HG3	16:V:31:ARG:HE	5.01	0.51
13:O:36:GLN:OE1	13:O:37:THR:N	2.35	0.51
16:V:38:ALA:O	16:V:42:VAL:HG23	2.10	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.51
19:Z:33:TRP:CZ3	19:Z:37:LYS:HB2	9.88	0.51
3:C:90:PRO:HB3	3:C:301:PHE:HB3	2.04	0.51
7:H:49:TYR:CE2	33:H:102:DGD:HG32	2.93	0.51
13:O:103:PHE:HB3	13:O:123:LYS:HE2	2.30	0.51
3:C:437:PHE:CZ	25:C:510:CLA:HMB3	2.45	0.51
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.00	0.51
13:O:15:LEU:HA	13:O:18:LYS:HG3	2.50	0.51
3:C:429:SER:HB3	33:C:517:DGD:HBT2	1.93	0.50
1:A:308:ASP:OD1	1:A:312:ASN:N	2.45	0.50
1:A:224:ILE:HG23	2:B:484:PRO:HA	1.94	0.50
3:C:216:SER:HB3	3:C:221:GLU:HG3	2.00	0.50
4:D:350:ASN:O	4:D:352:LEU:N	2.46	0.50
2:B:49:ASP:CG	13:O:57:LYS:HD2	46.32	0.50
2:B:62:VAL:HB	25:B:605:CLA:HED3	1.92	0.50
2:B:474:LEU:O	4:D:134:ARG:NH1	2.44	0.50
25:C:502:CLA:H61	25:C:512:CLA:H42	2.01	0.50
3:C:285:ILE:HA	33:C:516:DGD:HB31	1.94	0.50
5:E:26:THR:HA	20:R:15:ALA:HB1	1.97	0.50
16:V:5:PRO:O	16:V:9:THR:OG1	2.58	0.50
33:C:517:DGD:HB22	23:C:519:LMG:H302	1.94	0.50
3:C:132:HIS:HE1	25:C:513:CLA:NA	2.08	0.49
3:C:346:THR:OG1	3:C:348:GLU:OE2	2.27	0.49
3:C:406:SER:HA	3:C:420:VAL:HG23	1.99	0.49
25:B:615:CLA:H2	25:B:616:CLA:HBB2	2.01	0.49
3:C:402:GLY:HA3	3:C:420:VAL:HG22	2.01	0.49
20:R:20:VAL:O	20:R:24:LEU:N	2.51	0.49
14:T:15:ALA:HB2	26:T:101:BCR:H14C	1.94	0.49
25:C:512:CLA:HMA2	25:C:513:CLA:H203	1.94	0.49
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.59	0.49
14:T:18:PHE:HB2	26:T:101:BCR:HC8	1.93	0.49
15:U:57:SER:HA	15:U:84:VAL:HG21	1.98	0.49
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.40	0.49
2:B:479:PHE:O	4:D:139:ARG:NH2	2.46	0.49
13:O:60:ARG:HG3	13:O:60:ARG:O	2.12	0.49
16:V:22:THR:HG23	16:V:25:GLN:HE21	6.12	0.49
2:B:475:PHE:HB2	2:B:479:PHE:HE2	5.27	0.49
3:C:154:LYS:HB3	3:C:256:PRO:HG2	2.05	0.49
6:F:24:HIS:HA	6:F:27:ALA:HB3	1.95	0.49
13:O:90:ASP:OD1	13:O:92:SER:N	3.65	0.49
2:B:476:ARG:NH1	36:B:733:HOH:O	2.42	0.49
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.07	0.48
2:B:399:VAL:HG12	2:B:417:VAL:HG22	2.16	0.48
2:B:475:PHE:HB2	2:B:479:PHE:HE1	1.76	0.48
3:C:195:ASP:OD1	3:C:196:VAL:N	2.81	0.48
25:B:601:CLA:H122	26:H:101:BCR:H19C	2.79	0.48
10:K:25:LEU:HD22	26:K:101:BCR:H332	1.94	0.48
13:O:224:ASP:HB3	13:O:227:ALA:HB3	1.94	0.48
25:B:601:CLA:H42	25:B:601:CLA:HBD	3.57	0.48
3:C:311:GLN:NE2	3:C:358:PHE:O	4.02	0.48
3:C:455:PHE:HD2	8:I:33:LYS:HD3	4.63	0.48
10:K:31:LEU:HD22	26:K:101:BCR:H363	1.94	0.48
3:C:444:HIS:HE1	25:C:508:CLA:C1A	2.27	0.48
29:A:614:LHG:H383	25:C:510:CLA:H43	1.95	0.48
3:C:52:ALA:HB1	25:C:509:CLA:HBB1	1.96	0.48
2:B:113:TRP:CD1	25:B:616:CLA:HBA2	2.49	0.48
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	2.14	0.48
29:A:613:LHG:H371	29:A:613:LHG:HC82	1.95	0.48
25:C:503:CLA:HAB	25:C:512:CLA:H41	3.32	0.48
16:V:22:THR:H	16:V:25:GLN:NE2	4.68	0.48
1:A:191:ASN:HB2	3:C:411:ALA:HB1	2.19	0.48
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.95	0.48
5:E:36:LEU:HD13	20:R:7:VAL:HG12	1.96	0.48
5:E:57:ALA:H	5:E:60:GLN:HG2	1.78	0.48
1:A:132:GLU:O	1:A:136:ARG:HG2	2.17	0.48
2:B:462:PHE:CZ	25:B:613:CLA:HMB3	2.49	0.48
19:Z:29:SER:O	19:Z:33:TRP:NE1	2.47	0.48
16:V:34:GLN:HA	16:V:38:ALA:HB2	1.96	0.47
2:B:498:LYS:HE3	4:D:23:LYS:HD2	2.64	0.47
3:C:318:LEU:HD21	3:C:328:VAL:HG21	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:609:BCR:H351	26:A:609:BCR:H15C	1.73	0.47
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.03	0.47
3:C:88:LEU:HB3	25:C:503:CLA:HED3	1.96	0.47
15:U:57:SER:OG	15:U:60:ASP:OD2	2.27	0.47
1:A:270:SER:OG	28:A:611:SQD:O49	2.24	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.96	0.47
25:B:605:CLA:HBB1	25:B:606:CLA:H51	2.64	0.47
2:B:86:ILE:H	2:B:86:ILE:HG13	1.69	0.47
2:B:103:LEU:HB2	25:B:606:CLA:H62	2.68	0.47
2:B:154:GLY:HA2	2:B:158:LEU:HD12	2.05	0.47
2:B:242:ILE:HG23	2:B:462:PHE:HD2	1.97	0.47
34:D:402:PHO:H3A	34:D:402:PHO:HBA2	1.69	0.47
25:B:614:CLA:H41	25:B:614:CLA:H62	2.03	0.47
3:C:42:LEU:HD21	25:C:511:CLA:H2A	2.01	0.47
4:D:270:PHE:HZ	27:D:407:PL9:H203	1.79	0.47
28:L:101:SQD:H461	28:L:101:SQD:H92	1.96	0.47
2:B:496:TYR:CZ	2:B:502:VAL:HA	2.50	0.47
3:C:237:HIS:HA	3:C:240:ILE:HG22	4.42	0.47
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.49	0.47
25:D:403:CLA:H92	29:D:408:LHG:H172	1.95	0.47
1:A:223:LEU:HD13	4:D:265:ARG:HD3	2.13	0.47
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.84	0.47
13:O:4:THR:OG1	13:O:5:LEU:N	4.62	0.47
1:A:201:GLY:HA3	1:A:286:THR:HB	2.05	0.46
2:B:281:GLN:O	2:B:285:ASN:ND2	2.38	0.46
3:C:57:ALA:O	3:C:61:VAL:HG23	2.15	0.46
27:A:610:PL9:H502	4:D:39:PRO:HG3	1.98	0.46
2:B:388:SER:O	2:B:389:LYS:HD3	2.14	0.46
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.96	0.46
15:U:92:VAL:HG12	15:U:97:ARG:HD2	2.31	0.46
1:A:286:THR:HG21	25:A:606:CLA:HMA2	1.96	0.46
1:A:305:SER:HA	9:J:39:SER:HB3	2.19	0.46
26:C:514:BCR:H11C	26:C:514:BCR:H341	1.75	0.46
4:D:19:ASP:O	4:D:23:LYS:HG2	4.30	0.46
15:U:31:ASN:ND2	15:U:96:ASP:O	2.46	0.46
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.45	0.46
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.02	0.46
29:A:614:LHG:H121	29:A:614:LHG:H312	1.97	0.46
26:B:619:BCR:H351	26:B:619:BCR:H15C	1.76	0.46
3:C:377:LEU:HG	3:C:381:LYS:HE3	2.13	0.46
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:NH1	4:D:254:SER:O	2.65	0.46
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.98	0.46
19:Z:33:TRP:HZ3	19:Z:37:LYS:HG3	9.87	0.46
19:Z:3:ILE:O	19:Z:7:LEU:HB2	2.14	0.46
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.50	0.46
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.81	0.46
3:C:279:LEU:HD22	25:C:509:CLA:HED2	2.01	0.46
25:B:616:CLA:H11	25:B:616:CLA:H52	1.74	0.46
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.97	0.46
1:A:283:VAL:HA	1:A:286:THR:HG22	1.97	0.46
4:D:149:PRO:HB3	25:D:404:CLA:H41	1.98	0.46
25:B:608:CLA:H162	25:D:405:CLA:H3A	1.98	0.46
26:T:101:BCR:H351	26:T:101:BCR:H15C	1.71	0.46
26:B:618:BCR:H11C	26:B:618:BCR:H341	1.81	0.46
25:C:503:CLA:H192	25:C:509:CLA:H12	3.07	0.46
3:C:79:LYS:HD2	16:V:35:TYR:HE1	1.81	0.46
2:B:193:TYR:HH	7:H:49:TYR:HH	2.57	0.46
19:Z:42:LEU:HA	19:Z:42:LEU:HD12	1.81	0.46
13:O:158:ASP:OD2	13:O:162:ARG:HB2	2.82	0.45
14:T:24:ARG:NH1	36:T:202:HOH:O	2.34	0.45
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.97	0.45
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.99	0.45
2:B:109:LEU:O	26:B:619:BCR:H21C	2.19	0.45
26:D:406:BCR:H351	26:D:406:BCR:H15C	1.75	0.45
35:E:102:HEM:C3C	6:F:27:ALA:HB1	2.51	0.45
2:B:149:LEU:HD22	25:B:604:CLA:H152	1.97	0.45
25:B:605:CLA:H62	25:B:605:CLA:H41	1.75	0.45
3:C:343:ARG:NH1	3:C:347:GLY:O	2.49	0.45
26:B:617:BCR:HC32	23:B:620:LMG:H322	1.99	0.45
23:B:620:LMG:H411	12:M:17:VAL:HG11	1.98	0.45
2:B:125:ASP:HB2	2:B:132:ALA:HB3	2.33	0.45
13:O:127:ALA:HA	13:O:144:GLY:HA3	1.99	0.45
1:A:308:ASP:O	6:F:45:ARG:NH1	2.46	0.45
2:B:475:PHE:HB2	2:B:479:PHE:CE2	4.51	0.45
3:C:199:ILE:HG13	3:C:234:VAL:HG21	1.97	0.45
25:C:501:CLA:C2D	25:C:503:CLA:H2	2.50	0.45
3:C:168:LEU:HD21	25:C:509:CLA:H61	2.08	0.45
4:D:103:ARG:HE	5:E:77:GLU:HG3	2.02	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.99	0.45
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H:101:BCR:H341	26:H:101:BCR:H11C	1.79	0.45
13:O:99:ASP:OD1	13:O:100:GLY:N	2.44	0.45
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.99	0.45
19:Z:58:ASN:O	19:Z:61:VAL:HG12	2.17	0.45
1:A:221:SER:HB2	4:D:139:ARG:O	2.17	0.45
26:A:609:BCR:H24C	26:A:609:BCR:H371	1.82	0.45
2:B:208:VAL:HG21	25:B:602:CLA:HMC1	1.99	0.45
2:B:30:VAL:HG12	25:B:605:CLA:HHD	1.98	0.45
25:C:506:CLA:H41	25:C:506:CLA:H62	1.74	0.45
29:A:613:LHG:O4	4:D:141:TYR:OH	2.18	0.45
4:D:74:LEU:HD22	4:D:175:VAL:HG11	2.31	0.45
35:E:102:HEM:CAC	6:F:27:ALA:HB1	2.47	0.45
13:O:118:LEU:HD22	13:O:233:VAL:HG11	2.04	0.45
2:B:307:GLU:OE1	13:O:59:LYS:HD2	55.47	0.45
3:C:251:HIS:HE1	25:C:506:CLA:C1A	2.30	0.44
25:C:512:CLA:H93	25:C:513:CLA:H202	1.99	0.44
25:A:606:CLA:H151	25:D:403:CLA:H151	1.98	0.44
16:V:19:ILE:HD11	16:V:69:ILE:HG13	5.54	0.44
26:B:619:BCR:H11C	26:B:619:BCR:H341	1.79	0.44
3:C:162:GLY:HA3	3:C:252:ILE:HG13	2.21	0.44
3:C:179:ALA:HA	3:C:184:GLY:HA2	1.98	0.44
3:C:371:GLY:N	3:C:374:GLY:O	2.48	0.44
19:Z:33:TRP:HZ3	19:Z:37:LYS:HB2	10.26	0.44
3:C:429:SER:HB3	33:C:516:DGD:HBT2	15.05	0.44
25:C:507:CLA:H62	25:C:507:CLA:H41	1.86	0.44
26:C:514:BCR:H15C	26:C:514:BCR:H351	1.75	0.44
4:D:79:SER:HA	4:D:172:SER:HB3	2.04	0.44
5:E:61:ARG:HH12	16:V:127:GLY:HA3	3.07	0.44
27:A:610:PL9:H252	34:D:402:PHO:HBA1	1.99	0.44
2:B:149:LEU:HD23	25:B:603:CLA:HBC1	1.99	0.44
2:B:227:LYS:HD3	2:B:227:LYS:HA	4.47	0.44
2:B:235:GLU:OE1	2:B:472:ARG:NH2	5.24	0.44
26:C:514:BCR:H24C	26:C:514:BCR:H371	1.84	0.44
16:V:129:LYS:HG2	16:V:136:TYR:HB3	2.05	0.44
1:A:269:ARG:HE	4:D:243:THR:HG1	1.80	0.44
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.93	0.44
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.03	0.44
13:O:199:LEU:HD23	13:O:215:PHE:HB3	4.14	0.44
2:B:65:PHE:HE1	25:B:604:CLA:HED2	5.08	0.44
16:V:12:LEU:HD12	16:V:69:ILE:HB	2.38	0.44
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:617:BCR:H351	26:B:617:BCR:H15C	1.76	0.44
2:B:192:PRO:HG2	7:H:49:TYR:CE1	2.53	0.44
13:O:79:ASP:OD1	13:O:80:GLN:N	2.74	0.44
19:Z:25:VAL:O	19:Z:29:SER:HB2	2.69	0.44
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.58	0.44
25:B:614:CLA:HBA1	28:L:101:SQD:H82	2.00	0.44
13:O:169:ASP:N	13:O:169:ASP:OD1	2.51	0.44
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.96	0.43
26:H:101:BCR:H20C	26:H:101:BCR:H361	1.84	0.43
15:U:76:ARG:HA	15:U:79:LEU:HG	2.08	0.43
17:Y:18:VAL:O	17:Y:21:GLN:HB3	2.18	0.43
29:A:613:LHG:H223	25:B:613:CLA:H192	1.98	0.43
2:B:357:ARG:NH1	36:B:720:HOH:O	13.74	0.43
3:C:228:ASN:HB3	33:C:516:DGD:HE62	1.99	0.43
3:C:38:GLY:HA3	25:C:511:CLA:HMD3	1.99	0.43
25:C:508:CLA:H13	25:C:510:CLA:H202	3.39	0.43
16:V:42:VAL:O	16:V:45:ILE:HG12	2.18	0.43
16:V:87:GLU:OE1	16:V:96:ARG:NH1	2.87	0.43
1:A:140:ARG:NH2	29:A:614:LHG:HC41	2.32	0.43
33:C:516:DGD:HA62	33:C:516:DGD:HA31	4.79	0.43
4:D:24:ARG:HB2	4:D:26:ARG:HE	1.82	0.43
1:A:131:TRP:HZ2	3:C:449:ARG:HG3	2.04	0.43
4:D:342:PRO:O	4:D:345:VAL:HG22	2.18	0.43
26:D:406:BCR:H341	26:D:406:BCR:H11C	1.78	0.43
8:I:2:GLU:O	8:I:6:ILE:HG12	3.95	0.43
11:L:4:ASN:O	11:L:7:ARG:HG3	2.69	0.43
3:C:334:PRO:HA	13:O:153:THR:OG1	2.19	0.43
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.65	0.43
2:B:497:GLN:HE22	18:X:38:GLN:CB	3.90	0.43
26:B:619:BCR:H24C	26:B:619:BCR:H371	1.84	0.43
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.01	0.43
3:C:211:GLY:O	3:C:215:LYS:HG3	2.18	0.43
26:C:522:BCR:H15C	26:C:522:BCR:H351	1.76	0.43
13:O:86:LYS:HA	13:O:86:LYS:HD2	4.55	0.43
19:Z:33:TRP:HZ3	19:Z:37:LYS:CB	10.55	0.43
1:A:300:PHE:HZ	33:C:518:DGD:HB61	1.84	0.43
1:A:343:LEU:HD12	3:C:310:SER:HA	2.06	0.43
1:A:264:SER:OG	27:A:610:PL9:O2	2.32	0.43
25:C:513:CLA:C4B	26:C:514:BCR:H383	2.49	0.43
4:D:126:MET:HE3	4:D:143:ALA:O	2.18	0.43
4:D:27:PHE:HD2	4:D:28:VAL:HG23	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ASN:HB2	7:H:58:VAL:HG13	2.01	0.43
19:Z:46:LEU:HD23	19:Z:50:LEU:HG	2.00	0.43
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.43
25:B:613:CLA:H191	26:B:618:BCR:H333	2.01	0.43
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.53	0.43
3:C:31:SER:HB3	3:C:41:ARG:HG2	2.01	0.43
26:C:515:BCR:H24C	26:C:515:BCR:H371	1.85	0.43
34:D:401:PHO:H2	34:D:401:PHO:H61	1.82	0.43
17:Y:19:ILE:H	17:Y:19:ILE:HD12	1.84	0.43
17:Y:44:GLY:HA2	19:Z:30:PRO:HD3	3.20	0.43
3:C:363:GLY:O	3:C:367:GLU:HG2	2.19	0.42
25:C:507:CLA:HAA2	25:C:507:CLA:HBD	2.03	0.42
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.67	0.42
25:C:501:CLA:H71	25:C:501:CLA:CBB	2.45	0.42
1:A:202:VAL:HG11	25:A:607:CLA:C3D	2.50	0.42
27:A:610:PL9:H171	27:A:610:PL9:H151	1.71	0.42
25:C:508:CLA:H141	25:C:510:CLA:H18	2.01	0.42
1:A:179:THR:O	1:A:183:MET:HG3	2.24	0.42
1:A:46:ILE:HD13	23:A:603:LMG:H421	2.01	0.42
26:A:609:BCR:H341	26:A:609:BCR:H11C	1.85	0.42
26:H:101:BCR:H351	26:H:101:BCR:H15C	1.79	0.42
12:M:31:SER:HG	12:M:31:SER:HG	0.00	0.42
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.01	0.42
1:A:217:SER:HA	4:D:272:LEU:HD12	2.00	0.42
2:B:363:PHE:HB3	2:B:365:SER:O	2.33	0.42
2:B:490:GLN:HB3	2:B:496:TYR:HE2	4.02	0.42
25:B:605:CLA:H122	25:B:610:CLA:HMA2	2.11	0.42
25:B:614:CLA:H72	26:B:617:BCR:H362	2.01	0.42
23:C:521:LMG:H391	23:C:521:LMG:H362	1.75	0.42
34:D:402:PHO:H3A	25:D:404:CLA:H142	2.00	0.42
5:E:8:ARG:HA	5:E:9:PRO:HD3	1.95	0.42
1:A:227:THR:HB	1:A:231:GLU:HG3	2.03	0.42
1:A:45:THR:HG23	25:A:607:CLA:H201	48.62	0.42
2:B:141:ILE:HD11	7:H:14:LEU:HD22	2.17	0.42
3:C:256:PRO:HA	25:C:506:CLA:HED2	2.02	0.42
7:H:62:TRP:HD1	33:H:102:DGD:HO5E	1.67	0.42
12:M:31:SER:HB2	12:M:32:GLN:HG3	5.11	0.42
15:U:42:TYR:HA	15:U:43:PRO:HA	1.80	0.42
25:C:505:CLA:H43	26:C:514:BCR:HC7	45.35	0.42
25:C:506:CLA:C3D	25:C:507:CLA:H193	5.70	0.42
25:D:403:CLA:H91	29:D:408:LHG:H191	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.01	0.42
2:B:84:THR:HG21	13:O:67:PRO:HD2	68.17	0.42
2:B:469:HIS:HE1	25:B:611:CLA:C1A	2.32	0.42
25:B:603:CLA:H41	25:B:603:CLA:H61	3.67	0.42
2:B:150:CYS:HB2	25:B:603:CLA:HMC3	2.00	0.42
26:B:617:BCR:H371	26:B:617:BCR:H24C	1.81	0.42
5:E:14:ILE:O	5:E:20:TRP:NE1	2.44	0.42
5:E:56:TYR:C	5:E:83:LEU:HD21	3.45	0.42
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.79	0.42
16:V:26:TYR:OH	16:V:122:GLU:OE2	2.49	0.42
18:X:3:ILE:HA	18:X:7:LEU:HD23	2.22	0.42
2:B:141:ILE:HG21	25:B:615:CLA:HBB1	5.02	0.42
2:B:201:HIS:HB2	25:B:602:CLA:CHB	2.52	0.42
4:D:56:THR:OG1	4:D:57:SER:N	2.52	0.42
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.91	0.42
29:A:613:LHG:H351	29:A:613:LHG:H101	2.02	0.41
25:C:504:CLA:C1D	33:C:517:DGD:HB21	2.50	0.41
25:C:504:CLA:H41	25:C:504:CLA:H62	1.91	0.41
16:V:45:ILE:HG13	16:V:45:ILE:H	3.01	0.41
1:A:121:LEU:HD11	25:C:505:CLA:H171	2.03	0.41
25:B:604:CLA:H62	25:B:604:CLA:H41	1.91	0.41
2:B:466:HIS:HE1	25:B:608:CLA:C4D	2.36	0.41
25:C:506:CLA:H192	25:C:506:CLA:H13	4.36	0.41
1:A:218:LEU:HD12	27:A:610:PL9:C3	2.51	0.41
27:A:610:PL9:H121	27:A:610:PL9:HC8	1.72	0.41
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.24	0.41
1:A:136:ARG:NH1	8:I:27:ASP:OD1	2.49	0.41
20:R:23:ILE:O	20:R:27:ALA:N	2.54	0.41
2:B:487:SER:HA	2:B:488:PRO:HD3	2.08	0.41
25:B:616:CLA:H142	26:B:619:BCR:H14C	2.02	0.41
2:B:472:ARG:HA	2:B:479:PHE:CE1	2.55	0.41
25:B:601:CLA:H8	25:B:601:CLA:C4D	2.50	0.41
5:E:57:ALA:HB3	5:E:60:GLN:HB2	4.52	0.41
5:E:61:ARG:NH1	16:V:127:GLY:HA3	3.66	0.41
11:L:18:TYR:OH	28:L:101:SQD:H241	29.54	0.41
2:B:216:HIS:HE1	25:B:609:CLA:CHA	2.39	0.41
3:C:87:ILE:O	3:C:91:HIS:ND1	2.47	0.41
29:A:613:LHG:H361	25:B:613:CLA:H51	2.02	0.41
2:B:419:SER:O	2:B:423:LYS:HG2	2.42	0.41
26:B:618:BCR:H371	26:B:618:BCR:H24C	1.83	0.41
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.58	0.41
19:Z:58:ASN:O	19:Z:62:VAL:HG22	5.47	0.41
1:A:289:GLY:O	1:A:293:MET:HE3	2.38	0.41
2:B:191:ASN:HA	2:B:192:PRO:HD2	2.63	0.41
25:B:607:CLA:H41	25:B:607:CLA:H62	1.85	0.41
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.03	0.41
7:H:22:ALA:HA	7:H:23:PRO:HD3	1.91	0.41
20:R:8:VAL:O	20:R:11:PRO:HD2	2.21	0.41
17:Y:20:ALA:O	17:Y:24:MET:HG2	3.46	0.41
25:A:608:CLA:H202	25:C:506:CLA:H101	2.01	0.41
16:V:100:ILE:HG13	16:V:101:PHE:CD2	2.57	0.41
25:B:612:CLA:H61	25:B:612:CLA:H102	2.09	0.41
25:C:512:CLA:O2D	25:C:513:CLA:HBB2	2.21	0.41
12:M:23:ILE:O	12:M:27:VAL:HG23	2.21	0.41
29:D:408:LHG:H201	14:T:13:ILE:HG21	2.01	0.41
25:C:508:CLA:H203	33:C:516:DGD:HA92	36.43	0.40
33:C:516:DGD:HAT2	33:C:516:DGD:HAH1	1.88	0.40
4:D:23:LYS:HE2	4:D:23:LYS:HB3	4.21	0.40
5:E:9:PRO:O	5:E:13:ILE:HG13	2.21	0.40
4:D:87:HIS:HB2	33:H:102:DGD:HG11	2.39	0.40
13:O:53:LYS:HB2	13:O:65:PHE:CE1	3.64	0.40
14:T:26:PRO:HA	14:T:27:PRO:HD2	1.98	0.40
2:B:201:HIS:HE2	25:B:603:CLA:C2B	2.34	0.40
3:C:346:THR:HG21	13:O:12:GLY:HA2	2.02	0.40
29:D:408:LHG:H171	29:D:408:LHG:H142	1.93	0.40
4:D:261:PHE:CZ	29:D:408:LHG:HC81	2.56	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.09	0.40
3:C:296:VAL:HG11	25:C:501:CLA:HMA2	2.36	0.40
25:C:505:CLA:H43	26:C:515:BCR:HC7	2.04	0.40
25:C:508:CLA:H72	25:C:510:CLA:HED3	2.04	0.40
23:C:521:LMG:H382	23:C:521:LMG:H411	1.74	0.40
23:C:521:LMG:O2	23:C:521:LMG:HC71	2.21	0.40
26:T:101:BCR:H11C	26:T:101:BCR:H341	1.76	0.40
1:A:240:GLY:HA3	14:T:29:ILE:HG23	2.81	0.40
2:B:156:PHE:HB3	2:B:162:PHE:HB3	2.08	0.40
11:L:22:LEU:HG	29:L:102:LHG:H181	2.03	0.40
19:Z:38:GLN:O	19:Z:42:LEU:N	2.81	0.40
2:B:305:ILE:HA	2:B:306:PRO:HD3	2.02	0.40
25:B:615:CLA:H161	7:H:7:LEU:HD21	3.21	0.40
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.04	0.40
3:C:62:PHE:HZ	10:K:28:ILE:HD12	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:LEU:HD23	5:E:80:LEU:HA	2.24	0.40
28:F:101:SQD:H332	28:F:101:SQD:H361	1.88	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	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	44	54
1	a	331/344 (96%)	324 (98%)	6 (2%)	1 (0%)	44	54
2	B	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
2	b	501/510 (98%)	482 (96%)	18 (4%)	1 (0%)	51	62
3	C	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	51	62
3	c	446/461 (97%)	435 (98%)	9 (2%)	2 (0%)	38	47
4	D	338/352 (96%)	326 (96%)	12 (4%)	0	100	100
4	d	338/352 (96%)	323 (96%)	14 (4%)	1 (0%)	44	54
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	31/38 (82%)	31 (100%)	0	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/40 (80%)	32 (100%)	0	0	100	100
9	j	31/40 (78%)	31 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	34/46 (74%)	31 (91%)	3 (9%)	0	100	100
10	k	34/46 (74%)	34 (100%)	0	0	100	100
11	L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	228 (95%)	11 (5%)	1 (0%)	38	47
13	o	241/272 (89%)	225 (93%)	13 (5%)	3 (1%)	15	16
14	T	27/32 (84%)	27 (100%)	0	0	100	100
14	t	27/32 (84%)	26 (96%)	1 (4%)	0	100	100
15	U	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
15	u	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	25	31
17	Y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
17	y	27/46 (59%)	24 (89%)	2 (7%)	1 (4%)	4	1
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	9
19	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	4	2
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	31/41 (76%)	29 (94%)	2 (6%)	0	100	100
All	All	5199/5700 (91%)	5010 (96%)	173 (3%)	16 (0%)	44	54

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	30	PRO
13	o	57	LYS
3	c	416	SER
13	o	58	ASN
13	o	61	GLN
17	y	21	GLN

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Mol	Chain	Res	Type
19	z	31	GLN
3	C	416	SER
3	c	135	ARG
4	d	351	ALA
2	b	126	PRO
19	z	30	PRO
1	A	259	ILE
1	a	259	ILE
16	v	45	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	93	95
1	a	270/280 (96%)	270 (100%)	0	100	100
2	B	403/407 (99%)	401 (100%)	2 (0%)	91	95
2	b	401/407 (98%)	399 (100%)	2 (0%)	91	95
3	C	350/362 (97%)	349 (100%)	1 (0%)	94	96
3	c	350/362 (97%)	350 (100%)	0	100	100
4	D	275/283 (97%)	274 (100%)	1 (0%)	93	95
4	d	275/283 (97%)	275 (100%)	0	100	100
5	E	71/73 (97%)	70 (99%)	1 (1%)	71	82
5	e	70/73 (96%)	69 (99%)	1 (1%)	71	82
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	52 (98%)	1 (2%)	62	75
7	h	53/55 (96%)	53 (100%)	0	100	100
8	I	30/35 (86%)	30 (100%)	0	100	100
8	i	32/35 (91%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	206/228 (90%)	205 (100%)	1 (0%)	91	95
13	o	206/228 (90%)	206 (100%)	0	100	100
14	T	26/29 (90%)	26 (100%)	0	100	100
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	83 (100%)	0	100	100
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	117 (100%)	0	100	100
17	Y	22/37 (60%)	21 (96%)	1 (4%)	32	44
17	y	22/37 (60%)	21 (96%)	1 (4%)	32	44
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	62	75
19	z	52/52 (100%)	49 (94%)	3 (6%)	23	32
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	28/33 (85%)	28 (100%)	0	100	100
All	All	4318/4660 (93%)	4301 (100%)	17 (0%)	93	95

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
2	B	223	GLN
2	B	362	PHE
3	C	289	PHE
4	D	180	ARG
5	E	5	THR

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Mol	Chain	Res	Type
7	H	49	TYR
13	O	61	GLN
17	Y	23	THR
19	Z	31	GLN
2	b	362	PHE
2	b	490	GLN
5	e	7	GLU
17	y	22	LEU
19	z	2	THR
19	z	31	GLN
19	z	33	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	223	GLN
13	o	61	GLN
16	v	25	GLN
20	r	30	GLN
19	z	31	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 191 ligands modelled in this entry, 29 are unknown and 6 are monoatomic - leaving 156 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	1,3,36	0,15,15	0.00	-	0,32,32	0.00	-
23	LMG	A	603	-	51,51,55	0.92	2 (3%)	59,59,63	1.05	3 (5%)
25	CLA	A	606	-	56,73,73	1.14	2 (3%)	65,113,113	1.24	7 (10%)
25	CLA	A	607	-	56,73,73	1.19	2 (3%)	65,113,113	1.22	7 (10%)
25	CLA	A	608	-	56,73,73	1.20	3 (5%)	65,113,113	1.25	6 (9%)
26	BCR	A	609	-	41,41,41	0.67	0	56,56,56	1.85	12 (21%)
27	PL9	A	610	-	55,55,55	0.60	1 (1%)	69,69,69	1.69	20 (28%)
28	SQD	A	611	-	53,54,54	1.17	4 (7%)	63,65,65	1.38	8 (12%)
23	LMG	A	612	-	51,51,55	0.92	2 (3%)	59,59,63	1.03	3 (5%)
29	LHG	A	613	-	48,48,48	0.91	2 (4%)	49,54,54	1.04	3 (6%)
29	LHG	A	614	-	48,48,48	0.93	2 (4%)	49,54,54	1.05	2 (4%)
30	SO4	A	615	-	4,4,4	0.15	0	6,6,6	0.06	0
31	BCT	A	616	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	B	601	-	56,73,73	1.18	3 (5%)	65,113,113	1.27	6 (9%)
25	CLA	B	602	-	56,73,73	1.19	3 (5%)	65,113,113	1.23	9 (13%)
25	CLA	B	603	-	56,73,73	1.13	3 (5%)	65,113,113	1.29	7 (10%)
25	CLA	B	604	-	56,73,73	1.19	3 (5%)	65,113,113	1.37	6 (9%)
25	CLA	B	605	-	56,73,73	1.18	3 (5%)	65,113,113	1.30	6 (9%)
25	CLA	B	606	-	56,73,73	1.18	3 (5%)	65,113,113	1.28	7 (10%)
25	CLA	B	607	36	56,73,73	1.17	3 (5%)	65,113,113	1.30	7 (10%)
25	CLA	B	608	-	56,73,73	1.18	3 (5%)	65,113,113	1.23	5 (7%)
25	CLA	B	609	-	56,73,73	1.22	3 (5%)	65,113,113	1.29	7 (10%)
25	CLA	B	610	-	56,73,73	1.20	3 (5%)	65,113,113	1.28	8 (12%)
25	CLA	B	611	-	56,73,73	1.19	3 (5%)	65,113,113	1.31	7 (10%)
25	CLA	B	612	-	56,73,73	1.17	2 (3%)	65,113,113	1.27	7 (10%)
25	CLA	B	613	-	56,73,73	1.17	3 (5%)	65,113,113	1.31	7 (10%)
25	CLA	B	614	-	56,73,73	1.16	3 (5%)	65,113,113	1.24	7 (10%)
25	CLA	B	615	-	56,73,73	1.20	3 (5%)	65,113,113	1.33	5 (7%)
25	CLA	B	616	-	56,73,73	1.17	3 (5%)	65,113,113	1.33	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	B	617	-	41,41,41	0.68	0	56,56,56	1.96	16 (28%)
26	BCR	B	618	-	41,41,41	0.67	0	56,56,56	1.86	12 (21%)
26	BCR	B	619	-	41,41,41	0.73	0	56,56,56	1.94	14 (25%)
23	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.00	3 (5%)
23	LMG	B	624	-	51,51,55	0.92	2 (3%)	59,59,63	1.00	3 (5%)
25	CLA	C	501	-	56,73,73	1.18	3 (5%)	65,113,113	1.31	7 (10%)
25	CLA	C	502	-	56,73,73	1.20	3 (5%)	65,113,113	1.29	7 (10%)
25	CLA	C	503	-	56,73,73	1.19	3 (5%)	65,113,113	1.34	7 (10%)
25	CLA	C	504	-	56,73,73	1.17	3 (5%)	65,113,113	1.24	6 (9%)
25	CLA	C	505	-	56,73,73	1.15	3 (5%)	65,113,113	1.24	6 (9%)
25	CLA	C	506	-	56,73,73	1.16	3 (5%)	65,113,113	1.29	7 (10%)
25	CLA	C	507	-	56,73,73	1.16	3 (5%)	65,113,113	1.31	6 (9%)
25	CLA	C	508	-	56,73,73	1.17	3 (5%)	65,113,113	1.26	7 (10%)
25	CLA	C	509	-	56,73,73	1.19	3 (5%)	65,113,113	1.28	6 (9%)
25	CLA	C	510	-	56,73,73	1.18	3 (5%)	65,113,113	1.27	7 (10%)
25	CLA	C	511	3	56,73,73	1.18	3 (5%)	65,113,113	1.30	6 (9%)
25	CLA	C	512	-	56,73,73	1.17	3 (5%)	65,113,113	1.32	6 (9%)
25	CLA	C	513	-	56,73,73	1.18	2 (3%)	65,113,113	1.26	7 (10%)
26	BCR	C	514	-	41,41,41	0.69	0	56,56,56	1.93	13 (23%)
26	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.83	13 (23%)
33	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	4 (5%)
33	DGD	C	517	-	63,63,67	0.86	2 (3%)	77,77,81	0.97	3 (3%)
33	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.92	3 (3%)
23	LMG	C	519	-	51,51,55	0.93	2 (3%)	59,59,63	1.00	3 (5%)
23	LMG	C	521	-	51,51,55	0.96	3 (5%)	59,59,63	1.13	4 (6%)
26	BCR	C	522	-	41,41,41	0.65	0	56,56,56	2.07	15 (26%)
34	PHO	D	401	-	67,69,69	0.65	3 (4%)	87,99,99	0.93	4 (4%)
34	PHO	D	402	-	67,69,69	0.64	3 (4%)	87,99,99	0.96	5 (5%)
25	CLA	D	403	36	56,73,73	1.17	2 (3%)	65,113,113	1.26	8 (12%)
25	CLA	D	404	-	56,73,73	1.15	3 (5%)	65,113,113	1.24	7 (10%)
25	CLA	D	405	-	56,73,73	1.18	3 (5%)	65,113,113	1.27	7 (10%)
26	BCR	D	406	-	41,41,41	0.68	0	56,56,56	2.22	15 (26%)
27	PL9	D	407	-	55,55,55	0.60	1 (1%)	69,69,69	1.63	17 (24%)
29	LHG	D	408	-	48,48,48	0.91	2 (4%)	49,54,54	1.06	3 (6%)
23	LMG	D	409	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LHG	E	101	-	41,41,48	1.00	2 (4%)	42,47,54	1.14	3 (7%)
35	HEM	E	102	5,6	28,50,50	1.46	3 (10%)	17,82,82	1.27	2 (11%)
28	SQD	F	101	-	42,43,54	1.31	4 (9%)	52,54,65	1.45	9 (17%)
26	BCR	H	101	-	41,41,41	0.65	0	56,56,56	2.05	14 (25%)
33	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	0.91	3 (3%)
26	BCR	K	101	-	41,41,41	0.71	0	56,56,56	1.79	14 (25%)
28	SQD	L	101	-	53,54,54	1.20	4 (7%)	63,65,65	4.36	8 (12%)
29	LHG	L	102	-	48,48,48	0.91	2 (4%)	49,54,54	1.14	3 (6%)
28	SQD	L	103	-	53,54,54	1.19	4 (7%)	63,65,65	1.59	6 (9%)
30	SO4	O	301	-	4,4,4	0.14	0	6,6,6	0.07	0
30	SO4	O	302	-	4,4,4	0.14	0	6,6,6	0.05	0
26	BCR	T	101	-	41,41,41	0.67	0	56,56,56	2.06	13 (23%)
30	SO4	U	201	-	4,4,4	0.15	0	6,6,6	0.07	0
35	HEM	V	201	16	28,50,50	1.80	4 (14%)	17,82,82	1.32	2 (11%)
30	SO4	V	202	-	4,4,4	0.14	0	6,6,6	0.09	0
21	OEX	a	601	1,3,36	0,15,15	0.00	-	0,32,32	0.00	-
23	LMG	a	603	-	51,51,55	0.92	2 (3%)	59,59,63	1.11	6 (10%)
25	CLA	a	606	-	56,73,73	1.12	2 (3%)	65,113,113	1.27	7 (10%)
25	CLA	a	607	36	56,73,73	1.16	2 (3%)	65,113,113	1.23	8 (12%)
25	CLA	a	608	-	56,73,73	1.21	3 (5%)	65,113,113	1.28	7 (10%)
34	PHO	a	609	-	67,69,69	0.64	2 (2%)	87,99,99	0.92	4 (4%)
25	CLA	a	610	-	56,73,73	1.19	3 (5%)	65,113,113	1.26	7 (10%)
26	BCR	a	611	-	41,41,41	0.67	0	56,56,56	1.80	11 (19%)
27	PL9	a	612	-	55,55,55	0.61	1 (1%)	69,69,69	1.62	19 (27%)
28	SQD	a	613	-	53,54,54	1.18	4 (7%)	63,65,65	1.37	9 (14%)
23	LMG	a	614	-	51,51,55	0.90	2 (3%)	59,59,63	1.06	3 (5%)
29	LHG	a	615	-	48,48,48	0.92	2 (4%)	49,54,54	1.06	3 (6%)
29	LHG	a	616	-	41,41,48	0.99	2 (4%)	42,47,54	1.15	3 (7%)
30	SO4	a	617	-	4,4,4	0.15	0	6,6,6	0.06	0
31	BCT	a	618	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	b	601	-	56,73,73	1.18	3 (5%)	65,113,113	1.27	6 (9%)
25	CLA	b	602	-	56,73,73	1.18	2 (3%)	65,113,113	1.24	8 (12%)
25	CLA	b	603	-	56,73,73	1.17	3 (5%)	65,113,113	1.26	6 (9%)
25	CLA	b	604	-	56,73,73	1.18	3 (5%)	65,113,113	1.35	6 (9%)
25	CLA	b	605	-	56,73,73	1.20	3 (5%)	65,113,113	1.25	6 (9%)
25	CLA	b	606	-	56,73,73	1.17	3 (5%)	65,113,113	1.26	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	b	607	36	56,73,73	1.14	3 (5%)	65,113,113	1.28	7 (10%)
25	CLA	b	608	-	56,73,73	1.18	3 (5%)	65,113,113	1.23	7 (10%)
25	CLA	b	609	-	56,73,73	1.20	3 (5%)	65,113,113	1.33	6 (9%)
25	CLA	b	610	36	56,73,73	1.20	3 (5%)	65,113,113	1.28	7 (10%)
25	CLA	b	611	-	56,73,73	1.20	3 (5%)	65,113,113	1.30	7 (10%)
25	CLA	b	612	-	56,73,73	1.17	2 (3%)	65,113,113	1.29	7 (10%)
25	CLA	b	613	-	56,73,73	1.17	2 (3%)	65,113,113	1.31	7 (10%)
25	CLA	b	614	-	56,73,73	1.18	3 (5%)	65,113,113	1.24	7 (10%)
25	CLA	b	615	-	56,73,73	1.21	3 (5%)	65,113,113	1.30	6 (9%)
25	CLA	b	616	-	56,73,73	1.17	3 (5%)	65,113,113	1.27	7 (10%)
26	BCR	b	617	-	41,41,41	0.66	0	56,56,56	2.02	15 (26%)
26	BCR	b	618	-	41,41,41	0.65	0	56,56,56	1.96	17 (30%)
26	BCR	b	619	-	41,41,41	0.71	0	56,56,56	1.93	12 (21%)
23	LMG	b	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.06	3 (5%)
23	LMG	b	624	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	3 (5%)
25	CLA	c	501	-	56,73,73	1.19	3 (5%)	65,113,113	1.30	7 (10%)
25	CLA	c	502	-	56,73,73	1.21	3 (5%)	65,113,113	1.30	7 (10%)
25	CLA	c	503	-	56,73,73	1.22	3 (5%)	65,113,113	1.35	7 (10%)
25	CLA	c	504	-	56,73,73	1.17	3 (5%)	65,113,113	1.27	6 (9%)
25	CLA	c	505	-	56,73,73	1.15	3 (5%)	65,113,113	1.24	6 (9%)
25	CLA	c	506	-	56,73,73	1.16	3 (5%)	65,113,113	1.27	7 (10%)
25	CLA	c	507	-	56,73,73	1.19	3 (5%)	65,113,113	1.30	7 (10%)
25	CLA	c	508	-	56,73,73	1.17	3 (5%)	65,113,113	1.25	7 (10%)
25	CLA	c	509	-	56,73,73	1.17	3 (5%)	65,113,113	1.27	6 (9%)
25	CLA	c	510	-	56,73,73	1.17	3 (5%)	65,113,113	1.31	7 (10%)
25	CLA	c	511	3	56,73,73	1.21	3 (5%)	65,113,113	1.30	5 (7%)
25	CLA	c	512	-	56,73,73	1.20	3 (5%)	65,113,113	1.31	6 (9%)
25	CLA	c	513	-	56,73,73	1.20	3 (5%)	65,113,113	1.25	6 (9%)
26	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.82	12 (21%)
33	DGD	c	515	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	4 (5%)
33	DGD	c	516	-	63,63,67	0.86	2 (3%)	77,77,81	0.94	2 (2%)
33	DGD	c	517	-	63,63,67	0.86	2 (3%)	77,77,81	0.91	3 (3%)
23	LMG	c	518	-	51,51,55	0.92	2 (3%)	59,59,63	1.00	3 (5%)
23	LMG	c	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.06	4 (6%)
26	BCR	c	521	-	41,41,41	0.65	0	56,56,56	2.06	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	d	401	-	56,73,73	1.14	3 (5%)	65,113,113	1.24	7 (10%)
34	PHO	d	402	-	67,69,69	0.64	3 (4%)	87,99,99	0.97	5 (5%)
25	CLA	d	403	-	56,73,73	1.20	3 (5%)	65,113,113	1.28	6 (9%)
26	BCR	d	404	-	41,41,41	0.70	0	56,56,56	2.04	13 (23%)
27	PL9	d	405	-	55,55,55	0.60	1 (1%)	69,69,69	1.64	18 (26%)
29	LHG	d	406	-	48,48,48	0.92	2 (4%)	49,54,54	1.06	3 (6%)
29	LHG	d	407	-	48,48,48	0.92	2 (4%)	49,54,54	1.03	2 (4%)
23	LMG	d	408	-	51,51,55	0.93	2 (3%)	59,59,63	1.00	3 (5%)
30	SO4	d	410	-	4,4,4	0.14	0	6,6,6	0.06	0
35	HEM	e	101	5,6	28,50,50	1.49	3 (10%)	17,82,82	1.27	3 (17%)
28	SQD	f	101	-	42,43,54	1.33	4 (9%)	52,54,65	1.47	8 (15%)
26	BCR	h	101	-	41,41,41	0.66	0	56,56,56	1.98	14 (25%)
33	DGD	h	102	-	63,63,67	0.86	2 (3%)	77,77,81	0.92	2 (2%)
26	BCR	k	102	-	41,41,41	0.71	0	56,56,56	1.84	16 (28%)
29	LHG	l	101	-	48,48,48	0.93	2 (4%)	49,54,54	1.12	3 (6%)
30	SO4	o	301	-	4,4,4	0.14	0	6,6,6	0.06	0
26	BCR	t	102	-	41,41,41	0.65	0	56,56,56	2.06	15 (26%)
30	SO4	u	201	-	4,4,4	0.15	0	6,6,6	0.06	0
30	SO4	u	202	-	4,4,4	0.14	0	6,6,6	0.07	0
35	HEM	v	201	16	28,50,50	1.79	4 (14%)	17,82,82	1.31	2 (11%)
26	BCR	z	101	-	41,41,41	0.69	0	56,56,56	1.86	9 (16%)

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	1,3,36	-	0/0/68/68	0/0/6/6
23	LMG	A	603	-	-	0/46/66/70	0/1/1/1
25	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	608	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	A	609	-	-	0/29/63/63	0/2/2/2
27	PL9	A	610	-	-	0/53/73/73	0/1/1/1
28	SQD	A	611	-	-	0/49/69/69	0/1/1/1
23	LMG	A	612	-	-	0/46/66/70	0/1/1/1
29	LHG	A	613	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	A	614	-	-	0/53/53/53	0/0/0/0
30	SO4	A	615	-	-	0/0/0/0	0/0/0/0
31	BCT	A	616	22	-	0/0/0/0	0/0/0/0
25	CLA	B	601	-	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	36	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	-	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
26	BCR	B	617	-	-	0/29/63/63	0/2/2/2
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	LMG	B	620	-	-	0/46/66/70	0/1/1/1
23	LMG	B	624	-	-	0/46/66/70	0/1/1/1
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	-	3/3/20/25	0/37/135/135	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	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	-	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	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
26	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
23	LMG	C	519	-	-	0/46/66/70	0/1/1/1
23	LMG	C	521	-	-	1/46/66/70	0/1/1/1
26	BCR	C	522	-	-	0/29/63/63	0/2/2/2
34	PHO	D	401	-	-	0/53/103/103	0/1/6/6
34	PHO	D	402	-	-	0/53/103/103	0/1/6/6
25	CLA	D	403	36	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
27	PL9	D	407	-	-	0/53/73/73	0/1/1/1
29	LHG	D	408	-	-	0/53/53/53	0/0/0/0
23	LMG	D	409	-	-	0/46/66/70	0/1/1/1
29	LHG	E	101	-	-	0/46/46/53	0/0/0/0
35	HEM	E	102	5,6	-	0/6/54/54	0/0/8/8
28	SQD	F	101	-	-	0/38/58/69	0/1/1/1
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
33	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	SQD	L	101	-	-	0/49/69/69	0/1/1/1
29	LHG	L	102	-	-	0/53/53/53	0/0/0/0
28	SQD	L	103	-	-	0/49/69/69	0/1/1/1
30	SO4	O	301	-	-	0/0/0/0	0/0/0/0
30	SO4	O	302	-	-	0/0/0/0	0/0/0/0
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
30	SO4	U	201	-	-	0/0/0/0	0/0/0/0
35	HEM	V	201	16	-	0/6/54/54	0/0/8/8
30	SO4	V	202	-	-	0/0/0/0	0/0/0/0
21	OEX	a	601	1,3,36	-	0/0/68/68	0/0/6/6
23	LMG	a	603	-	-	0/46/66/70	0/1/1/1
25	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	607	36	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	608	-	3/3/20/25	0/37/135/135	0/0/9/9
34	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	a	611	-	-	0/29/63/63	0/2/2/2
27	PL9	a	612	-	-	0/53/73/73	0/1/1/1
28	SQD	a	613	-	-	0/49/69/69	0/1/1/1
23	LMG	a	614	-	-	0/46/66/70	0/1/1/1
29	LHG	a	615	-	-	0/53/53/53	0/0/0/0
29	LHG	a	616	-	-	0/46/46/53	0/0/0/0
30	SO4	a	617	-	-	0/0/0/0	0/0/0/0
31	BCT	a	618	22	-	0/0/0/0	0/0/0/0
25	CLA	b	601	-	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	36	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	36	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
26	BCR	b	617	-	-	0/29/63/63	0/2/2/2
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
23	LMG	b	620	-	-	0/46/66/70	0/1/1/1
23	LMG	b	624	-	-	0/46/66/70	0/1/1/1
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	-	3/3/20/25	0/37/135/135	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	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	508	-	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	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
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
33	DGD	c	515	-	-	0/51/91/95	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
23	LMG	c	518	-	-	0/46/66/70	0/1/1/1
23	LMG	c	520	-	-	0/46/66/70	0/1/1/1
26	BCR	c	521	-	-	0/29/63/63	0/2/2/2
25	CLA	d	401	-	3/3/20/25	0/37/135/135	0/0/9/9
34	PHO	d	402	-	-	0/53/103/103	0/1/6/6
25	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	d	404	-	-	0/29/63/63	0/2/2/2
27	PL9	d	405	-	-	0/53/73/73	0/1/1/1
29	LHG	d	406	-	-	0/53/53/53	0/0/0/0
29	LHG	d	407	-	-	0/53/53/53	0/0/0/0
23	LMG	d	408	-	-	0/46/66/70	0/1/1/1
30	SO4	d	410	-	-	0/0/0/0	0/0/0/0
35	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
28	SQD	f	101	-	-	0/38/58/69	0/1/1/1
26	BCR	h	101	-	-	0/29/63/63	0/2/2/2
33	DGD	h	102	-	-	0/51/91/95	0/2/2/2
26	BCR	k	102	-	-	0/29/63/63	0/2/2/2
29	LHG	l	101	-	-	0/53/53/53	0/0/0/0
30	SO4	o	301	-	-	0/0/0/0	0/0/0/0
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
30	SO4	u	201	-	-	0/0/0/0	0/0/0/0
30	SO4	u	202	-	-	0/0/0/0	0/0/0/0
35	HEM	v	201	16	-	0/6/54/54	0/0/8/8
26	BCR	z	101	-	-	0/29/63/63	0/2/2/2

All (318) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	V	201	HEM	C3C-C2C	-5.34	1.33	1.40
35	e	101	HEM	C3C-C2C	-5.31	1.33	1.40
35	v	201	HEM	C3C-C2C	-5.25	1.33	1.40
35	E	102	HEM	C3C-C2C	-5.11	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	101	HEM	C3B-C2B	-3.32	1.36	1.40
35	E	102	HEM	C3B-C2B	-3.28	1.36	1.40
35	v	201	HEM	C3B-C2B	-3.22	1.36	1.40
35	V	201	HEM	C3B-C2B	-3.15	1.36	1.40
25	b	609	CLA	C3B-C2B	-3.05	1.36	1.40
25	B	615	CLA	C3B-C2B	-2.98	1.36	1.40
25	b	615	CLA	C3B-C2B	-2.93	1.36	1.40
25	B	609	CLA	C3B-C2B	-2.89	1.36	1.40
25	c	502	CLA	C3B-C2B	-2.78	1.36	1.40
25	c	512	CLA	C3B-C2B	-2.78	1.36	1.40
25	b	605	CLA	C3B-C2B	-2.77	1.36	1.40
28	L	103	SQD	C6-S	-2.77	1.66	1.77
25	c	503	CLA	C3B-C2B	-2.76	1.36	1.40
25	a	608	CLA	C3B-C2B	-2.74	1.36	1.40
25	c	507	CLA	C3B-C2B	-2.74	1.36	1.40
25	b	603	CLA	C3B-C2B	-2.72	1.36	1.40
25	b	611	CLA	C3B-C2B	-2.69	1.36	1.40
25	B	605	CLA	C3B-C2B	-2.69	1.36	1.40
25	B	606	CLA	C3B-C2B	-2.69	1.36	1.40
25	a	607	CLA	C3B-C2B	-2.69	1.36	1.40
25	b	610	CLA	C3B-C2B	-2.68	1.36	1.40
25	b	606	CLA	C3B-C2B	-2.68	1.36	1.40
25	D	403	CLA	C3B-C2B	-2.68	1.36	1.40
28	a	613	SQD	C6-S	-2.67	1.66	1.77
25	A	608	CLA	C3B-C2B	-2.67	1.36	1.40
28	f	101	SQD	C6-S	-2.65	1.66	1.77
25	c	513	CLA	C3B-C2B	-2.65	1.36	1.40
25	A	607	CLA	C3B-C2B	-2.64	1.36	1.40
25	B	607	CLA	C3B-C2B	-2.64	1.36	1.40
25	B	601	CLA	C3B-C2B	-2.64	1.36	1.40
28	F	101	SQD	C6-S	-2.64	1.66	1.77
25	C	502	CLA	C3B-C2B	-2.63	1.36	1.40
25	a	610	CLA	C3B-C2B	-2.63	1.36	1.40
25	B	604	CLA	C3B-C2B	-2.63	1.36	1.40
25	C	504	CLA	C3B-C2B	-2.63	1.36	1.40
25	b	601	CLA	C3B-C2B	-2.61	1.36	1.40
28	A	611	SQD	C6-S	-2.61	1.66	1.77
25	b	608	CLA	C3B-C2B	-2.61	1.36	1.40
25	c	505	CLA	C3B-C2B	-2.60	1.36	1.40
25	C	505	CLA	C3B-C2B	-2.58	1.36	1.40
25	B	602	CLA	C3B-C2B	-2.56	1.37	1.40
25	B	610	CLA	C3B-C2B	-2.50	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	C3B-C2B	-2.48	1.37	1.40
25	c	511	CLA	C3B-C2B	-2.44	1.37	1.40
25	c	504	CLA	C3B-C2B	-2.42	1.37	1.40
25	b	602	CLA	C3B-C2B	-2.40	1.37	1.40
25	b	604	CLA	C3B-C2B	-2.39	1.37	1.40
25	d	403	CLA	C3B-C2B	-2.39	1.37	1.40
25	c	506	CLA	C3B-C2B	-2.37	1.37	1.40
25	c	501	CLA	C3B-C2B	-2.36	1.37	1.40
25	C	503	CLA	C3B-C2B	-2.36	1.37	1.40
25	B	608	CLA	C3B-C2B	-2.35	1.37	1.40
25	b	614	CLA	C3B-C2B	-2.35	1.37	1.40
25	C	510	CLA	C3B-C2B	-2.33	1.37	1.40
25	C	506	CLA	C3B-C2B	-2.33	1.37	1.40
25	C	513	CLA	C3B-C2B	-2.32	1.37	1.40
25	B	603	CLA	C3B-C2B	-2.30	1.37	1.40
25	B	611	CLA	C3B-C2B	-2.29	1.37	1.40
25	D	404	CLA	C3B-C2B	-2.26	1.37	1.40
25	C	512	CLA	C3B-C2B	-2.25	1.37	1.40
25	C	511	CLA	C3B-C2B	-2.24	1.37	1.40
25	b	616	CLA	C3B-C2B	-2.23	1.37	1.40
25	B	613	CLA	C3B-C2B	-2.22	1.37	1.40
25	B	614	CLA	C3B-C2B	-2.21	1.37	1.40
28	L	101	SQD	C6-S	-2.20	1.68	1.77
25	b	612	CLA	CHD-C4C	-2.19	1.34	1.41
25	B	616	CLA	C3B-C2B	-2.19	1.37	1.40
25	B	612	CLA	CHD-C4C	-2.18	1.34	1.41
25	b	606	CLA	CHD-C4C	-2.17	1.34	1.41
25	b	615	CLA	CHD-C4C	-2.17	1.34	1.41
25	C	507	CLA	CHD-C4C	-2.17	1.34	1.41
25	c	503	CLA	CHD-C4C	-2.16	1.34	1.41
25	c	507	CLA	CHD-C4C	-2.15	1.34	1.41
25	b	613	CLA	CHD-C4C	-2.15	1.34	1.41
34	a	609	PHO	C1D-C2D	-2.15	1.41	1.45
25	b	610	CLA	CHD-C4C	-2.14	1.35	1.41
25	C	509	CLA	C3B-C2B	-2.14	1.37	1.40
25	b	604	CLA	CHD-C4C	-2.13	1.35	1.41
25	b	601	CLA	CHD-C4C	-2.13	1.35	1.41
25	c	502	CLA	CHD-C4C	-2.12	1.35	1.41
25	B	615	CLA	CHD-C4C	-2.12	1.35	1.41
25	C	501	CLA	CHD-C4C	-2.12	1.35	1.41
25	b	611	CLA	CHD-C4C	-2.12	1.35	1.41
25	C	508	CLA	C3B-C2B	-2.12	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	604	CLA	CHD-C4C	-2.11	1.35	1.41
25	C	512	CLA	CHD-C4C	-2.11	1.35	1.41
25	C	509	CLA	CHD-C4C	-2.11	1.35	1.41
25	b	609	CLA	CHD-C4C	-2.11	1.35	1.41
25	b	603	CLA	CHD-C4C	-2.11	1.35	1.41
25	C	511	CLA	CHD-C4C	-2.11	1.35	1.41
25	b	616	CLA	CHD-C4C	-2.11	1.35	1.41
25	c	512	CLA	CHD-C4C	-2.11	1.35	1.41
25	B	606	CLA	CHD-C4C	-2.11	1.35	1.41
25	c	511	CLA	CHD-C4C	-2.10	1.35	1.41
25	C	503	CLA	CHD-C4C	-2.10	1.35	1.41
25	D	405	CLA	CHD-C4C	-2.10	1.35	1.41
25	B	610	CLA	CHD-C4C	-2.10	1.35	1.41
25	C	505	CLA	CHD-C4C	-2.10	1.35	1.41
25	B	603	CLA	CHD-C4C	-2.10	1.35	1.41
25	B	611	CLA	CHD-C4C	-2.10	1.35	1.41
25	c	510	CLA	CHD-C4C	-2.10	1.35	1.41
25	B	616	CLA	CHD-C4C	-2.09	1.35	1.41
25	A	608	CLA	CHD-C4C	-2.09	1.35	1.41
25	B	609	CLA	CHD-C4C	-2.09	1.35	1.41
25	d	403	CLA	CHD-C4C	-2.09	1.35	1.41
25	c	508	CLA	C3B-C2B	-2.09	1.37	1.40
25	b	605	CLA	CHD-C4C	-2.09	1.35	1.41
25	c	508	CLA	CHD-C4C	-2.09	1.35	1.41
25	c	510	CLA	C3B-C2B	-2.09	1.37	1.40
25	d	401	CLA	CHD-C4C	-2.08	1.35	1.41
25	b	614	CLA	CHD-C4C	-2.08	1.35	1.41
25	C	508	CLA	CHD-C4C	-2.08	1.35	1.41
25	b	607	CLA	CHD-C4C	-2.08	1.35	1.41
25	d	401	CLA	C3B-C2B	-2.08	1.37	1.40
25	B	613	CLA	CHD-C4C	-2.08	1.35	1.41
25	B	614	CLA	CHD-C4C	-2.08	1.35	1.41
25	a	610	CLA	CHD-C4C	-2.07	1.35	1.41
25	B	607	CLA	CHD-C4C	-2.07	1.35	1.41
34	D	402	PHO	C1D-C2D	-2.07	1.41	1.45
25	B	608	CLA	CHD-C4C	-2.07	1.35	1.41
25	C	506	CLA	CHD-C4C	-2.07	1.35	1.41
25	a	606	CLA	CHD-C4C	-2.07	1.35	1.41
25	C	504	CLA	CHD-C4C	-2.06	1.35	1.41
25	c	509	CLA	CHD-C4C	-2.06	1.35	1.41
34	d	402	PHO	C1D-C2D	-2.06	1.41	1.45
25	c	505	CLA	CHD-C4C	-2.06	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	CHD-C4C	-2.06	1.35	1.41
25	C	501	CLA	C3B-C2B	-2.06	1.37	1.40
25	c	509	CLA	C3B-C2B	-2.06	1.37	1.40
25	B	601	CLA	CHD-C4C	-2.05	1.35	1.41
34	D	401	PHO	C1D-C2D	-2.05	1.41	1.45
25	D	405	CLA	C3B-C2B	-2.05	1.37	1.40
25	c	506	CLA	CHD-C4C	-2.05	1.35	1.41
25	B	605	CLA	CHD-C4C	-2.04	1.35	1.41
25	b	608	CLA	CHD-C4C	-2.04	1.35	1.41
25	C	510	CLA	CHD-C4C	-2.04	1.35	1.41
25	D	404	CLA	CHD-C4C	-2.04	1.35	1.41
25	c	501	CLA	CHD-C4C	-2.03	1.35	1.41
25	c	513	CLA	CHD-C4C	-2.03	1.35	1.41
25	A	606	CLA	CHD-C4C	-2.03	1.35	1.41
25	c	504	CLA	CHD-C4C	-2.02	1.35	1.41
25	a	608	CLA	CHD-C4C	-2.02	1.35	1.41
25	b	607	CLA	C3B-C2B	-2.01	1.37	1.40
25	B	602	CLA	CHD-C4C	-2.00	1.35	1.41
35	e	101	HEM	C3D-C2D	2.00	1.43	1.37
34	d	402	PHO	C3D-C2D	2.01	1.44	1.38
34	d	402	PHO	C3B-C4B	2.01	1.47	1.43
34	D	402	PHO	C3B-C4B	2.02	1.47	1.43
35	E	102	HEM	C3D-C2D	2.05	1.43	1.37
34	D	401	PHO	C3D-C2D	2.06	1.44	1.38
34	D	402	PHO	C3D-C2D	2.07	1.44	1.38
34	a	609	PHO	C3D-C2D	2.07	1.44	1.38
34	D	401	PHO	C3B-C4B	2.08	1.47	1.43
23	C	521	LMG	O1-C1	2.24	1.44	1.40
27	D	407	PL9	C6-C5	2.53	1.48	1.35
27	d	405	PL9	C6-C5	2.54	1.48	1.35
27	a	612	PL9	C6-C5	2.55	1.48	1.35
27	A	610	PL9	C6-C5	2.56	1.48	1.35
35	V	201	HEM	CBB-CAB	3.75	1.55	1.28
35	v	201	HEM	CBB-CAB	3.79	1.55	1.28
29	A	613	LHG	O7-C7	3.87	1.45	1.34
29	D	408	LHG	O7-C7	3.88	1.45	1.34
35	V	201	HEM	CBC-CAC	3.90	1.56	1.28
35	v	201	HEM	CBC-CAC	3.90	1.56	1.28
23	a	614	LMG	O7-C10	3.92	1.45	1.34
29	d	406	LHG	O7-C7	3.94	1.45	1.34
29	L	102	LHG	O7-C7	3.94	1.45	1.34
29	a	615	LHG	O7-C7	3.95	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	616	LHG	O7-C7	3.96	1.45	1.34
33	c	515	DGD	O2G-C1B	3.96	1.45	1.34
23	B	624	LMG	O7-C10	3.97	1.45	1.34
23	c	518	LMG	O7-C10	3.97	1.45	1.34
23	a	603	LMG	O7-C10	3.97	1.45	1.34
23	A	612	LMG	O7-C10	3.97	1.45	1.34
28	a	613	SQD	O47-C7	3.98	1.45	1.34
29	l	101	LHG	O7-C7	3.98	1.45	1.34
33	C	518	DGD	O2G-C1B	3.99	1.45	1.34
33	C	517	DGD	O2G-C1B	4.00	1.45	1.34
33	c	517	DGD	O2G-C1B	4.00	1.45	1.34
23	A	603	LMG	O7-C10	4.00	1.45	1.34
29	d	407	LHG	O7-C7	4.00	1.45	1.34
23	C	519	LMG	O7-C10	4.01	1.45	1.34
23	b	620	LMG	O7-C10	4.01	1.45	1.34
23	b	624	LMG	O7-C10	4.01	1.45	1.34
33	C	516	DGD	O2G-C1B	4.02	1.45	1.34
23	d	408	LMG	O7-C10	4.02	1.46	1.34
33	c	516	DGD	O2G-C1B	4.03	1.46	1.34
33	h	102	DGD	O2G-C1B	4.04	1.46	1.34
33	h	102	DGD	O1G-C1A	4.04	1.45	1.33
28	F	101	SQD	O47-C7	4.04	1.46	1.34
23	c	520	LMG	O7-C10	4.04	1.46	1.34
29	A	614	LHG	O7-C7	4.04	1.46	1.34
29	E	101	LHG	O7-C7	4.04	1.46	1.34
33	H	102	DGD	O2G-C1B	4.05	1.46	1.34
23	C	521	LMG	O7-C10	4.05	1.46	1.34
23	B	620	LMG	O7-C10	4.06	1.46	1.34
28	L	103	SQD	O47-C7	4.06	1.46	1.34
28	f	101	SQD	O47-C7	4.06	1.46	1.34
23	D	409	LMG	O7-C10	4.06	1.46	1.34
28	A	611	SQD	O47-C7	4.06	1.46	1.34
28	F	101	SQD	O48-C23	4.08	1.45	1.33
28	A	611	SQD	O48-C23	4.13	1.45	1.33
29	A	613	LHG	O8-C23	4.15	1.45	1.33
28	L	101	SQD	O47-C7	4.15	1.46	1.34
29	D	408	LHG	O8-C23	4.15	1.45	1.33
29	a	615	LHG	O8-C23	4.17	1.45	1.33
29	L	102	LHG	O8-C23	4.17	1.45	1.33
33	C	516	DGD	O1G-C1A	4.17	1.45	1.33
33	c	517	DGD	O1G-C1A	4.18	1.45	1.33
28	L	103	SQD	O48-C23	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	614	LMG	O8-C28	4.18	1.45	1.33
29	a	616	LHG	O8-C23	4.18	1.45	1.33
28	L	101	SQD	O48-C23	4.19	1.45	1.33
33	C	518	DGD	O1G-C1A	4.19	1.45	1.33
33	C	517	DGD	O1G-C1A	4.20	1.45	1.33
33	c	516	DGD	O1G-C1A	4.20	1.45	1.33
29	d	407	LHG	O8-C23	4.21	1.45	1.33
29	d	406	LHG	O8-C23	4.21	1.45	1.33
29	E	101	LHG	O8-C23	4.21	1.45	1.33
23	b	624	LMG	O8-C28	4.21	1.45	1.33
28	a	613	SQD	O48-C23	4.22	1.45	1.33
33	H	102	DGD	O1G-C1A	4.22	1.45	1.33
33	c	515	DGD	O1G-C1A	4.23	1.45	1.33
23	B	624	LMG	O8-C28	4.23	1.45	1.33
23	A	612	LMG	O8-C28	4.24	1.45	1.33
29	A	614	LHG	O8-C23	4.24	1.45	1.33
23	b	620	LMG	O8-C28	4.25	1.45	1.33
23	c	518	LMG	O8-C28	4.25	1.45	1.33
23	C	521	LMG	O8-C28	4.25	1.45	1.33
23	B	620	LMG	O8-C28	4.25	1.45	1.33
23	A	603	LMG	O8-C28	4.26	1.45	1.33
23	c	520	LMG	O8-C28	4.26	1.45	1.33
29	l	101	LHG	O8-C23	4.27	1.45	1.33
23	d	408	LMG	O8-C28	4.28	1.45	1.33
23	a	603	LMG	O8-C28	4.29	1.46	1.33
23	D	409	LMG	O8-C28	4.29	1.46	1.33
23	C	519	LMG	O8-C28	4.29	1.46	1.33
28	f	101	SQD	O48-C23	4.30	1.46	1.33
28	F	101	SQD	O8-S	4.82	1.63	1.47
28	A	611	SQD	O8-S	4.85	1.63	1.47
28	f	101	SQD	O8-S	4.88	1.63	1.47
28	L	103	SQD	O8-S	4.88	1.63	1.47
28	a	613	SQD	O8-S	4.89	1.64	1.47
28	L	101	SQD	O8-S	5.31	1.65	1.47
25	c	505	CLA	C4C-NC	7.01	1.48	1.37
25	a	607	CLA	C4C-NC	7.04	1.48	1.37
25	B	603	CLA	C4C-NC	7.05	1.48	1.37
25	C	507	CLA	C4C-NC	7.07	1.48	1.37
25	C	505	CLA	C4C-NC	7.07	1.48	1.37
25	d	401	CLA	C4C-NC	7.12	1.48	1.37
25	D	404	CLA	C4C-NC	7.12	1.48	1.37
25	a	606	CLA	C4C-NC	7.14	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	403	CLA	C4C-NC	7.16	1.48	1.37
25	b	606	CLA	C4C-NC	7.16	1.48	1.37
25	b	601	CLA	C4C-NC	7.17	1.48	1.37
25	c	507	CLA	C4C-NC	7.17	1.48	1.37
25	B	605	CLA	C4C-NC	7.17	1.48	1.37
25	b	603	CLA	C4C-NC	7.19	1.48	1.37
25	B	607	CLA	C4C-NC	7.19	1.48	1.37
25	b	609	CLA	C4C-NC	7.19	1.48	1.37
25	c	506	CLA	C4C-NC	7.19	1.48	1.37
25	C	504	CLA	C4C-NC	7.21	1.48	1.37
25	b	608	CLA	C4C-NC	7.21	1.48	1.37
25	b	607	CLA	C4C-NC	7.21	1.48	1.37
25	B	606	CLA	C4C-NC	7.22	1.48	1.37
25	B	601	CLA	C4C-NC	7.24	1.48	1.37
25	B	613	CLA	C4C-NC	7.24	1.48	1.37
25	C	506	CLA	C4C-NC	7.25	1.48	1.37
25	b	602	CLA	C4C-NC	7.25	1.48	1.37
25	B	604	CLA	C4C-NC	7.26	1.48	1.37
25	c	512	CLA	C4C-NC	7.27	1.48	1.37
25	B	616	CLA	C4C-NC	7.27	1.49	1.37
25	b	616	CLA	C4C-NC	7.28	1.49	1.37
25	b	605	CLA	C4C-NC	7.28	1.49	1.37
25	b	604	CLA	C4C-NC	7.29	1.49	1.37
25	B	615	CLA	C4C-NC	7.30	1.49	1.37
25	B	610	CLA	C4C-NC	7.30	1.49	1.37
25	c	504	CLA	C4C-NC	7.30	1.49	1.37
25	B	608	CLA	C4C-NC	7.31	1.49	1.37
25	C	512	CLA	C4C-NC	7.31	1.49	1.37
25	B	614	CLA	C4C-NC	7.31	1.49	1.37
25	a	610	CLA	C4C-NC	7.31	1.49	1.37
25	b	615	CLA	C4C-NC	7.32	1.49	1.37
25	C	513	CLA	C4C-NC	7.32	1.49	1.37
25	b	610	CLA	C4C-NC	7.32	1.49	1.37
25	A	606	CLA	C4C-NC	7.34	1.49	1.37
25	c	502	CLA	C4C-NC	7.34	1.49	1.37
25	c	509	CLA	C4C-NC	7.34	1.49	1.37
25	B	602	CLA	C4C-NC	7.34	1.49	1.37
25	C	511	CLA	C4C-NC	7.34	1.49	1.37
25	b	614	CLA	C4C-NC	7.35	1.49	1.37
25	C	509	CLA	C4C-NC	7.35	1.49	1.37
25	A	607	CLA	C4C-NC	7.36	1.49	1.37
25	c	510	CLA	C4C-NC	7.36	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	501	CLA	C4C-NC	7.36	1.49	1.37
25	C	502	CLA	C4C-NC	7.36	1.49	1.37
25	C	503	CLA	C4C-NC	7.36	1.49	1.37
25	B	612	CLA	C4C-NC	7.37	1.49	1.37
25	C	510	CLA	C4C-NC	7.37	1.49	1.37
25	A	608	CLA	C4C-NC	7.38	1.49	1.37
25	b	611	CLA	C4C-NC	7.38	1.49	1.37
25	c	513	CLA	C4C-NC	7.38	1.49	1.37
25	b	613	CLA	C4C-NC	7.39	1.49	1.37
25	b	612	CLA	C4C-NC	7.40	1.49	1.37
25	C	508	CLA	C4C-NC	7.40	1.49	1.37
25	c	508	CLA	C4C-NC	7.40	1.49	1.37
25	c	501	CLA	C4C-NC	7.42	1.49	1.37
25	a	608	CLA	C4C-NC	7.43	1.49	1.37
25	B	611	CLA	C4C-NC	7.44	1.49	1.37
25	D	405	CLA	C4C-NC	7.44	1.49	1.37
25	d	403	CLA	C4C-NC	7.45	1.49	1.37
25	c	503	CLA	C4C-NC	7.46	1.49	1.37
25	B	609	CLA	C4C-NC	7.47	1.49	1.37
25	c	511	CLA	C4C-NC	7.52	1.49	1.37

All (1014) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	101	SQD	O9-S-C6	-24.65	85.76	106.83
28	L	101	SQD	O8-S-O9	-12.55	82.59	111.37
28	L	101	SQD	O9-S-O7	-9.20	81.97	113.86
25	b	609	CLA	C1C-NC-C4C	-7.74	102.60	107.06
28	L	103	SQD	C5-C6-S	-7.64	103.70	114.34
25	B	615	CLA	C1C-NC-C4C	-7.63	102.66	107.06
25	C	512	CLA	C1C-NC-C4C	-7.63	102.67	107.06
25	c	503	CLA	C1C-NC-C4C	-7.61	102.68	107.06
25	B	604	CLA	C1C-NC-C4C	-7.57	102.70	107.06
25	b	615	CLA	C1C-NC-C4C	-7.55	102.71	107.06
25	b	604	CLA	C1C-NC-C4C	-7.51	102.74	107.06
25	C	503	CLA	C1C-NC-C4C	-7.50	102.74	107.06
25	c	512	CLA	C1C-NC-C4C	-7.48	102.75	107.06
25	C	507	CLA	C1C-NC-C4C	-7.46	102.77	107.06
25	c	507	CLA	C1C-NC-C4C	-7.44	102.78	107.06
25	b	613	CLA	C1C-NC-C4C	-7.36	102.82	107.06
25	c	511	CLA	C1C-NC-C4C	-7.36	102.82	107.06
25	B	605	CLA	C1C-NC-C4C	-7.36	102.82	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	609	CLA	C1C-NC-C4C	-7.33	102.84	107.06
25	C	506	CLA	C1C-NC-C4C	-7.33	102.84	107.06
25	c	501	CLA	C1C-NC-C4C	-7.30	102.86	107.06
25	C	511	CLA	C1C-NC-C4C	-7.30	102.86	107.06
25	C	501	CLA	C1C-NC-C4C	-7.27	102.87	107.06
25	d	403	CLA	C1C-NC-C4C	-7.26	102.88	107.06
25	c	502	CLA	C1C-NC-C4C	-7.24	102.89	107.06
25	b	616	CLA	C1C-NC-C4C	-7.23	102.90	107.06
25	B	616	CLA	C1C-NC-C4C	-7.22	102.90	107.06
25	b	612	CLA	C1C-NC-C4C	-7.22	102.90	107.06
25	b	611	CLA	C1C-NC-C4C	-7.21	102.91	107.06
25	c	506	CLA	C1C-NC-C4C	-7.20	102.92	107.06
25	c	510	CLA	C1C-NC-C4C	-7.19	102.92	107.06
25	B	601	CLA	C1C-NC-C4C	-7.19	102.92	107.06
25	D	404	CLA	C1C-NC-C4C	-7.19	102.92	107.06
25	b	601	CLA	C1C-NC-C4C	-7.18	102.93	107.06
25	B	610	CLA	C1C-NC-C4C	-7.18	102.93	107.06
25	B	613	CLA	C1C-NC-C4C	-7.18	102.93	107.06
25	A	608	CLA	C1C-NC-C4C	-7.17	102.93	107.06
25	b	610	CLA	C1C-NC-C4C	-7.15	102.94	107.06
25	c	505	CLA	C1C-NC-C4C	-7.15	102.94	107.06
25	B	612	CLA	C1C-NC-C4C	-7.15	102.94	107.06
25	B	606	CLA	C1C-NC-C4C	-7.13	102.95	107.06
25	a	610	CLA	C1C-NC-C4C	-7.13	102.96	107.06
25	B	611	CLA	C1C-NC-C4C	-7.12	102.96	107.06
25	b	606	CLA	C1C-NC-C4C	-7.12	102.96	107.06
25	C	502	CLA	C1C-NC-C4C	-7.11	102.96	107.06
25	C	505	CLA	C1C-NC-C4C	-7.11	102.97	107.06
25	C	509	CLA	C1C-NC-C4C	-7.10	102.97	107.06
25	B	607	CLA	C1C-NC-C4C	-7.10	102.97	107.06
25	B	603	CLA	C1C-NC-C4C	-7.09	102.98	107.06
25	d	401	CLA	C1C-NC-C4C	-7.07	102.99	107.06
25	b	603	CLA	C1C-NC-C4C	-7.07	102.99	107.06
25	c	509	CLA	C1C-NC-C4C	-7.06	102.99	107.06
25	b	605	CLA	C1C-NC-C4C	-7.06	103.00	107.06
25	D	405	CLA	C1C-NC-C4C	-7.05	103.00	107.06
25	b	607	CLA	C1C-NC-C4C	-7.04	103.01	107.06
25	a	606	CLA	C1C-NC-C4C	-7.01	103.02	107.06
25	C	513	CLA	C1C-NC-C4C	-6.97	103.05	107.06
25	c	504	CLA	C1C-NC-C4C	-6.95	103.06	107.06
25	B	614	CLA	C1C-NC-C4C	-6.94	103.06	107.06
25	B	608	CLA	C1C-NC-C4C	-6.91	103.08	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	614	CLA	C1C-NC-C4C	-6.90	103.08	107.06
25	a	608	CLA	C1C-NC-C4C	-6.85	103.11	107.06
25	C	508	CLA	C1C-NC-C4C	-6.83	103.13	107.06
25	b	608	CLA	C1C-NC-C4C	-6.82	103.13	107.06
25	C	510	CLA	C1C-NC-C4C	-6.82	103.14	107.06
25	c	513	CLA	C1C-NC-C4C	-6.82	103.14	107.06
25	C	504	CLA	C1C-NC-C4C	-6.81	103.14	107.06
25	c	508	CLA	C1C-NC-C4C	-6.80	103.15	107.06
25	b	602	CLA	C1C-NC-C4C	-6.78	103.16	107.06
25	D	403	CLA	C1C-NC-C4C	-6.72	103.19	107.06
25	B	602	CLA	C1C-NC-C4C	-6.66	103.23	107.06
25	A	606	CLA	C1C-NC-C4C	-6.65	103.23	107.06
25	A	607	CLA	C1C-NC-C4C	-6.63	103.24	107.06
25	a	607	CLA	C1C-NC-C4C	-6.50	103.31	107.06
26	t	102	BCR	C24-C23-C22	-6.41	116.58	126.21
26	d	404	BCR	C7-C8-C9	-5.88	117.38	126.21
26	t	102	BCR	C20-C21-C22	-5.69	119.19	127.31
26	D	406	BCR	C7-C8-C9	-5.65	117.72	126.21
26	c	521	BCR	C7-C8-C9	-5.34	118.19	126.21
26	h	101	BCR	C7-C8-C9	-5.33	118.20	126.21
26	H	101	BCR	C11-C10-C9	-5.26	119.80	127.31
26	D	406	BCR	C28-C27-C26	-5.25	104.75	113.78
26	b	617	BCR	C28-C27-C26	-5.14	104.93	113.78
26	T	101	BCR	C15-C14-C13	-5.00	120.17	127.31
26	D	406	BCR	C15-C14-C13	-4.99	120.19	127.31
26	T	101	BCR	C7-C8-C9	-4.97	118.75	126.21
26	H	101	BCR	C7-C8-C9	-4.95	118.78	126.21
26	z	101	BCR	C15-C14-C13	-4.94	120.26	127.31
26	C	515	BCR	C15-C14-C13	-4.92	120.28	127.31
26	T	101	BCR	C24-C23-C22	-4.90	118.85	126.21
26	c	521	BCR	C11-C10-C9	-4.88	120.35	127.31
26	h	101	BCR	C11-C10-C9	-4.86	120.38	127.31
26	A	609	BCR	C15-C14-C13	-4.83	120.42	127.31
26	C	522	BCR	C20-C21-C22	-4.83	120.42	127.31
26	k	102	BCR	C33-C5-C6	-4.81	119.12	124.51
26	K	101	BCR	C33-C5-C6	-4.80	119.13	124.51
26	b	618	BCR	C15-C14-C13	-4.74	120.54	127.31
26	t	102	BCR	C15-C14-C13	-4.72	120.57	127.31
26	C	514	BCR	C15-C14-C13	-4.71	120.59	127.31
26	T	101	BCR	C33-C5-C6	-4.66	119.29	124.51
26	C	514	BCR	C11-C10-C9	-4.65	120.67	127.31
26	C	522	BCR	C15-C14-C13	-4.65	120.68	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	102	BCR	C16-C17-C18	-4.63	120.70	127.31
26	C	522	BCR	C11-C10-C9	-4.63	120.71	127.31
26	K	101	BCR	C16-C17-C18	-4.61	120.73	127.31
26	T	101	BCR	C20-C21-C22	-4.61	120.73	127.31
26	H	101	BCR	C16-C17-C18	-4.61	120.74	127.31
26	c	514	BCR	C33-C5-C6	-4.58	119.38	124.51
26	c	521	BCR	C20-C21-C22	-4.57	120.78	127.31
26	T	101	BCR	C11-C10-C9	-4.57	120.78	127.31
26	d	404	BCR	C11-C10-C9	-4.57	120.79	127.31
26	D	406	BCR	C24-C23-C22	-4.54	119.39	126.21
27	D	407	PL9	C7-C8-C9	-4.54	119.12	126.71
34	a	609	PHO	CBD-CHA-C4D	-4.54	103.43	108.54
34	d	402	PHO	CBD-CHA-C4D	-4.53	103.44	108.54
26	B	619	BCR	C15-C14-C13	-4.52	120.86	127.31
26	C	515	BCR	C33-C5-C6	-4.52	119.45	124.51
26	c	514	BCR	C15-C14-C13	-4.51	120.87	127.31
26	t	102	BCR	C33-C5-C6	-4.51	119.46	124.51
26	B	618	BCR	C15-C14-C13	-4.51	120.88	127.31
26	a	611	BCR	C15-C14-C13	-4.49	120.90	127.31
26	B	617	BCR	C15-C14-C13	-4.49	120.91	127.31
26	C	522	BCR	C7-C8-C9	-4.46	119.52	126.21
34	D	401	PHO	CBD-CHA-C4D	-4.44	103.54	108.54
27	A	610	PL9	C7-C8-C9	-4.43	119.30	126.71
26	B	619	BCR	C38-C26-C25	-4.42	119.56	124.51
26	h	101	BCR	C15-C14-C13	-4.42	121.01	127.31
26	B	617	BCR	C28-C27-C26	-4.39	106.24	113.78
26	d	404	BCR	C24-C23-C22	-4.38	119.62	126.21
26	b	617	BCR	C15-C14-C13	-4.38	121.05	127.31
26	b	619	BCR	C16-C17-C18	-4.38	121.06	127.31
26	C	514	BCR	C16-C17-C18	-4.37	121.08	127.31
26	b	617	BCR	C33-C5-C6	-4.36	119.63	124.51
34	D	402	PHO	CBD-CHA-C4D	-4.36	103.63	108.54
26	B	617	BCR	C33-C5-C6	-4.35	119.64	124.51
26	D	406	BCR	C11-C10-C9	-4.34	121.11	127.31
27	d	405	PL9	C7-C8-C9	-4.33	119.47	126.71
26	T	101	BCR	C16-C17-C18	-4.33	121.13	127.31
26	D	406	BCR	C33-C5-C6	-4.32	119.67	124.51
26	c	521	BCR	C24-C23-C22	-4.32	119.72	126.21
26	C	522	BCR	C24-C23-C22	-4.32	119.72	126.21
26	b	619	BCR	C15-C14-C13	-4.32	121.15	127.31
26	B	619	BCR	C7-C8-C9	-4.31	119.73	126.21
26	c	514	BCR	C7-C8-C9	-4.31	119.73	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	521	BCR	C16-C17-C18	-4.28	121.20	127.31
26	c	521	BCR	C15-C14-C13	-4.26	121.23	127.31
26	b	617	BCR	C11-C10-C9	-4.26	121.23	127.31
26	d	404	BCR	C15-C14-C13	-4.24	121.26	127.31
26	b	619	BCR	C38-C26-C25	-4.22	119.78	124.51
26	d	404	BCR	C33-C5-C6	-4.19	119.81	124.51
26	k	102	BCR	C15-C14-C13	-4.18	121.35	127.31
26	b	619	BCR	C7-C8-C9	-4.17	119.95	126.21
26	d	404	BCR	C38-C26-C25	-4.16	119.85	124.51
26	C	515	BCR	C7-C8-C9	-4.15	119.98	126.21
26	H	101	BCR	C15-C14-C13	-4.14	121.40	127.31
26	d	404	BCR	C16-C17-C18	-4.13	121.41	127.31
26	b	619	BCR	C11-C10-C9	-4.12	121.43	127.31
26	b	618	BCR	C28-C27-C26	-4.12	106.70	113.78
26	z	101	BCR	C16-C17-C18	-4.09	121.48	127.31
26	h	101	BCR	C16-C17-C18	-4.07	121.50	127.31
26	H	101	BCR	C20-C21-C22	-4.06	121.52	127.31
26	C	514	BCR	C7-C8-C9	-4.06	120.12	126.21
26	B	617	BCR	C11-C10-C9	-4.05	121.53	127.31
26	b	618	BCR	C16-C17-C18	-4.03	121.56	127.31
26	K	101	BCR	C15-C14-C13	-4.03	121.56	127.31
26	B	619	BCR	C16-C17-C18	-4.02	121.57	127.31
26	B	619	BCR	C11-C10-C9	-4.02	121.58	127.31
26	D	406	BCR	C16-C17-C18	-3.99	121.62	127.31
26	b	618	BCR	C11-C10-C9	-3.98	121.63	127.31
26	C	522	BCR	C16-C17-C18	-3.95	121.68	127.31
26	c	514	BCR	C11-C10-C9	-3.94	121.68	127.31
26	t	102	BCR	C11-C10-C9	-3.94	121.69	127.31
26	z	101	BCR	C11-C10-C9	-3.92	121.72	127.31
27	a	612	PL9	C7-C8-C9	-3.92	120.16	126.71
26	B	618	BCR	C11-C10-C9	-3.85	121.81	127.31
26	z	101	BCR	C20-C21-C22	-3.82	121.85	127.31
26	h	101	BCR	C20-C21-C22	-3.82	121.85	127.31
26	H	101	BCR	C28-C27-C26	-3.81	107.23	113.78
26	h	101	BCR	C24-C23-C22	-3.80	120.50	126.21
26	C	514	BCR	C33-C5-C6	-3.80	120.25	124.51
26	t	102	BCR	C16-C17-C18	-3.78	121.92	127.31
26	b	618	BCR	C3-C4-C5	-3.77	107.29	113.78
26	a	611	BCR	C16-C17-C18	-3.77	121.93	127.31
26	B	618	BCR	C33-C5-C6	-3.73	120.33	124.51
26	H	101	BCR	C24-C23-C22	-3.73	120.61	126.21
26	b	617	BCR	C16-C17-C18	-3.67	122.07	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C24-C23-C22	-3.67	120.70	126.21
26	B	618	BCR	C16-C17-C18	-3.65	122.10	127.31
26	C	514	BCR	C20-C21-C22	-3.63	122.13	127.31
26	z	101	BCR	C24-C23-C22	-3.62	120.77	126.21
26	a	611	BCR	C11-C10-C9	-3.61	122.16	127.31
26	A	609	BCR	C38-C26-C25	-3.60	120.48	124.51
26	b	619	BCR	C24-C23-C22	-3.60	120.81	126.21
26	b	618	BCR	C20-C21-C22	-3.59	122.18	127.31
26	B	618	BCR	C7-C8-C9	-3.59	120.82	126.21
26	B	618	BCR	C24-C23-C22	-3.58	120.84	126.21
26	B	618	BCR	C20-C21-C22	-3.56	122.23	127.31
26	z	101	BCR	C7-C8-C9	-3.54	120.89	126.21
26	B	617	BCR	C24-C23-C22	-3.54	120.89	126.21
26	B	618	BCR	C28-C27-C26	-3.53	107.71	113.78
26	b	619	BCR	C20-C21-C22	-3.52	122.29	127.31
26	z	101	BCR	C33-C5-C6	-3.51	120.58	124.51
26	C	515	BCR	C11-C10-C9	-3.51	122.30	127.31
26	A	609	BCR	C20-C21-C22	-3.50	122.32	127.31
26	A	609	BCR	C16-C17-C18	-3.49	122.33	127.31
26	b	618	BCR	C7-C8-C9	-3.48	120.98	126.21
26	c	521	BCR	C33-C5-C6	-3.47	120.62	124.51
26	D	406	BCR	C20-C21-C22	-3.47	122.36	127.31
26	A	609	BCR	C7-C8-C9	-3.46	121.01	126.21
26	A	609	BCR	C33-C5-C6	-3.46	120.63	124.51
26	B	617	BCR	C16-C17-C18	-3.45	122.39	127.31
26	a	611	BCR	C33-C5-C6	-3.44	120.66	124.51
26	A	609	BCR	C24-C23-C22	-3.40	121.10	126.21
26	a	611	BCR	C38-C26-C25	-3.38	120.72	124.51
26	c	521	BCR	C28-C27-C26	-3.35	108.02	113.78
26	C	522	BCR	C3-C4-C5	-3.35	108.02	113.78
26	C	514	BCR	C24-C23-C22	-3.34	121.20	126.21
26	K	101	BCR	C38-C26-C25	-3.32	120.79	124.51
26	b	617	BCR	C7-C8-C9	-3.32	121.23	126.21
26	A	609	BCR	C11-C10-C9	-3.31	122.58	127.31
26	H	101	BCR	C3-C4-C5	-3.29	108.12	113.78
27	D	407	PL9	C37-C38-C39	-3.26	119.49	127.68
26	k	102	BCR	C38-C26-C25	-3.26	120.86	124.51
26	C	522	BCR	C28-C27-C26	-3.26	108.18	113.78
26	a	611	BCR	C7-C8-C9	-3.26	121.32	126.21
28	a	613	SQD	C5-C6-S	-3.25	109.81	114.34
26	B	619	BCR	C20-C21-C22	-3.22	122.72	127.31
26	a	611	BCR	C20-C21-C22	-3.18	122.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C24-C23-C22	-3.17	121.45	126.21
26	a	611	BCR	C24-C23-C22	-3.17	121.45	126.21
27	a	612	PL9	C37-C38-C39	-3.14	119.78	127.68
26	C	515	BCR	C24-C23-C22	-3.14	121.49	126.21
26	h	101	BCR	C3-C4-C5	-3.13	108.40	113.78
27	d	405	PL9	C37-C38-C39	-3.12	119.83	127.68
26	C	514	BCR	C38-C26-C25	-3.12	121.01	124.51
26	t	102	BCR	C20-C19-C18	-3.11	117.67	126.42
26	b	617	BCR	C20-C21-C22	-3.10	122.89	127.31
26	B	617	BCR	C7-C8-C9	-3.09	121.57	126.21
29	L	102	LHG	C5-O7-C7	-3.09	110.58	117.88
26	B	617	BCR	C20-C21-C22	-3.08	122.92	127.31
26	d	404	BCR	C20-C21-C22	-3.06	122.94	127.31
26	b	618	BCR	C24-C23-C22	-3.05	121.62	126.21
26	c	514	BCR	C16-C17-C18	-3.04	122.97	127.31
26	b	617	BCR	C27-C26-C25	-3.03	118.30	122.74
27	A	610	PL9	C32-C33-C34	-3.02	120.09	127.68
25	B	611	CLA	C1-C2-C3	-3.02	120.39	125.96
26	z	101	BCR	C38-C26-C25	-3.01	121.14	124.51
26	b	619	BCR	C33-C5-C6	-2.99	121.17	124.51
26	K	101	BCR	C24-C23-C22	-2.97	121.75	126.21
26	h	101	BCR	C38-C26-C25	-2.97	121.18	124.51
26	A	609	BCR	C3-C4-C5	-2.96	108.69	113.78
27	A	610	PL9	C22-C23-C24	-2.95	120.26	127.68
27	d	405	PL9	C27-C28-C29	-2.95	120.26	127.68
26	C	515	BCR	C20-C21-C22	-2.94	123.11	127.31
27	A	610	PL9	C37-C38-C39	-2.93	120.31	127.68
25	b	611	CLA	C1-C2-C3	-2.93	120.55	125.96
29	a	616	LHG	C5-O7-C7	-2.88	111.07	117.88
25	c	510	CLA	C1-C2-C3	-2.87	120.66	125.96
29	l	101	LHG	C5-O7-C7	-2.87	111.10	117.88
33	c	515	DGD	C2G-O2G-C1B	-2.85	111.13	117.88
26	C	522	BCR	C33-C5-C6	-2.84	121.33	124.51
26	k	102	BCR	C24-C23-C22	-2.83	121.97	126.21
26	C	515	BCR	C15-C16-C17	-2.81	117.45	123.46
23	a	614	LMG	C8-O7-C10	-2.81	111.25	117.88
26	B	619	BCR	C1-C6-C5	-2.80	118.66	122.59
29	d	406	LHG	C5-O7-C7	-2.80	111.27	117.88
26	b	617	BCR	C24-C23-C22	-2.80	122.01	126.21
26	D	406	BCR	C38-C26-C25	-2.78	121.40	124.51
26	D	406	BCR	C27-C26-C25	-2.76	118.69	122.74
27	D	407	PL9	C27-C28-C29	-2.76	120.76	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	612	PL9	C22-C23-C24	-2.75	120.78	127.68
25	B	616	CLA	C1-C2-C3	-2.75	120.90	125.96
27	a	612	PL9	C17-C18-C19	-2.75	120.78	127.68
27	A	610	PL9	C17-C18-C19	-2.74	120.80	127.68
26	C	515	BCR	C16-C17-C18	-2.74	123.40	127.31
23	A	612	LMG	C8-O7-C10	-2.73	111.42	117.88
25	C	510	CLA	C1-C2-C3	-2.73	120.92	125.96
33	C	516	DGD	C2G-O2G-C1B	-2.73	111.42	117.88
25	c	502	CLA	C1-C2-C3	-2.73	120.94	125.96
27	a	612	PL9	C42-C43-C44	-2.73	120.83	127.68
25	C	502	CLA	C1-C2-C3	-2.73	120.94	125.96
29	D	408	LHG	C5-O7-C7	-2.72	111.45	117.88
23	c	520	LMG	C8-O7-C10	-2.71	111.47	117.88
28	F	101	SQD	C5-C6-S	-2.71	110.56	114.34
23	B	624	LMG	C8-O7-C10	-2.68	111.53	117.88
26	B	618	BCR	C38-C26-C25	-2.67	121.52	124.51
26	c	514	BCR	C20-C21-C22	-2.67	123.50	127.31
27	A	610	PL9	C42-C43-C44	-2.65	121.02	127.68
23	b	624	LMG	C8-O7-C10	-2.65	111.61	117.88
26	k	102	BCR	C11-C10-C9	-2.64	123.55	127.31
26	k	102	BCR	C8-C7-C6	-2.63	119.88	127.25
27	a	612	PL9	C32-C33-C34	-2.63	121.07	127.68
25	A	606	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
26	C	515	BCR	C38-C26-C25	-2.63	121.56	124.51
27	d	405	PL9	C17-C18-C19	-2.63	121.08	127.68
23	d	408	LMG	C8-O7-C10	-2.62	111.67	117.88
25	c	503	CLA	C1-C2-C3	-2.62	121.12	125.96
25	b	610	CLA	C1-C2-C3	-2.62	121.13	125.96
25	b	602	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
25	a	607	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
26	h	101	BCR	C33-C5-C6	-2.60	121.60	124.51
27	A	610	PL9	C12-C13-C14	-2.60	121.15	127.68
29	a	615	LHG	C5-O7-C7	-2.59	111.76	117.88
26	H	101	BCR	C33-C5-C6	-2.58	121.62	124.51
26	K	101	BCR	C8-C7-C6	-2.58	120.04	127.25
26	a	611	BCR	C3-C4-C5	-2.57	109.36	113.78
27	a	612	PL9	C27-C28-C29	-2.57	121.22	127.68
25	B	610	CLA	C1-C2-C3	-2.56	121.24	125.96
27	d	405	PL9	C22-C23-C24	-2.56	121.26	127.68
25	B	602	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
34	d	402	PHO	C1-C2-C3	-2.55	121.26	125.96
28	f	101	SQD	C45-O47-C7	-2.55	111.86	117.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	C3D-CAD-CBD	-2.54	104.00	107.60
25	a	606	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
26	h	101	BCR	C28-C27-C26	-2.53	109.43	113.78
26	B	619	BCR	C3-C4-C5	-2.52	109.44	113.78
28	F	101	SQD	C45-O47-C7	-2.52	111.92	117.88
25	b	604	CLA	CHC-C1C-C2C	-2.52	119.78	126.65
25	B	603	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	D	409	LMG	C8-O7-C10	-2.51	111.94	117.88
25	c	503	CLA	C3D-CAD-CBD	-2.51	104.05	107.60
35	E	102	HEM	CMA-C3A-C4A	-2.51	124.61	128.46
25	B	604	CLA	CHC-C1C-C2C	-2.50	119.82	126.65
26	c	514	BCR	C15-C16-C17	-2.50	118.13	123.46
26	c	521	BCR	C3-C4-C5	-2.48	109.51	113.78
25	b	614	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
28	a	613	SQD	C45-O47-C7	-2.48	112.01	117.88
27	D	407	PL9	C22-C23-C24	-2.48	121.46	127.68
25	D	403	CLA	C1-C2-C3	-2.47	121.40	125.96
26	K	101	BCR	C20-C21-C22	-2.47	123.79	127.31
25	B	607	CLA	C1-C2-C3	-2.46	121.42	125.96
35	e	101	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
25	D	403	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
25	C	506	CLA	C1-C2-C3	-2.45	121.44	125.96
27	D	407	PL9	C17-C18-C19	-2.45	121.52	127.68
26	b	619	BCR	C3-C4-C5	-2.45	109.57	113.78
25	c	507	CLA	C3D-CAD-CBD	-2.45	104.14	107.60
25	B	607	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
25	B	604	CLA	C3D-CAD-CBD	-2.44	104.15	107.60
26	K	101	BCR	C7-C8-C9	-2.44	122.55	126.21
26	B	617	BCR	C27-C26-C25	-2.44	119.16	122.74
26	A	609	BCR	C15-C16-C17	-2.44	118.26	123.46
29	E	101	LHG	C5-O7-C7	-2.44	112.12	117.88
25	a	608	CLA	CHC-C1C-C2C	-2.44	120.01	126.65
25	b	608	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
26	t	102	BCR	C3-C4-C5	-2.43	109.61	113.78
23	a	603	LMG	C8-O7-C10	-2.43	112.14	117.88
27	D	407	PL9	C12-C13-C14	-2.42	121.59	127.68
25	B	608	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	d	405	PL9	C12-C13-C14	-2.41	121.63	127.68
28	f	101	SQD	C5-C6-S	-2.41	110.98	114.34
26	c	514	BCR	C21-C20-C19	-2.40	115.86	123.23
25	b	604	CLA	C3D-CAD-CBD	-2.40	104.20	107.60
26	k	102	BCR	C23-C24-C25	-2.40	120.53	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C10-C11-C12	-2.40	115.87	123.23
27	A	610	PL9	C7-C3-C2	-2.40	119.82	123.23
25	c	513	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
25	C	508	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
25	d	401	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
25	c	504	CLA	CHC-C1C-C2C	-2.39	120.14	126.65
25	A	608	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
25	a	608	CLA	C1-C2-C3	-2.39	121.56	125.96
28	F	101	SQD	C44-O6-C1	-2.38	108.88	113.76
26	C	515	BCR	C21-C20-C19	-2.38	115.93	123.23
26	k	102	BCR	C20-C21-C22	-2.38	123.92	127.31
25	c	507	CLA	C1-C2-C3	-2.38	121.58	125.96
25	B	607	CLA	CHC-C1C-C2C	-2.38	120.17	126.65
27	A	610	PL9	C27-C28-C29	-2.37	121.71	127.68
25	a	610	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	c	506	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	B	614	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	C	521	LMG	O2-C2-C3	-2.37	105.20	110.36
25	D	404	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
26	T	101	BCR	C28-C27-C26	-2.37	109.71	113.78
25	B	604	CLA	C1-C2-C3	-2.37	121.59	125.96
25	b	601	CLA	C3D-CAD-CBD	-2.37	104.25	107.60
26	t	102	BCR	C28-C27-C26	-2.36	109.72	113.78
25	b	613	CLA	C3D-CAD-CBD	-2.36	104.26	107.60
25	B	613	CLA	CHC-C1C-C2C	-2.36	120.21	126.65
25	b	607	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	C	505	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	b	605	CLA	C3D-CAD-CBD	-2.36	104.26	107.60
25	C	505	CLA	C3D-CAD-CBD	-2.36	104.26	107.60
23	b	620	LMG	C8-O7-C10	-2.36	112.31	117.88
26	B	619	BCR	C33-C5-C6	-2.36	121.87	124.51
25	c	505	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
25	C	511	CLA	CHC-C1C-C2C	-2.35	120.23	126.65
25	B	601	CLA	C3D-CAD-CBD	-2.35	104.27	107.60
25	c	511	CLA	C3D-CAD-CBD	-2.35	104.27	107.60
26	C	522	BCR	C15-C16-C17	-2.35	118.45	123.46
25	b	606	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	C	501	CLA	CHC-C1C-C2C	-2.35	120.25	126.65
25	B	615	CLA	CHC-C1C-C2C	-2.35	120.25	126.65
25	C	507	CLA	C3D-CAD-CBD	-2.34	104.28	107.60
27	d	405	PL9	C32-C33-C34	-2.34	121.79	127.68
25	b	609	CLA	C3D-CAD-CBD	-2.34	104.29	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	512	CLA	C3D-CAD-CBD	-2.34	104.29	107.60
25	C	507	CLA	CHC-C1C-C2C	-2.34	120.27	126.65
25	B	613	CLA	C3D-CAD-CBD	-2.34	104.30	107.60
25	b	603	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
25	b	602	CLA	C1-C2-C3	-2.33	121.66	125.96
35	v	201	HEM	CMA-C3A-C4A	-2.33	124.88	128.46
27	a	612	PL9	C12-C13-C14	-2.33	121.82	127.68
26	t	102	BCR	C8-C7-C6	-2.33	120.72	127.25
26	k	102	BCR	C16-C15-C14	-2.33	118.49	123.46
25	B	605	CLA	C3D-CAD-CBD	-2.33	104.31	107.60
25	c	501	CLA	CHC-C1C-C2C	-2.32	120.31	126.65
25	C	512	CLA	CHC-C1C-C2C	-2.32	120.31	126.65
25	C	504	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
25	C	509	CLA	C3D-CAD-CBD	-2.32	104.31	107.60
25	B	606	CLA	CHC-C1C-C2C	-2.32	120.32	126.65
26	k	102	BCR	C7-C8-C9	-2.32	122.72	126.21
25	A	606	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
25	c	512	CLA	CHC-C1C-C2C	-2.32	120.32	126.65
25	B	613	CLA	C1-C2-C3	-2.32	121.69	125.96
25	C	503	CLA	CHC-C1C-C2C	-2.32	120.33	126.65
25	A	607	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
25	d	403	CLA	CHC-C1C-C2C	-2.31	120.34	126.65
25	C	509	CLA	CHC-C1C-C2C	-2.31	120.34	126.65
25	B	605	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
25	b	609	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
25	B	605	CLA	CHC-C1C-C2C	-2.31	120.35	126.65
25	b	606	CLA	CHC-C1C-C2C	-2.31	120.35	126.65
25	B	612	CLA	C1-C2-C3	-2.31	121.70	125.96
35	V	201	HEM	CMA-C3A-C4A	-2.31	124.92	128.46
25	D	405	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
33	C	517	DGD	C2G-O2G-C1B	-2.31	112.43	117.88
27	D	407	PL9	C32-C33-C34	-2.31	121.89	127.68
25	c	513	CLA	CHC-C1C-C2C	-2.30	120.36	126.65
25	C	513	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
25	B	615	CLA	C3D-CAD-CBD	-2.30	104.34	107.60
25	b	607	CLA	CHC-C1C-C2C	-2.30	120.37	126.65
25	C	513	CLA	CHC-C1C-C2C	-2.30	120.37	126.65
25	C	504	CLA	CHC-C1C-C2C	-2.30	120.37	126.65
25	C	511	CLA	C3D-CAD-CBD	-2.30	104.35	107.60
25	c	501	CLA	C1-C2-C3	-2.29	121.73	125.96
25	C	512	CLA	C3D-CAD-CBD	-2.29	104.36	107.60
25	c	511	CLA	CHC-C1C-C2C	-2.29	120.40	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	608	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
25	C	510	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
25	B	601	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
26	B	617	BCR	C38-C26-C25	-2.29	121.95	124.51
26	t	102	BCR	C11-C12-C13	-2.29	120.00	126.42
25	c	510	CLA	CHC-C1C-C2C	-2.29	120.42	126.65
25	c	505	CLA	C3D-CAD-CBD	-2.28	104.37	107.60
25	c	508	CLA	C3D-CAD-CBD	-2.28	104.37	107.60
25	b	612	CLA	C3D-CAD-CBD	-2.28	104.37	107.60
25	B	616	CLA	CHC-C1C-C2C	-2.28	120.42	126.65
25	B	611	CLA	CHC-C1C-C2C	-2.28	120.42	126.65
25	B	609	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
26	T	101	BCR	C20-C19-C18	-2.28	120.01	126.42
25	c	509	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
25	C	503	CLA	C1-C2-C3	-2.28	121.76	125.96
25	B	606	CLA	C1-C2-C3	-2.28	121.76	125.96
25	B	603	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
26	b	619	BCR	C23-C24-C25	-2.28	120.87	127.25
23	c	518	LMG	C8-O7-C10	-2.28	112.49	117.88
25	b	603	CLA	CHC-C1C-C2C	-2.28	120.44	126.65
26	c	514	BCR	C38-C26-C25	-2.28	121.96	124.51
26	K	101	BCR	C23-C24-C25	-2.28	120.88	127.25
25	b	613	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
25	c	508	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
27	d	405	PL9	C42-C43-C44	-2.27	121.97	127.68
25	b	613	CLA	CHC-C1C-C2C	-2.27	120.45	126.65
34	D	401	PHO	C2B-C1B-NB	-2.27	106.46	109.82
25	d	401	CLA	C3D-CAD-CBD	-2.27	104.39	107.60
25	B	609	CLA	C3D-CAD-CBD	-2.27	104.39	107.60
25	c	509	CLA	C3D-CAD-CBD	-2.27	104.39	107.60
25	D	404	CLA	C3D-CAD-CBD	-2.27	104.39	107.60
25	D	403	CLA	CHC-C1C-C2C	-2.27	120.47	126.65
26	k	102	BCR	C10-C11-C12	-2.27	116.28	123.23
26	k	102	BCR	C21-C20-C19	-2.27	116.28	123.23
26	k	102	BCR	C28-C27-C26	-2.26	109.89	113.78
25	b	615	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
25	B	606	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	c	510	CLA	C3D-CAD-CBD	-2.26	104.40	107.60
25	a	606	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
33	C	518	DGD	C2G-O2G-C1B	-2.26	112.54	117.88
25	c	503	CLA	CHC-C1C-C2C	-2.26	120.49	126.65
25	b	611	CLA	CHC-C1C-C2C	-2.26	120.50	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	506	CLA	C3D-CAD-CBD	-2.26	104.41	107.60
25	C	506	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
29	A	613	LHG	C5-O7-C7	-2.25	112.55	117.88
25	b	605	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
25	D	405	CLA	CHC-C1C-C2C	-2.25	120.52	126.65
25	C	502	CLA	CHC-C1C-C2C	-2.25	120.52	126.65
25	B	612	CLA	C3D-CAD-CBD	-2.25	104.42	107.60
25	C	501	CLA	C1-C2-C3	-2.25	121.82	125.96
25	c	504	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
25	c	508	CLA	C1-C2-C3	-2.24	121.82	125.96
34	D	402	PHO	C1-C2-C3	-2.24	121.82	125.96
25	B	614	CLA	C3D-CAD-CBD	-2.24	104.42	107.60
25	b	615	CLA	CHC-C1C-C2C	-2.24	120.53	126.65
25	b	614	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
25	c	507	CLA	CHC-C1C-C2C	-2.24	120.53	126.65
25	D	405	CLA	CMB-C2B-C1B	-2.24	125.02	128.46
25	b	606	CLA	C3D-CAD-CBD	-2.24	104.43	107.60
25	B	611	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
25	b	616	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
26	T	101	BCR	C3-C4-C5	-2.24	109.94	113.78
25	c	502	CLA	CHC-C1C-C2C	-2.23	120.56	126.65
25	A	606	CLA	C4A-NA-C1A	-2.23	103.68	106.45
25	d	403	CLA	C3D-CAD-CBD	-2.23	104.44	107.60
26	B	617	BCR	C8-C7-C6	-2.23	121.01	127.25
25	b	602	CLA	C4A-NA-C1A	-2.23	103.69	106.45
25	b	601	CLA	CHC-C1C-C2C	-2.23	120.57	126.65
25	A	606	CLA	C3D-CAD-CBD	-2.23	104.45	107.60
25	a	607	CLA	C1-C2-C3	-2.23	121.86	125.96
25	B	609	CLA	CHC-C1C-C2C	-2.22	120.58	126.65
25	c	502	CLA	C3D-CAD-CBD	-2.22	104.45	107.60
25	b	607	CLA	C3D-CAD-CBD	-2.22	104.46	107.60
25	c	506	CLA	C1-C2-C3	-2.22	121.87	125.96
25	C	508	CLA	C1-C2-C3	-2.22	121.87	125.96
25	A	607	CLA	C1-C2-C3	-2.22	121.87	125.96
25	C	508	CLA	CHC-C1C-C2C	-2.22	120.61	126.65
28	A	611	SQD	C45-O47-C7	-2.21	112.64	117.88
33	c	517	DGD	C2G-O2G-C1B	-2.21	112.64	117.88
25	b	609	CLA	CHC-C1C-C2C	-2.21	120.62	126.65
25	A	608	CLA	CHC-C1C-C2C	-2.21	120.62	126.65
25	b	612	CLA	CHC-C1C-C2C	-2.21	120.62	126.65
25	B	603	CLA	C1-C2-C3	-2.21	121.89	125.96
25	c	506	CLA	C3D-CAD-CBD	-2.21	104.48	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	608	CLA	CHC-C1C-C2C	-2.21	120.63	126.65
25	c	504	CLA	C3D-CAD-CBD	-2.21	104.48	107.60
26	b	617	BCR	C23-C24-C25	-2.21	121.08	127.25
23	B	620	LMG	C8-O7-C10	-2.20	112.67	117.88
25	a	607	CLA	CHC-C1C-C2C	-2.20	120.64	126.65
25	a	610	CLA	CHC-C1C-C2C	-2.20	120.64	126.65
25	b	607	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
25	b	610	CLA	C3D-CAD-CBD	-2.20	104.48	107.60
25	c	506	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
25	B	601	CLA	CHC-C1C-C2C	-2.20	120.66	126.65
34	D	402	PHO	C2B-C1B-NB	-2.20	106.57	109.82
25	c	508	CLA	CHC-C1C-C2C	-2.19	120.67	126.65
25	a	606	CLA	C3D-CAD-CBD	-2.19	104.50	107.60
25	B	602	CLA	C3D-CAD-CBD	-2.19	104.50	107.60
25	B	616	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
25	B	610	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
26	b	618	BCR	C15-C16-C17	-2.19	118.79	123.46
26	B	617	BCR	C15-C16-C17	-2.19	118.79	123.46
25	C	510	CLA	C3D-CAD-CBD	-2.19	104.50	107.60
34	d	402	PHO	C2B-C1B-NB	-2.19	106.58	109.82
25	b	611	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
25	A	607	CLA	CHC-C1C-C2C	-2.19	120.68	126.65
25	C	510	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
25	c	501	CLA	C3D-CAD-CBD	-2.19	104.50	107.60
25	B	606	CLA	C3D-CAD-CBD	-2.19	104.51	107.60
26	z	101	BCR	C15-C16-C17	-2.19	118.80	123.46
25	a	606	CLA	CHC-C1C-C2C	-2.19	120.69	126.65
25	C	508	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
23	A	603	LMG	C8-O7-C10	-2.18	112.72	117.88
26	B	619	BCR	C4-C5-C6	-2.18	119.54	122.74
25	A	606	CLA	CHC-C1C-C2C	-2.18	120.70	126.65
25	C	506	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
25	C	504	CLA	C3D-CAD-CBD	-2.18	104.51	107.60
25	B	611	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
25	a	610	CLA	C3D-CAD-CBD	-2.18	104.51	107.60
25	b	608	CLA	C1-C2-C3	-2.18	121.94	125.96
27	D	407	PL9	C42-C43-C44	-2.18	122.20	127.68
25	C	506	CLA	CHC-C1C-C2C	-2.18	120.71	126.65
25	b	611	CLA	C3D-CAD-CBD	-2.18	104.52	107.60
25	c	508	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
25	C	502	CLA	C3D-CAD-CBD	-2.17	104.53	107.60
25	b	613	CLA	C1-C2-C3	-2.17	121.96	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	601	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
26	B	619	BCR	C23-C24-C25	-2.17	121.18	127.25
25	B	607	CLA	C3D-CAD-CBD	-2.17	104.53	107.60
25	b	603	CLA	C3D-CAD-CBD	-2.17	104.53	107.60
25	b	612	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
25	B	603	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
25	b	610	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
25	c	507	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
25	b	605	CLA	CHC-C1C-C2C	-2.16	120.75	126.65
25	C	510	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
25	D	405	CLA	C3D-CAD-CBD	-2.16	104.54	107.60
25	b	612	CLA	C1-C2-C3	-2.16	121.98	125.96
25	B	610	CLA	CHC-C1C-C2C	-2.16	120.76	126.65
25	B	615	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
25	B	616	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
25	b	604	CLA	C1-C2-C3	-2.16	121.98	125.96
25	C	513	CLA	C1-C2-C3	-2.16	121.98	125.96
23	C	519	LMG	C8-O7-C10	-2.16	112.78	117.88
25	B	611	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
25	C	508	CLA	C3D-CAD-CBD	-2.15	104.55	107.60
25	b	615	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
25	D	404	CLA	C1-C2-C3	-2.15	121.99	125.96
25	C	501	CLA	C3D-CAD-CBD	-2.15	104.56	107.60
25	C	502	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
25	B	608	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
25	b	616	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
25	B	608	CLA	CHC-C1C-C2C	-2.15	120.79	126.65
25	b	616	CLA	CHC-C1C-C2C	-2.15	120.79	126.65
25	B	614	CLA	CMB-C2B-C1B	-2.15	125.17	128.46
25	D	405	CLA	C1-C2-C3	-2.14	122.00	125.96
25	b	604	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
26	t	102	BCR	C35-C13-C14	-2.14	119.92	122.92
25	a	606	CLA	C4A-NA-C1A	-2.14	103.80	106.45
25	C	512	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
25	B	610	CLA	C3D-CAD-CBD	-2.14	104.57	107.60
25	C	513	CLA	C3D-CAD-CBD	-2.14	104.58	107.60
25	C	504	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
25	B	612	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
26	K	101	BCR	C21-C20-C19	-2.13	116.68	123.23
27	a	612	PL9	C7-C3-C2	-2.13	120.19	123.23
25	B	603	CLA	C3D-CAD-CBD	-2.13	104.58	107.60
25	c	503	CLA	C1B-CHB-C4A	-2.13	125.89	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
25	b	602	CLA	C3D-CAD-CBD	-2.13	104.58	107.60
25	b	614	CLA	C4A-NA-C1A	-2.13	103.81	106.45
25	B	614	CLA	CHC-C1C-C2C	-2.13	120.84	126.65
25	c	513	CLA	C3D-CAD-CBD	-2.13	104.59	107.60
26	c	514	BCR	C28-C27-C26	-2.13	110.12	113.78
25	A	608	CLA	C3D-CAD-CBD	-2.13	104.59	107.60
25	B	613	CLA	CMB-C2B-C1B	-2.13	125.20	128.46
25	C	501	CLA	CMB-C2B-C1B	-2.13	125.20	128.46
25	B	612	CLA	CHC-C1C-C2C	-2.13	120.85	126.65
26	b	617	BCR	C3-C4-C5	-2.12	110.13	113.78
25	c	510	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
25	a	607	CLA	C3D-CAD-CBD	-2.12	104.59	107.60
25	b	610	CLA	CHC-C1C-C2C	-2.12	120.86	126.65
25	c	501	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
25	a	610	CLA	C1-C2-C3	-2.12	122.05	125.96
25	b	608	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
26	K	101	BCR	C16-C15-C14	-2.12	118.94	123.46
25	d	403	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
25	c	504	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
28	a	613	SQD	O48-C23-O10	-2.11	118.31	123.55
25	B	616	CLA	C4A-NA-C1A	-2.11	103.83	106.45
25	a	607	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
26	T	101	BCR	C35-C13-C14	-2.11	119.97	122.92
25	b	616	CLA	C3D-CAD-CBD	-2.11	104.61	107.60
25	C	503	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
33	H	102	DGD	C2G-O2G-C1B	-2.11	112.89	117.88
25	d	401	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
25	c	512	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
25	c	509	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
25	B	602	CLA	CHC-C1C-C2C	-2.10	120.92	126.65
25	c	511	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
25	D	403	CLA	C3D-CAD-CBD	-2.10	104.62	107.60
26	C	514	BCR	C8-C7-C6	-2.10	121.37	127.25
25	b	614	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
25	d	403	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
25	C	509	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
25	c	506	CLA	CHC-C1C-C2C	-2.10	120.93	126.65
25	A	607	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
25	c	502	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
26	C	514	BCR	C11-C12-C13	-2.09	120.53	126.42
26	B	618	BCR	C15-C16-C17	-2.09	119.00	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	607	CLA	C3D-CAD-CBD	-2.09	104.64	107.60
25	C	507	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
26	t	102	BCR	C7-C6-C5	-2.09	116.56	121.54
26	H	101	BCR	C11-C12-C13	-2.09	120.55	126.42
25	B	616	CLA	C3D-CAD-CBD	-2.09	104.64	107.60
25	d	401	CLA	C1-C2-C3	-2.09	122.11	125.96
25	C	513	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
25	c	510	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
25	B	613	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
25	B	609	CLA	C1-C2-C3	-2.08	122.12	125.96
25	c	501	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
25	B	604	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
26	C	515	BCR	C8-C7-C6	-2.08	121.44	127.25
26	C	514	BCR	C3-C4-C5	-2.08	110.21	113.78
25	B	609	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
26	d	404	BCR	C11-C12-C13	-2.07	120.60	126.42
25	C	512	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
25	b	607	CLA	C1-C2-C3	-2.07	122.14	125.96
25	D	404	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
26	H	101	BCR	C34-C9-C10	-2.07	120.03	122.92
26	b	618	BCR	C33-C5-C6	-2.06	122.20	124.51
25	b	602	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
26	A	609	BCR	C8-C7-C6	-2.06	121.48	127.25
25	C	507	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
25	a	607	CLA	C4A-NA-C1A	-2.06	103.90	106.45
26	b	618	BCR	C38-C26-C25	-2.06	122.20	124.51
25	b	609	CLA	C1-C2-C3	-2.06	122.16	125.96
25	b	610	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
25	B	602	CLA	CAA-C2A-C1A	-2.06	105.23	111.97
25	b	602	CLA	CHC-C1C-C2C	-2.06	121.04	126.65
25	A	608	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
23	c	520	LMG	O8-C28-O10	-2.06	118.44	123.55
25	b	614	CLA	CHC-C1C-C2C	-2.06	121.04	126.65
25	c	505	CLA	CHC-C1C-C2C	-2.06	121.04	126.65
26	C	522	BCR	C38-C26-C25	-2.05	122.21	124.51
26	b	617	BCR	C8-C7-C6	-2.05	121.50	127.25
25	C	502	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
25	C	509	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
25	C	501	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
25	c	509	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
26	D	406	BCR	C3-C4-C5	-2.05	110.26	113.78
26	h	101	BCR	C34-C9-C10	-2.05	120.05	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C28-C27-C26	-2.05	110.26	113.78
25	C	505	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
26	D	406	BCR	C23-C24-C25	-2.04	121.53	127.25
25	B	614	CLA	C4A-NA-C1A	-2.04	103.92	106.45
25	B	607	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
25	B	610	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
25	c	502	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
25	a	608	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
25	B	602	CLA	C4A-NA-C1A	-2.04	103.92	106.45
25	b	616	CLA	C4A-NA-C1A	-2.04	103.92	106.45
26	b	618	BCR	C21-C20-C19	-2.04	116.98	123.23
25	C	511	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
25	C	505	CLA	CHC-C1C-C2C	-2.04	121.10	126.65
26	d	404	BCR	C3-C4-C5	-2.04	110.28	113.78
25	C	511	CLA	C1-C2-C3	-2.04	122.21	125.96
25	b	605	CLA	CMB-C2B-C1B	-2.04	125.34	128.46
26	h	101	BCR	C39-C30-C25	-2.04	107.01	110.31
25	b	613	CLA	C1B-CHB-C4A	-2.04	126.09	130.12
26	t	102	BCR	C37-C22-C21	-2.03	120.07	122.92
25	a	610	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
26	d	404	BCR	C23-C24-C25	-2.03	121.56	127.25
25	b	603	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
25	B	601	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
25	a	608	CLA	C3D-CAD-CBD	-2.03	104.73	107.60
25	D	403	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
25	b	606	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
25	b	611	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
26	T	101	BCR	C11-C12-C13	-2.02	120.73	126.42
25	D	404	CLA	CHC-C1C-C2C	-2.02	121.13	126.65
25	c	503	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
26	B	617	BCR	C39-C30-C25	-2.02	107.03	110.31
25	B	602	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
28	A	611	SQD	O48-C23-O10	-2.02	118.54	123.55
25	D	403	CLA	C4A-NA-C1A	-2.02	103.95	106.45
25	c	512	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
23	a	603	LMG	O8-C28-O10	-2.02	118.54	123.55
25	d	401	CLA	CHC-C1C-C2C	-2.02	121.15	126.65
26	b	618	BCR	C23-C24-C25	-2.02	121.61	127.25
26	c	521	BCR	C16-C15-C14	-2.02	119.16	123.46
25	b	615	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
25	B	610	CLA	C4A-NA-C1A	-2.01	103.95	106.45
25	b	612	CLA	C1B-CHB-C4A	-2.01	126.13	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	605	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
25	c	513	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
25	c	505	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
25	c	507	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
26	a	611	BCR	C8-C7-C6	-2.01	121.63	127.25
26	C	522	BCR	C10-C11-C12	-2.01	117.07	123.23
25	B	602	CLA	C1-C2-C3	-2.01	122.26	125.96
25	B	606	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
28	L	103	SQD	C46-C45-C44	-2.00	107.33	111.86
25	b	608	CLA	C3D-CAD-CBD	-2.00	104.76	107.60
26	C	514	BCR	C23-C24-C25	-2.00	121.64	127.25
25	b	601	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
25	B	612	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
28	A	611	SQD	C5-C6-S	-2.00	111.55	114.34
35	e	101	HEM	C4A-C3A-C2A	2.01	108.39	107.00
23	a	603	LMG	O6-C5-C4	2.02	113.38	109.66
34	a	609	PHO	C4A-NA-C1A	2.02	109.80	108.16
26	c	521	BCR	C38-C26-C27	2.04	117.32	113.45
35	v	201	HEM	CMC-C2C-C3C	2.06	128.71	124.89
26	C	515	BCR	C36-C18-C19	2.06	121.38	118.10
26	B	618	BCR	C33-C5-C4	2.09	117.42	113.45
26	K	101	BCR	C33-C5-C4	2.11	117.45	113.45
27	d	405	PL9	C51-C49-C50	2.12	119.55	114.60
33	C	516	DGD	O6D-C5D-C6D	2.12	110.87	106.64
26	b	618	BCR	C33-C5-C4	2.12	117.48	113.45
27	d	405	PL9	C40-C39-C41	2.12	118.97	115.29
26	h	101	BCR	C33-C5-C4	2.13	117.48	113.45
35	V	201	HEM	C4C-C3C-C2C	2.15	108.40	106.90
26	C	522	BCR	C38-C26-C27	2.15	117.53	113.45
35	e	101	HEM	CMC-C2C-C3C	2.16	128.91	124.89
26	k	102	BCR	C33-C5-C4	2.18	117.58	113.45
28	a	613	SQD	O6-C1-C2	2.18	111.80	108.23
27	A	610	PL9	C51-C49-C50	2.19	119.72	114.60
27	D	407	PL9	C51-C49-C50	2.21	119.76	114.60
28	A	611	SQD	O8-S-C6	2.22	108.72	106.01
26	b	618	BCR	C29-C30-C25	2.22	113.95	110.48
27	a	612	PL9	C35-C34-C36	2.23	119.15	115.29
26	H	101	BCR	C33-C5-C4	2.23	117.68	113.45
26	b	617	BCR	C33-C5-C4	2.24	117.70	113.45
28	F	101	SQD	O8-S-C6	2.25	108.75	106.01
26	H	101	BCR	C38-C26-C27	2.25	117.72	113.45
26	D	406	BCR	C33-C5-C4	2.25	117.72	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	617	BCR	C33-C5-C4	2.25	117.73	113.45
26	d	404	BCR	C33-C5-C4	2.26	117.73	113.45
27	a	612	PL9	C51-C49-C50	2.26	119.87	114.60
27	a	612	PL9	C30-C29-C31	2.26	119.21	115.29
26	K	101	BCR	C38-C26-C27	2.26	117.74	113.45
34	D	402	PHO	CBD-CHA-C1A	2.27	131.70	126.36
23	a	603	LMG	C3-C4-C5	2.27	114.21	110.22
26	b	619	BCR	C38-C26-C27	2.29	117.80	113.45
26	h	101	BCR	C29-C30-C25	2.29	114.06	110.48
27	a	612	PL9	C10-C9-C11	2.29	119.27	115.29
26	t	102	BCR	C33-C5-C4	2.33	117.87	113.45
26	b	618	BCR	C38-C26-C27	2.33	117.87	113.45
28	F	101	SQD	O48-C23-C24	2.34	118.69	111.90
27	d	405	PL9	C10-C9-C11	2.35	119.36	115.29
34	D	401	PHO	CBD-CHA-C1A	2.35	131.90	126.36
34	d	402	PHO	CBD-CHA-C1A	2.35	131.90	126.36
26	a	611	BCR	C33-C5-C4	2.36	117.92	113.45
23	d	408	LMG	O8-C28-C29	2.36	118.77	111.90
27	A	610	PL9	C35-C34-C36	2.36	119.39	115.29
26	c	514	BCR	C33-C5-C4	2.39	117.99	113.45
34	d	402	PHO	C3D-C4D-CHA	2.39	116.16	109.97
34	D	402	PHO	C3D-C4D-CHA	2.40	116.18	109.97
34	a	609	PHO	CBD-CHA-C1A	2.40	132.02	126.36
25	D	404	CLA	C2C-C1C-NC	2.41	111.88	110.22
34	a	609	PHO	C3D-C4D-CHA	2.41	116.20	109.97
33	c	515	DGD	O6D-C5D-C6D	2.43	111.48	106.64
26	C	515	BCR	C33-C5-C4	2.43	118.06	113.45
25	d	401	CLA	C2C-C1C-NC	2.43	111.90	110.22
26	B	618	BCR	C38-C26-C27	2.44	118.08	113.45
25	C	505	CLA	C2C-C1C-NC	2.44	111.91	110.22
35	E	102	HEM	CMC-C2C-C3C	2.45	129.43	124.89
34	D	401	PHO	C3D-C4D-CHA	2.45	116.31	109.97
26	B	619	BCR	C38-C26-C27	2.45	118.09	113.45
27	A	610	PL9	C40-C39-C41	2.45	119.54	115.29
28	F	101	SQD	O6-C1-C2	2.46	112.24	108.23
27	D	407	PL9	C10-C9-C11	2.46	119.55	115.29
27	A	610	PL9	C30-C29-C31	2.48	119.59	115.29
27	A	610	PL9	C10-C9-C11	2.48	119.59	115.29
25	c	505	CLA	C2C-C1C-NC	2.48	111.93	110.22
29	D	408	LHG	O8-C23-C24	2.50	119.16	111.90
25	B	602	CLA	C2C-C1C-NC	2.50	111.94	110.22
27	a	612	PL9	C40-C39-C41	2.50	119.63	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	613	SQD	O8-S-C6	2.51	109.07	106.01
27	D	407	PL9	C45-C44-C46	2.51	119.65	115.29
26	A	609	BCR	C33-C5-C4	2.51	118.22	113.45
26	c	521	BCR	C33-C5-C4	2.51	118.22	113.45
29	d	406	LHG	O8-C23-C24	2.52	119.25	111.90
27	A	610	PL9	C20-C19-C21	2.53	119.68	115.29
26	k	102	BCR	C38-C26-C27	2.53	118.25	113.45
23	D	409	LMG	O8-C28-C29	2.54	119.28	111.90
27	a	612	PL9	C25-C24-C26	2.54	119.69	115.29
28	f	101	SQD	O8-S-C6	2.54	109.11	106.01
26	C	522	BCR	C29-C30-C25	2.54	114.45	110.48
29	a	616	LHG	O8-C23-C24	2.54	119.30	111.90
27	A	610	PL9	C25-C24-C26	2.56	119.73	115.29
23	B	624	LMG	O8-C28-C29	2.57	119.38	111.90
27	d	405	PL9	C30-C29-C31	2.58	119.76	115.29
26	c	521	BCR	C29-C30-C25	2.58	114.51	110.48
23	a	614	LMG	O8-C28-C29	2.58	119.41	111.90
25	b	602	CLA	C2C-C1C-NC	2.60	112.01	110.22
26	d	404	BCR	C38-C26-C27	2.60	118.38	113.45
27	D	407	PL9	C25-C24-C26	2.60	119.80	115.29
33	c	515	DGD	O1G-C1A-C2A	2.61	119.50	111.90
26	B	617	BCR	C29-C30-C25	2.61	114.56	110.48
27	A	610	PL9	C15-C14-C16	2.62	119.83	115.29
25	c	506	CLA	C2C-C1C-NC	2.62	112.03	110.22
28	L	101	SQD	O48-C23-C24	2.63	119.55	111.90
23	b	624	LMG	O8-C28-C29	2.63	119.57	111.90
27	D	407	PL9	C30-C29-C31	2.64	119.88	115.29
25	b	614	CLA	C2C-C1C-NC	2.65	112.05	110.22
33	h	102	DGD	O1G-C1A-C2A	2.65	119.62	111.90
27	a	612	PL9	C45-C44-C46	2.66	119.90	115.29
27	d	405	PL9	C35-C34-C36	2.66	119.91	115.29
27	D	407	PL9	C53-C6-C1	2.66	120.49	114.84
26	H	101	BCR	C29-C30-C25	2.67	114.65	110.48
26	B	619	BCR	C33-C5-C4	2.68	118.53	113.45
27	d	405	PL9	C45-C44-C46	2.68	119.94	115.29
26	b	619	BCR	C33-C5-C4	2.69	118.56	113.45
26	b	618	BCR	C2-C1-C6	2.70	114.69	110.48
29	d	407	LHG	O8-C23-C24	2.71	119.77	111.90
28	f	101	SQD	C3-C4-C5	2.71	114.99	110.22
27	d	405	PL9	C25-C24-C26	2.72	120.00	115.29
27	d	405	PL9	C53-C6-C1	2.72	120.61	114.84
26	D	406	BCR	C29-C30-C25	2.72	114.73	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	610	PL9	C45-C44-C46	2.72	120.01	115.29
29	E	101	LHG	O8-C23-C24	2.73	119.85	111.90
27	D	407	PL9	C35-C34-C36	2.74	120.04	115.29
27	a	612	PL9	C53-C6-C1	2.74	120.67	114.84
26	T	101	BCR	C33-C5-C4	2.75	118.67	113.45
33	H	102	DGD	O1G-C1A-C2A	2.76	119.92	111.90
25	B	614	CLA	C2C-C1C-NC	2.77	112.13	110.22
25	b	616	CLA	C2C-C1C-NC	2.77	112.13	110.22
29	A	614	LHG	O8-C23-C24	2.78	119.98	111.90
27	d	405	PL9	C15-C14-C16	2.78	120.11	115.29
27	a	612	PL9	C7-C3-C4	2.79	119.15	116.88
27	a	612	PL9	C20-C19-C21	2.79	120.14	115.29
25	B	612	CLA	C2C-C1C-NC	2.82	112.16	110.22
27	A	610	PL9	C53-C6-C1	2.82	120.83	114.84
29	a	615	LHG	O8-C23-C24	2.82	120.12	111.90
33	C	517	DGD	O1G-C1A-C2A	2.83	120.13	111.90
25	c	508	CLA	C2C-C1C-NC	2.84	112.18	110.22
26	C	522	BCR	C33-C5-C4	2.84	118.85	113.45
29	L	102	LHG	O8-C23-C24	2.84	120.18	111.90
26	B	617	BCR	C38-C26-C27	2.85	118.85	113.45
27	d	405	PL9	C20-C19-C21	2.85	120.23	115.29
25	a	607	CLA	C2C-C1C-NC	2.86	112.19	110.22
27	D	407	PL9	C15-C14-C16	2.88	120.28	115.29
23	A	612	LMG	O8-C28-C29	2.88	120.28	111.90
33	c	517	DGD	O1G-C1A-C2A	2.88	120.29	111.90
25	b	608	CLA	C2C-C1C-NC	2.89	112.21	110.22
25	B	608	CLA	C2C-C1C-NC	2.90	112.22	110.22
28	f	101	SQD	O48-C23-C24	2.90	120.35	111.90
26	b	617	BCR	C29-C30-C25	2.91	115.02	110.48
28	L	103	SQD	O48-C23-C24	2.92	120.39	111.90
25	b	605	CLA	C2C-C1C-NC	2.92	112.23	110.22
29	l	101	LHG	O8-C23-C24	2.93	120.42	111.90
25	b	612	CLA	C2C-C1C-NC	2.93	112.24	110.22
33	C	516	DGD	O1G-C1A-C2A	2.93	120.44	111.90
25	A	607	CLA	C2C-C1C-NC	2.94	112.24	110.22
23	C	521	LMG	O8-C28-C29	2.94	120.45	111.90
25	a	610	CLA	C2C-C1C-NC	2.95	112.25	110.22
29	A	613	LHG	O8-C23-C24	2.95	120.48	111.90
25	b	610	CLA	C2C-C1C-NC	2.96	112.26	110.22
25	A	606	CLA	C2C-C1C-NC	2.96	112.26	110.22
23	B	620	LMG	O8-C28-C29	2.97	120.55	111.90
25	C	508	CLA	C2C-C1C-NC	2.98	112.27	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	606	CLA	C2C-C1C-NC	2.98	112.27	110.22
23	c	518	LMG	O8-C28-C29	2.98	120.56	111.90
25	C	506	CLA	C2C-C1C-NC	2.99	112.28	110.22
25	b	601	CLA	C2C-C1C-NC	3.01	112.29	110.22
27	A	610	PL9	C7-C3-C4	3.01	119.32	116.88
33	C	518	DGD	O1G-C1A-C2A	3.02	120.70	111.90
25	B	610	CLA	C2C-C1C-NC	3.02	112.30	110.22
25	B	609	CLA	C2C-C1C-NC	3.03	112.31	110.22
23	C	521	LMG	O1-C1-C2	3.03	113.18	108.23
25	A	608	CLA	C2C-C1C-NC	3.04	112.31	110.22
25	B	601	CLA	C2C-C1C-NC	3.04	112.31	110.22
25	b	615	CLA	C2C-C1C-NC	3.05	112.32	110.22
25	C	502	CLA	C2C-C1C-NC	3.05	112.32	110.22
28	A	611	SQD	O48-C23-C24	3.06	120.80	111.90
25	D	405	CLA	C2C-C1C-NC	3.06	112.33	110.22
25	D	403	CLA	C2C-C1C-NC	3.06	112.33	110.22
25	B	616	CLA	C2C-C1C-NC	3.07	112.33	110.22
27	D	407	PL9	C20-C19-C21	3.08	120.62	115.29
28	a	613	SQD	O7-S-C6	3.09	109.47	106.83
33	c	516	DGD	O1G-C1A-C2A	3.09	120.90	111.90
23	b	620	LMG	O8-C28-C29	3.10	120.91	111.90
26	b	617	BCR	C38-C26-C27	3.11	119.36	113.45
23	A	603	LMG	O8-C28-C29	3.12	120.97	111.90
25	c	502	CLA	C2C-C1C-NC	3.12	112.37	110.22
25	c	507	CLA	C2C-C1C-NC	3.14	112.38	110.22
25	b	606	CLA	C2C-C1C-NC	3.14	112.39	110.22
25	c	513	CLA	C2C-C1C-NC	3.15	112.39	110.22
28	a	613	SQD	O48-C23-C24	3.15	121.08	111.90
25	b	603	CLA	C2C-C1C-NC	3.17	112.40	110.22
25	B	611	CLA	C2C-C1C-NC	3.19	112.42	110.22
25	C	510	CLA	C2C-C1C-NC	3.20	112.42	110.22
25	C	513	CLA	C2C-C1C-NC	3.21	112.43	110.22
23	C	519	LMG	O8-C28-C29	3.21	121.23	111.90
25	B	606	CLA	C2C-C1C-NC	3.22	112.44	110.22
23	a	603	LMG	O8-C28-C29	3.22	121.28	111.90
25	B	603	CLA	C2C-C1C-NC	3.22	112.44	110.22
23	c	520	LMG	O8-C28-C29	3.23	121.29	111.90
25	C	504	CLA	C2C-C1C-NC	3.23	112.44	110.22
25	b	607	CLA	C2C-C1C-NC	3.23	112.45	110.22
25	b	609	CLA	C2C-C1C-NC	3.25	112.46	110.22
25	b	611	CLA	C2C-C1C-NC	3.26	112.47	110.22
25	c	509	CLA	C2C-C1C-NC	3.26	112.47	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	511	CLA	C2C-C1C-NC	3.28	112.48	110.22
25	b	613	CLA	C2C-C1C-NC	3.28	112.48	110.22
28	f	101	SQD	O7-S-C6	3.31	109.65	106.83
25	d	403	CLA	C2C-C1C-NC	3.32	112.50	110.22
25	C	509	CLA	C2C-C1C-NC	3.34	112.52	110.22
25	c	510	CLA	C2C-C1C-NC	3.34	112.52	110.22
25	C	512	CLA	C2C-C1C-NC	3.34	112.52	110.22
25	c	501	CLA	C2C-C1C-NC	3.36	112.53	110.22
25	c	503	CLA	C2C-C1C-NC	3.36	112.53	110.22
25	B	605	CLA	C2C-C1C-NC	3.37	112.54	110.22
25	C	503	CLA	C2C-C1C-NC	3.38	112.55	110.22
25	c	504	CLA	C2C-C1C-NC	3.38	112.55	110.22
26	D	406	BCR	C38-C26-C27	3.39	119.88	113.45
25	C	511	CLA	C2C-C1C-NC	3.40	112.56	110.22
25	C	507	CLA	C2C-C1C-NC	3.40	112.56	110.22
25	B	613	CLA	C2C-C1C-NC	3.41	112.57	110.22
25	B	607	CLA	C2C-C1C-NC	3.41	112.57	110.22
25	B	615	CLA	C2C-C1C-NC	3.41	112.57	110.22
25	c	512	CLA	C2C-C1C-NC	3.43	112.58	110.22
28	F	101	SQD	O7-S-C6	3.45	109.78	106.83
25	a	608	CLA	C2C-C1C-NC	3.48	112.61	110.22
28	A	611	SQD	O7-S-C6	3.48	109.81	106.83
28	L	101	SQD	O47-C7-C8	3.49	118.81	111.55
28	L	101	SQD	O8-S-O7	3.50	119.40	111.37
25	C	501	CLA	C2C-C1C-NC	3.54	112.66	110.22
33	c	516	DGD	O2G-C1B-C2B	3.54	118.91	111.55
28	a	613	SQD	O9-S-C6	3.63	109.93	106.83
25	b	604	CLA	C2C-C1C-NC	3.64	112.73	110.22
23	C	521	LMG	O7-C10-C11	3.76	119.36	111.55
29	A	613	LHG	O7-C7-C8	3.77	119.39	111.55
28	F	101	SQD	O9-S-C6	3.79	110.07	106.83
28	f	101	SQD	O9-S-C6	3.82	110.09	106.83
28	L	103	SQD	O9-S-C6	3.83	110.10	106.83
25	B	604	CLA	C2C-C1C-NC	3.86	112.88	110.22
23	C	519	LMG	O7-C10-C11	3.88	119.61	111.55
29	D	408	LHG	O7-C7-C8	3.89	119.64	111.55
29	d	407	LHG	O7-C7-C8	3.90	119.65	111.55
33	h	102	DGD	O2G-C1B-C2B	3.92	119.69	111.55
29	a	615	LHG	O7-C7-C8	3.94	119.74	111.55
23	c	518	LMG	O7-C10-C11	3.94	119.74	111.55
33	c	517	DGD	O2G-C1B-C2B	3.95	119.76	111.55
33	C	518	DGD	O2G-C1B-C2B	3.96	119.77	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	620	LMG	O7-C10-C11	3.97	119.79	111.55
29	d	406	LHG	O7-C7-C8	3.97	119.80	111.55
23	A	603	LMG	O7-C10-C11	4.02	119.91	111.55
23	a	603	LMG	O7-C10-C11	4.04	119.94	111.55
33	H	102	DGD	O2G-C1B-C2B	4.04	119.95	111.55
28	F	101	SQD	O47-C7-C8	4.10	120.06	111.55
33	C	517	DGD	O2G-C1B-C2B	4.11	120.08	111.55
23	d	408	LMG	O7-C10-C11	4.12	120.10	111.55
33	C	516	DGD	O2G-C1B-C2B	4.14	120.15	111.55
29	a	616	LHG	O7-C7-C8	4.16	120.18	111.55
33	c	515	DGD	O2G-C1B-C2B	4.16	120.19	111.55
23	b	624	LMG	O7-C10-C11	4.17	120.21	111.55
29	A	614	LHG	O7-C7-C8	4.17	120.22	111.55
23	b	620	LMG	O7-C10-C11	4.19	120.24	111.55
23	B	624	LMG	O7-C10-C11	4.20	120.27	111.55
28	A	611	SQD	O9-S-C6	4.21	110.42	106.83
29	L	102	LHG	O7-C7-C8	4.21	120.30	111.55
23	A	612	LMG	O7-C10-C11	4.22	120.32	111.55
28	f	101	SQD	O47-C7-C8	4.23	120.33	111.55
28	A	611	SQD	O47-C7-C8	4.24	120.35	111.55
29	E	101	LHG	O7-C7-C8	4.24	120.35	111.55
23	D	409	LMG	O7-C10-C11	4.24	120.36	111.55
23	c	520	LMG	O7-C10-C11	4.25	120.37	111.55
28	L	103	SQD	O8-S-C6	4.28	111.23	106.01
28	L	103	SQD	O47-C7-C8	4.29	120.45	111.55
28	a	613	SQD	O47-C7-C8	4.31	120.50	111.55
29	l	101	LHG	O7-C7-C8	4.33	120.55	111.55
23	a	614	LMG	O7-C10-C11	4.34	120.57	111.55
28	L	101	SQD	O8-S-C6	10.02	118.24	106.01
28	L	101	SQD	O7-S-C6	13.65	118.49	106.83

All (210) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	b	609	CLA	NC
25	b	609	CLA	ND
25	b	609	CLA	NA
25	C	503	CLA	NC
25	C	503	CLA	ND
25	C	503	CLA	NA
25	a	610	CLA	NC
25	a	610	CLA	ND

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Mol	Chain	Res	Type	Atom
25	a	610	CLA	NA
25	b	610	CLA	NC
25	b	610	CLA	ND
25	b	610	CLA	NA
25	c	506	CLA	NC
25	c	506	CLA	ND
25	c	506	CLA	NA
25	b	615	CLA	NC
25	b	615	CLA	ND
25	b	615	CLA	NA
25	c	501	CLA	NC
25	c	501	CLA	ND
25	c	501	CLA	NA
25	B	612	CLA	NC
25	B	612	CLA	ND
25	B	612	CLA	NA
25	C	507	CLA	NC
25	C	507	CLA	ND
25	C	507	CLA	NA
25	C	511	CLA	NC
25	C	511	CLA	ND
25	C	511	CLA	NA
25	B	614	CLA	NC
25	B	614	CLA	ND
25	B	614	CLA	NA
25	c	502	CLA	NC
25	c	502	CLA	ND
25	c	502	CLA	NA
25	c	508	CLA	NC
25	c	508	CLA	ND
25	c	508	CLA	NA
25	C	504	CLA	NC
25	C	504	CLA	ND
25	C	504	CLA	NA
25	a	608	CLA	NC
25	a	608	CLA	ND
25	a	608	CLA	NA
25	b	602	CLA	NC
25	b	602	CLA	ND
25	b	602	CLA	NA
25	B	616	CLA	NC
25	B	616	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	616	CLA	NA
25	d	401	CLA	NC
25	d	401	CLA	ND
25	d	401	CLA	NA
25	B	613	CLA	NC
25	B	613	CLA	ND
25	B	613	CLA	NA
25	B	611	CLA	NC
25	B	611	CLA	ND
25	B	611	CLA	NA
25	c	505	CLA	NC
25	c	505	CLA	ND
25	c	505	CLA	NA
25	c	504	CLA	NC
25	c	504	CLA	ND
25	c	504	CLA	NA
25	A	608	CLA	NC
25	A	608	CLA	ND
25	A	608	CLA	NA
25	C	510	CLA	NC
25	C	510	CLA	ND
25	C	510	CLA	NA
25	D	405	CLA	NC
25	D	405	CLA	ND
25	D	405	CLA	NA
25	C	512	CLA	NC
25	C	512	CLA	ND
25	C	512	CLA	NA
25	b	606	CLA	NC
25	b	606	CLA	ND
25	b	606	CLA	NA
25	b	612	CLA	NC
25	b	612	CLA	ND
25	b	612	CLA	NA
25	B	609	CLA	NC
25	B	609	CLA	ND
25	B	609	CLA	NA
25	B	605	CLA	NC
25	B	605	CLA	ND
25	B	605	CLA	NA
25	b	614	CLA	NC
25	b	614	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	614	CLA	NA
25	C	502	CLA	NC
25	C	502	CLA	ND
25	C	502	CLA	NA
25	C	508	CLA	NC
25	C	508	CLA	ND
25	C	508	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	b	603	CLA	NC
25	b	603	CLA	ND
25	b	603	CLA	NA
25	B	601	CLA	NC
25	B	601	CLA	ND
25	B	601	CLA	NA
25	d	403	CLA	NC
25	d	403	CLA	ND
25	d	403	CLA	NA
25	B	603	CLA	NC
25	B	603	CLA	ND
25	B	603	CLA	NA
25	a	607	CLA	NC
25	a	607	CLA	ND
25	a	607	CLA	NA
25	c	512	CLA	NC
25	c	512	CLA	ND
25	c	512	CLA	NA
25	C	506	CLA	NC
25	C	506	CLA	ND
25	C	506	CLA	NA
25	A	607	CLA	NC
25	A	607	CLA	ND
25	A	607	CLA	NA
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

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Mol	Chain	Res	Type	Atom
25	C	509	CLA	NA
25	D	404	CLA	NC
25	D	404	CLA	ND
25	D	404	CLA	NA
25	B	607	CLA	NC
25	B	607	CLA	ND
25	B	607	CLA	NA
25	B	606	CLA	NC
25	B	606	CLA	ND
25	B	606	CLA	NA
25	b	616	CLA	NC
25	b	616	CLA	ND
25	b	616	CLA	NA
25	b	601	CLA	NC
25	b	601	CLA	ND
25	b	601	CLA	NA
25	b	604	CLA	NC
25	b	604	CLA	ND
25	b	604	CLA	NA
25	b	611	CLA	NC
25	b	611	CLA	ND
25	b	611	CLA	NA
25	C	505	CLA	NC
25	C	505	CLA	ND
25	C	505	CLA	NA
25	c	513	CLA	NC
25	c	513	CLA	ND
25	c	513	CLA	NA
25	B	608	CLA	NC
25	B	608	CLA	ND
25	B	608	CLA	NA
25	B	602	CLA	NC
25	B	602	CLA	ND
25	B	602	CLA	NA
25	b	605	CLA	NC
25	b	605	CLA	ND
25	b	605	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

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Mol	Chain	Res	Type	Atom
25	C	513	CLA	NA
25	C	501	CLA	NC
25	C	501	CLA	ND
25	C	501	CLA	NA
25	c	511	CLA	NC
25	c	511	CLA	ND
25	c	511	CLA	NA
25	b	613	CLA	NC
25	b	613	CLA	ND
25	b	613	CLA	NA
25	B	610	CLA	NC
25	B	610	CLA	ND
25	B	610	CLA	NA
25	B	615	CLA	NC
25	B	615	CLA	ND
25	B	615	CLA	NA
25	D	403	CLA	NC
25	D	403	CLA	ND
25	D	403	CLA	NA
25	a	606	CLA	NC
25	a	606	CLA	ND
25	a	606	CLA	NA
25	c	510	CLA	NC
25	c	510	CLA	ND
25	c	510	CLA	NA
25	c	507	CLA	NC
25	c	507	CLA	ND
25	c	507	CLA	NA
25	B	604	CLA	NC
25	B	604	CLA	ND
25	B	604	CLA	NA
25	A	606	CLA	NC
25	A	606	CLA	ND
25	A	606	CLA	NA

All (1) torsion outliers are listed below:

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

There are no ring outliers.

68 monomers are involved in 220 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	603	LMG	2	0
25	A	606	CLA	4	0
25	A	607	CLA	3	0
25	A	608	CLA	2	0
26	A	609	BCR	3	0
27	A	610	PL9	6	0
28	A	611	SQD	2	0
29	A	613	LHG	5	0
29	A	614	LHG	8	0
25	B	601	CLA	4	0
25	B	602	CLA	4	0
25	B	603	CLA	5	0
25	B	604	CLA	5	0
25	B	605	CLA	7	0
25	B	606	CLA	3	0
25	B	607	CLA	2	0
25	B	608	CLA	3	0
25	B	609	CLA	4	0
25	B	610	CLA	1	0
25	B	611	CLA	3	0
25	B	612	CLA	3	0
25	B	613	CLA	6	0
25	B	614	CLA	4	0
25	B	615	CLA	3	0
25	B	616	CLA	4	0
26	B	617	BCR	6	0
26	B	618	BCR	4	0
26	B	619	BCR	5	0
23	B	620	LMG	3	0
23	B	624	LMG	1	0
25	C	501	CLA	6	0
25	C	502	CLA	2	0
25	C	503	CLA	6	0
25	C	504	CLA	2	0
25	C	505	CLA	7	0
25	C	506	CLA	8	0
25	C	507	CLA	5	0
25	C	508	CLA	6	0
25	C	509	CLA	4	0
25	C	510	CLA	8	0
25	C	511	CLA	4	0
25	C	512	CLA	6	0
25	C	513	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	514	BCR	7	0
26	C	515	BCR	2	0
33	C	516	DGD	7	0
33	C	517	DGD	4	0
33	C	518	DGD	1	0
23	C	519	LMG	1	0
23	C	521	LMG	3	0
26	C	522	BCR	2	0
34	D	401	PHO	1	0
34	D	402	PHO	5	0
25	D	403	CLA	4	0
25	D	404	CLA	6	0
25	D	405	CLA	1	0
26	D	406	BCR	2	0
27	D	407	PL9	3	0
29	D	408	LHG	5	0
35	E	102	HEM	3	0
28	F	101	SQD	2	0
26	H	101	BCR	5	0
33	H	102	DGD	3	0
26	K	101	BCR	4	0
28	L	101	SQD	6	0
29	L	102	LHG	4	0
28	L	103	SQD	4	0
26	T	101	BCR	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	333/344 (96%)	0.11	10 (3%) 51 46	24, 32, 54, 72	0
1	a	333/344 (96%)	-0.00	5 (1%) 74 72	24, 34, 62, 76	0
2	B	505/510 (99%)	0.05	26 (5%) 29 27	24, 35, 61, 84	0
2	b	503/510 (98%)	0.14	32 (6%) 20 17	26, 38, 67, 87	0
3	C	448/461 (97%)	0.09	12 (2%) 55 50	24, 40, 59, 77	0
3	c	448/461 (97%)	0.04	12 (2%) 55 50	29, 42, 60, 80	0
4	D	340/352 (96%)	-0.01	8 (2%) 59 55	25, 34, 52, 70	0
4	d	340/352 (96%)	-0.13	5 (1%) 74 72	26, 37, 59, 74	0
5	E	82/84 (97%)	1.02	15 (18%) 1 1	39, 57, 71, 75	0
5	e	79/84 (94%)	0.56	9 (11%) 6 4	43, 58, 71, 81	0
6	F	33/45 (73%)	-0.15	0 100 100	42, 49, 63, 71	0
6	f	33/45 (73%)	-0.09	1 (3%) 51 46	46, 52, 73, 82	0
7	H	63/66 (95%)	0.11	3 (4%) 31 29	34, 41, 48, 60	0
7	h	63/66 (95%)	0.49	9 (14%) 3 2	39, 48, 59, 69	0
8	I	33/38 (86%)	-0.34	0 100 100	30, 36, 44, 55	0
8	i	35/38 (92%)	-0.23	0 100 100	31, 39, 56, 66	0
9	J	34/40 (85%)	0.13	5 (14%) 3 1	40, 53, 64, 78	0
9	j	33/40 (82%)	0.14	1 (3%) 51 46	43, 52, 61, 65	0
10	K	36/46 (78%)	0.43	2 (5%) 25 22	52, 61, 75, 77	0
10	k	36/46 (78%)	0.16	1 (2%) 53 49	48, 60, 76, 78	0
11	L	36/37 (97%)	-0.28	0 100 100	26, 33, 53, 59	0
11	l	36/37 (97%)	-0.09	2 (5%) 25 22	28, 35, 50, 62	0
12	M	32/36 (88%)	-0.13	0 100 100	30, 36, 56, 58	0
12	m	32/36 (88%)	0.10	3 (9%) 9 7	30, 38, 57, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	242/272 (88%)	0.47	25 (10%) 7 6	30, 44, 70, 104	0
13	o	243/272 (89%)	0.28	18 (7%) 15 13	28, 45, 72, 108	0
14	T	29/32 (90%)	0.20	2 (6%) 18 15	26, 35, 56, 62	0
14	t	29/32 (90%)	0.16	2 (6%) 18 15	31, 36, 55, 67	0
15	U	96/134 (71%)	0.39	8 (8%) 12 10	34, 43, 64, 72	0
15	u	96/134 (71%)	0.01	0 100 100	35, 45, 58, 65	0
16	V	137/163 (84%)	0.12	2 (1%) 74 72	33, 44, 56, 64	0
16	v	137/163 (84%)	0.72	19 (13%) 3 2	37, 50, 67, 82	0
17	Y	29/46 (63%)	2.58	17 (58%) 0 0	63, 76, 95, 96	0
17	y	29/46 (63%)	1.62	12 (41%) 0 0	61, 71, 90, 91	0
18	X	37/41 (90%)	0.23	5 (13%) 3 2	42, 50, 65, 79	0
18	x	38/41 (92%)	0.58	7 (18%) 1 1	41, 52, 74, 84	0
19	Z	62/62 (100%)	1.77	21 (33%) 0 0	57, 73, 104, 111	0
19	z	62/62 (100%)	2.28	32 (51%) 0 0	62, 74, 100, 107	0
20	R	34/41 (82%)	3.23	27 (79%) 0 0	61, 74, 88, 92	0
20	r	33/41 (80%)	3.01	26 (78%) 0 0	64, 73, 86, 91	0
All	All	5279/5700 (92%)	0.24	384 (7%) 16 13	24, 41, 72, 111	0

All (384) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	56	PRO	8.9
13	O	61	GLN	8.9
13	O	63	ALA	8.4
19	Z	33	TRP	7.4
17	Y	22	LEU	6.9
19	Z	30	PRO	6.8
19	Z	34	ASP	6.8
20	R	35	LEU	6.5
13	O	62	GLU	6.5
20	R	32	GLN	6.4
20	R	31	VAL	6.3
20	r	34	LEU	6.3
19	z	32	ASP	6.2
19	Z	31	GLN	5.9
17	Y	19	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
19	z	1	MET	5.9
2	b	126	PRO	5.9
20	r	5	VAL	5.8
13	o	5	LEU	5.8
13	o	57	LYS	5.8
13	O	58	ASN	5.7
20	R	34	LEU	5.6
19	z	39	LEU	5.6
2	b	495	PHE	5.6
2	b	128	THR	5.5
19	z	4	LEU	5.5
20	R	27	ALA	5.4
17	Y	18	VAL	5.4
17	Y	45	ASN	5.4
19	Z	32	ASP	5.3
19	Z	62	VAL	5.3
20	R	28	VAL	5.3
20	R	6	LEU	5.2
13	o	60	ARG	5.2
20	r	9	LEU	5.2
2	b	129	GLY	5.1
3	c	143	TYR	5.0
17	Y	26	ALA	5.0
19	z	30	PRO	5.0
2	b	499	VAL	5.0
17	Y	43	ARG	5.0
2	B	503	THR	4.9
13	o	63	ALA	4.9
19	z	31	GLN	4.9
5	E	79	PHE	4.7
2	B	484	PRO	4.6
2	B	490	GLN	4.6
20	R	25	PRO	4.5
19	z	3	ILE	4.5
20	r	26	TYR	4.4
7	h	49	TYR	4.4
20	r	24	LEU	4.4
10	K	46	ARG	4.4
18	x	38	GLN	4.4
13	O	35	SER	4.2
18	X	2	THR	4.2
17	y	20	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
13	O	64	GLU	4.2
19	z	33	TRP	4.2
20	r	14	LEU	4.2
1	A	245	THR	4.1
19	z	34	ASP	4.1
19	Z	41	PHE	4.1
19	Z	1	MET	4.1
20	r	3	TRP	4.1
19	Z	37	LYS	4.0
18	X	38	GLN	4.0
17	Y	44	GLY	4.0
5	E	82	GLN	4.0
5	e	74	GLN	4.0
18	x	2	THR	4.0
5	E	60	GLN	4.0
3	c	146	PHE	4.0
20	R	21	ARG	4.0
20	r	6	LEU	3.9
2	b	486	LEU	3.9
18	X	37	VAL	3.9
14	T	29	ILE	3.9
2	B	496	TYR	3.9
17	Y	20	ALA	3.9
14	t	28	ARG	3.9
16	v	21	LEU	3.9
13	O	54	GLU	3.8
16	V	1	ALA	3.8
2	b	488	PRO	3.8
13	o	59	LYS	3.8
19	Z	4	LEU	3.8
3	C	144	SER	3.8
17	y	41	VAL	3.8
2	B	495	PHE	3.8
17	y	40	ALA	3.8
13	o	62	GLU	3.8
18	x	39	ARG	3.7
19	z	41	PHE	3.7
20	r	31	VAL	3.7
13	O	60	ARG	3.7
14	T	28	ARG	3.7
13	o	56	PRO	3.7
16	v	12	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
16	v	17	LYS	3.7
2	b	503	THR	3.6
13	O	57	LYS	3.6
20	r	12	VAL	3.6
20	r	27	ALA	3.6
2	b	502	VAL	3.6
15	U	61	VAL	3.6
2	b	127	ARG	3.6
2	B	505	ARG	3.6
2	b	487	SER	3.6
16	v	14	SER	3.5
2	B	489	GLU	3.5
4	D	236	ASN	3.5
20	r	10	LEU	3.5
13	O	59	LYS	3.5
17	Y	25	ILE	3.5
19	z	47	TRP	3.5
20	R	3	TRP	3.5
5	E	68	ASP	3.5
18	X	3	ILE	3.4
20	r	28	VAL	3.4
16	v	3	LEU	3.4
20	R	2	ASP	3.4
1	A	227	THR	3.4
19	z	8	ALA	3.4
13	o	246	ALA	3.4
9	J	36	LEU	3.4
18	x	4	THR	3.4
2	b	490	GLN	3.4
18	x	37	VAL	3.4
20	R	14	LEU	3.4
20	R	8	VAL	3.4
17	y	45	ASN	3.4
19	z	61	VAL	3.4
19	Z	35	ARG	3.3
13	O	207	ARG	3.3
13	o	89	SER	3.3
2	b	125	ASP	3.3
20	r	13	LEU	3.3
20	R	30	GLN	3.3
1	A	225	ARG	3.3
19	z	46	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	b	84	THR	3.3
19	z	62	VAL	3.3
16	v	18	THR	3.3
2	B	485	GLU	3.3
20	R	11	PRO	3.3
4	D	240	ALA	3.3
17	y	37	PHE	3.3
1	a	230	THR	3.2
4	d	226	GLY	3.2
20	r	7	VAL	3.2
20	R	18	TRP	3.2
10	k	18	PHE	3.2
19	Z	60	PHE	3.2
3	c	142	GLU	3.2
17	y	19	ILE	3.2
2	B	296	ALA	3.1
5	e	83	LEU	3.2
16	v	2	GLU	3.1
17	y	44	GLY	3.1
2	b	296	ALA	3.1
7	h	2	ALA	3.1
13	o	54	GLU	3.1
17	Y	23	THR	3.1
19	z	42	LEU	3.1
16	v	71	GLY	3.1
2	B	292	LEU	3.1
13	o	4	THR	3.1
20	R	24	LEU	3.1
2	b	496	TYR	3.1
15	U	73	GLN	3.1
13	O	55	GLU	3.1
3	C	28	GLN	3.1
13	O	5	LEU	3.1
17	Y	46	LEU	3.1
6	f	13	TYR	3.1
19	Z	59	PHE	3.1
5	E	61	ARG	3.1
19	z	36	SER	3.1
5	E	64	PRO	3.0
2	b	494	GLY	3.0
3	C	148	GLY	3.0
20	R	17	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	a	228	THR	3.0
2	B	293	ALA	3.0
19	z	7	LEU	3.0
5	e	81	GLU	3.0
2	b	501	ASP	3.0
20	R	16	ALA	3.0
17	Y	24	MET	3.0
14	t	29	ILE	3.0
19	z	52	LEU	3.0
5	e	79	PHE	3.0
2	B	294	SER	2.9
20	r	8	VAL	2.9
17	Y	38	LEU	2.9
17	Y	40	ALA	2.9
13	o	61	GLN	2.9
13	o	58	ASN	2.9
20	r	33	LYS	2.9
3	C	143	TYR	2.9
2	B	500	GLY	2.9
2	b	295	GLY	2.9
7	h	19	GLY	2.9
16	v	15	GLU	2.9
19	z	9	LEU	2.9
2	B	479	PHE	2.9
19	Z	3	ILE	2.9
17	y	43	ARG	2.8
19	z	35	ARG	2.8
1	a	224	ILE	2.8
5	E	4	THR	2.8
3	C	30	SER	2.8
19	z	29	SER	2.8
1	A	226	GLU	2.8
5	E	80	LEU	2.8
19	z	56	VAL	2.8
5	e	59	GLU	2.8
19	Z	61	VAL	2.8
18	X	34	ILE	2.8
13	O	4	THR	2.8
15	U	62	LEU	2.8
3	c	462	GLU	2.8
19	z	38	GLN	2.8
2	B	499	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
20	R	12	VAL	2.8
20	r	11	PRO	2.8
5	E	2	ALA	2.8
2	b	292	LEU	2.8
13	O	38	TYR	2.7
19	z	51	VAL	2.7
19	z	60	PHE	2.7
3	c	429	SER	2.7
13	o	207	ARG	2.7
15	U	77	GLU	2.7
5	e	73	LYS	2.7
2	b	289	GLN	2.7
1	A	243	GLU	2.6
2	b	294	SER	2.6
20	R	26	TYR	2.6
2	B	501	ASP	2.6
2	b	130	GLU	2.6
5	e	72	ALA	2.6
9	j	40	LEU	2.6
2	b	485	GLU	2.6
2	b	293	ALA	2.6
13	o	37	THR	2.6
3	C	257	PHE	2.6
10	K	18	PHE	2.6
12	m	31	SER	2.6
3	c	433	LEU	2.6
11	l	3	PRO	2.6
20	r	18	TRP	2.6
4	D	237	PRO	2.6
16	v	107	LEU	2.6
1	A	249	VAL	2.5
20	R	9	LEU	2.5
20	r	21	ARG	2.5
2	b	302	TRP	2.5
19	z	28	ALA	2.5
2	B	502	VAL	2.5
16	v	25	GLN	2.5
19	Z	42	LEU	2.5
4	d	236	ASN	2.5
19	z	23	VAL	2.5
5	E	24	SER	2.5
16	v	11	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
17	Y	42	ARG	2.5
13	O	87	VAL	2.5
20	r	35	LEU	2.5
20	R	29	LYS	2.5
3	C	29	GLU	2.5
13	O	30	TYR	2.5
1	A	12	ASN	2.5
19	z	37	LYS	2.4
2	B	435	GLU	2.4
20	r	20	VAL	2.4
5	e	78	THR	2.4
4	d	234	ALA	2.4
5	e	82	GLN	2.4
2	B	486	LEU	2.4
20	r	23	ILE	2.4
4	d	227	GLU	2.4
4	D	13	GLY	2.3
5	E	63	ILE	2.3
16	v	19	ILE	2.3
2	b	492	GLU	2.3
12	m	30	GLU	2.3
13	o	21	THR	2.3
13	O	245	PRO	2.3
17	y	34	MET	2.3
9	J	40	LEU	2.3
17	Y	41	VAL	2.3
16	v	16	GLY	2.3
20	r	29	LYS	2.3
15	U	65	PRO	2.3
3	c	144	SER	2.3
19	Z	28	ALA	2.3
16	V	26	TYR	2.3
3	C	134	ILE	2.3
20	R	5	VAL	2.3
20	r	22	ASN	2.3
1	A	235	TYR	2.3
1	a	13	LEU	2.3
7	h	4	ARG	2.2
19	Z	26	ALA	2.2
1	a	235	TYR	2.2
2	b	85	GLY	2.2
16	v	62	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	124	ARG	2.2
4	D	239	GLN	2.2
17	Y	21	GLN	2.2
1	A	164	GLY	2.2
2	B	126	PRO	2.2
2	B	481	GLY	2.2
17	y	46	LEU	2.2
2	B	127	ARG	2.2
13	O	36	GLN	2.2
16	v	23	GLU	2.2
7	H	20	LYS	2.2
3	c	101	PRO	2.2
3	C	427	ALA	2.2
19	z	10	ALA	2.2
2	B	483	ASP	2.2
2	b	408	GLY	2.2
2	b	500	GLY	2.2
3	c	149	TYR	2.1
7	h	18	TYR	2.1
7	h	6	TRP	2.1
19	Z	18	VAL	2.1
9	J	7	ARG	2.1
3	c	276	LEU	2.1
19	z	12	LEU	2.1
20	R	33	LYS	2.1
5	E	6	GLY	2.1
18	x	33	GLN	2.1
20	r	32	GLN	2.1
13	O	39	ARG	2.1
11	l	2	GLU	2.1
4	D	121	GLY	2.1
4	d	240	ALA	2.1
4	D	238	THR	2.1
13	o	35	SER	2.1
16	v	90	GLU	2.1
2	B	494	GLY	2.1
3	c	432	VAL	2.1
5	E	74	GLN	2.1
19	Z	25	VAL	2.1
19	Z	38	GLN	2.1
16	v	65	PRO	2.1
15	U	64	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
17	y	36	ILE	2.1
1	A	242	GLU	2.1
3	c	279	LEU	2.1
3	C	424	SER	2.1
12	m	32	GLN	2.1
5	E	21	VAL	2.1
19	z	26	ALA	2.1
7	h	23	PRO	2.1
9	J	8	ILE	2.1
13	O	136	ILE	2.1
13	o	243	ILE	2.1
3	C	145	SER	2.1
20	R	10	LEU	2.1
7	H	26	GLY	2.1
4	D	227	GLU	2.1
2	B	504	THR	2.1
7	h	56	ASP	2.1
5	E	58	GLN	2.1
2	B	130	GLU	2.1
15	U	67	LEU	2.0
13	O	91	GLY	2.0
18	x	36	LYS	2.0
3	C	27	ASP	2.0
17	y	18	VAL	2.0
16	v	78	ASN	2.0
15	U	76	ARG	2.0
20	R	13	LEU	2.0
2	b	484	PRO	2.0
13	O	179	GLU	2.0
7	h	20	LYS	2.0
13	O	243	ILE	2.0
7	H	23	PRO	2.0
9	J	9	PRO	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
30	SO4	V	202	5/5	0.89	0.56	10.75	71,72,81,81	0
32	UNL	X	101	10/-	0.95	0.22	6.53	36,38,40,40	0
23	LMG	c	520	51/55	0.88	0.30	6.33	41,54,74,79	0
27	PL9	a	612	55/55	0.77	0.29	5.74	48,64,76,81	0
32	UNL	B	622	8/-	0.86	0.32	5.52	38,42,45,46	0
32	UNL	B	623	13/-	0.86	0.19	5.52	36,40,48,51	0
27	PL9	A	610	55/55	0.81	0.26	4.35	34,52,63,70	0
24	CL	a	604	1/1	0.93	0.22	4.35	40,40,40,40	0
23	LMG	a	603	51/55	0.82	0.21	4.29	37,52,70,80	0
32	UNL	b	622	12/-	0.86	0.23	4.28	37,47,51,51	0
23	LMG	b	624	51/55	0.84	0.26	3.82	43,59,69,72	0
26	BCR	d	404	40/40	0.86	0.22	3.60	38,50,62,67	0
32	UNL	d	409	15/-	0.86	0.25	3.38	39,45,52,53	0
23	LMG	a	614	51/55	0.84	0.23	3.34	34,50,68,75	0
32	UNL	B	621	10/-	0.91	0.19	3.10	34,41,45,46	0
23	LMG	C	521	51/55	0.85	0.27	3.09	38,51,63,67	0
32	UNL	J	101	11/-	0.84	0.25	2.93	48,58,64,67	0
32	UNL	b	621	10/-	0.85	0.20	2.81	32,41,44,46	0
26	BCR	t	102	40/40	0.87	0.22	2.80	28,39,45,49	0
23	LMG	A	612	51/55	0.82	0.25	2.80	38,52,61,63	0
29	LHG	a	616	42/49	0.85	0.23	2.67	53,71,80,87	0
23	LMG	B	624	51/55	0.88	0.22	2.55	41,50,60,66	0
27	PL9	D	407	55/55	0.92	0.19	2.51	21,37,44,47	0
32	UNL	D	410	15/-	0.82	0.21	2.48	36,44,67,68	0
27	PL9	d	405	55/55	0.89	0.20	2.40	29,37,50,55	0
29	LHG	d	407	49/49	0.92	0.22	2.37	38,50,68,76	0
23	LMG	B	620	51/55	0.82	0.25	2.33	27,50,57,64	0
32	UNL	T	102	15/-	0.86	0.24	2.31	36,46,51,51	0
32	UNL	T	103	12/-	0.86	0.23	2.28	35,42,49,49	0
26	BCR	D	406	40/40	0.88	0.21	2.24	28,45,64,66	0
23	LMG	A	603	51/55	0.83	0.20	2.23	36,49,64,72	0
28	SQD	L	101	54/54	0.81	0.23	2.20	34,54,89,94	0
28	SQD	L	103	54/54	0.73	0.28	2.06	34,53,92,102	0
26	BCR	b	617	40/40	0.91	0.21	2.02	31,41,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	A	609	40/40	0.90	0.17	1.98	24,34,39,40	0
29	LHG	d	406	49/49	0.92	0.16	1.87	25,41,48,53	0
28	SQD	a	613	54/54	0.87	0.21	1.80	37,65,73,77	0
32	UNL	x	101	16/-	0.85	0.18	1.76	31,42,52,54	0
25	CLA	a	610	65/65	0.94	0.16	1.74	23,30,65,76	0
32	UNL	B	627	12/-	0.88	0.24	1.74	33,39,45,50	0
30	SO4	u	202	5/5	0.75	0.23	1.65	64,73,90,96	0
25	CLA	A	608	65/65	0.95	0.17	1.64	14,27,68,74	0
25	CLA	b	601	65/65	0.87	0.23	1.64	39,59,77,84	0
25	CLA	c	506	65/65	0.93	0.17	1.52	35,44,66,73	0
26	BCR	T	101	40/40	0.89	0.21	1.51	30,41,48,50	0
26	BCR	K	101	40/40	0.81	0.22	1.50	51,61,70,73	0
25	CLA	B	616	65/65	0.91	0.18	1.42	26,36,78,87	0
26	BCR	B	619	40/40	0.89	0.17	1.40	33,39,46,50	0
23	LMG	b	620	51/55	0.86	0.23	1.36	31,44,58,60	0
28	SQD	f	101	43/54	0.87	0.34	1.34	55,77,85,88	0
25	CLA	C	512	65/65	0.86	0.23	1.32	45,56,66,71	0
32	UNL	j	101	15/-	0.86	0.20	1.30	43,53,57,59	0
26	BCR	B	617	40/40	0.92	0.17	1.30	32,38,44,47	0
25	CLA	b	607	65/65	0.95	0.21	1.21	22,29,42,44	0
29	LHG	a	615	49/49	0.91	0.20	1.21	32,42,53,62	0
26	BCR	a	611	40/40	0.91	0.15	1.21	26,35,41,44	0
32	UNL	c	519	15/-	0.88	0.18	1.18	40,46,51,53	0
26	BCR	c	514	40/40	0.93	0.16	1.14	26,42,50,53	0
32	UNL	t	101	15/-	0.87	0.21	1.14	31,49,57,57	0
29	LHG	A	613	49/49	0.92	0.18	1.14	21,37,47,56	0
25	CLA	b	604	65/65	0.91	0.23	1.12	23,34,50,58	0
23	LMG	d	408	51/55	0.92	0.17	1.10	35,49,72,80	0
26	BCR	b	618	40/40	0.93	0.21	1.07	27,36,41,48	0
25	CLA	b	606	65/65	0.92	0.15	1.06	24,35,55,62	0
25	CLA	d	403	65/65	0.92	0.17	1.05	28,39,77,85	0
29	LHG	E	101	42/49	0.84	0.23	1.04	44,67,78,83	0
26	BCR	C	514	40/40	0.87	0.23	1.03	50,58,65,66	0
25	CLA	b	605	65/65	0.95	0.18	1.03	24,33,42,47	0
33	DGD	H	102	62/66	0.90	0.23	1.02	27,36,47,58	0
26	BCR	k	102	40/40	0.86	0.19	0.98	48,59,65,65	0
26	BCR	b	619	40/40	0.93	0.16	0.96	35,44,50,54	0
25	CLA	c	510	65/65	0.93	0.25	0.96	41,46,53,57	0
25	CLA	b	616	65/65	0.90	0.19	0.94	28,42,62,69	0
34	PHO	d	402	64/64	0.93	0.17	0.92	29,40,48,54	0
29	LHG	D	408	49/49	0.95	0.15	0.92	20,36,45,51	0
25	CLA	D	405	65/65	0.91	0.19	0.92	24,35,63,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	c	508	65/65	0.92	0.21	0.91	35,44,73,77	0
26	BCR	C	515	40/40	0.93	0.16	0.88	30,40,50,54	0
25	CLA	c	502	65/65	0.88	0.24	0.87	31,41,49,55	0
25	CLA	B	606	65/65	0.91	0.16	0.85	25,33,57,62	0
33	DGD	c	515	62/66	0.94	0.18	0.83	26,37,70,73	0
34	PHO	D	402	64/64	0.94	0.20	0.82	24,33,41,49	0
25	CLA	a	608	65/65	0.92	0.18	0.81	28,36,75,85	0
25	CLA	B	605	65/65	0.94	0.17	0.81	21,30,37,42	0
25	CLA	c	504	65/65	0.93	0.23	0.80	35,42,61,74	0
26	BCR	c	521	40/40	0.82	0.23	0.78	43,53,62,66	0
25	CLA	b	612	65/65	0.94	0.21	0.76	24,34,43,48	0
25	CLA	C	505	65/65	0.92	0.17	0.72	29,39,49,57	0
25	CLA	C	508	65/65	0.91	0.20	0.70	36,43,79,88	0
29	LHG	A	614	49/49	0.91	0.20	0.70	29,48,70,78	0
25	CLA	C	513	65/65	0.88	0.21	0.68	51,62,77,82	0
33	DGD	C	518	62/66	0.89	0.20	0.68	30,46,63,70	0
26	BCR	z	101	40/40	0.86	0.25	0.67	49,59,63,67	0
26	BCR	C	522	40/40	0.91	0.19	0.66	45,55,63,64	0
25	CLA	c	503	65/65	0.89	0.20	0.66	33,43,50,57	0
29	LHG	l	101	49/49	0.92	0.17	0.65	28,39,50,53	0
25	CLA	c	513	65/65	0.88	0.24	0.62	45,60,76,79	0
25	CLA	c	501	65/65	0.93	0.18	0.61	27,39,45,54	0
33	DGD	c	516	62/66	0.88	0.24	0.59	32,46,78,87	0
23	LMG	c	518	51/55	0.86	0.23	0.59	38,58,76,80	0
25	CLA	b	613	65/65	0.93	0.23	0.58	21,29,52,58	0
33	DGD	C	517	62/66	0.87	0.21	0.58	36,50,69,82	0
33	DGD	C	516	62/66	0.95	0.18	0.57	25,35,67,72	0
25	CLA	b	603	65/65	0.94	0.18	0.56	24,36,50,60	0
32	UNL	m	102	15/-	0.87	0.19	0.55	34,43,51,52	0
34	PHO	a	609	64/64	0.94	0.15	0.55	24,30,39,42	0
29	LHG	L	102	49/49	0.91	0.17	0.54	27,39,46,50	0
25	CLA	C	507	65/65	0.92	0.16	0.53	26,41,51,57	0
25	CLA	c	509	65/65	0.93	0.20	0.51	32,45,56,61	0
25	CLA	B	607	65/65	0.96	0.16	0.49	19,28,53,54	0
25	CLA	b	610	65/65	0.95	0.18	0.48	23,35,45,48	0
25	CLA	b	609	65/65	0.94	0.15	0.48	28,41,55,60	0
25	CLA	a	607	65/65	0.93	0.17	0.45	22,30,37,45	0
25	CLA	A	607	65/65	0.94	0.19	0.44	23,36,71,74	0
25	CLA	B	601	65/65	0.89	0.16	0.43	36,49,72,80	0
25	CLA	C	510	65/65	0.91	0.22	0.43	36,46,58,68	0
25	CLA	c	505	65/65	0.92	0.16	0.43	32,40,48,51	0
23	LMG	D	409	51/55	0.93	0.17	0.42	31,48,74,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CLA	B	608	65/65	0.93	0.19	0.39	21,32,41,47	0
28	SQD	F	101	43/54	0.85	0.25	0.38	46,63,76,85	0
34	PHO	D	401	64/64	0.96	0.16	0.36	24,30,36,39	0
26	BCR	B	618	40/40	0.93	0.18	0.36	23,35,48,50	0
25	CLA	C	502	65/65	0.90	0.20	0.36	35,43,48,50	0
25	CLA	c	507	65/65	0.93	0.17	0.36	31,41,50,52	0
28	SQD	A	611	54/54	0.89	0.20	0.35	32,57,74,79	0
25	CLA	B	614	65/65	0.92	0.17	0.34	27,36,57,61	0
33	DGD	h	102	62/66	0.90	0.19	0.34	35,44,51,56	0
25	CLA	B	609	65/65	0.90	0.15	0.28	28,36,43,52	0
25	CLA	B	610	65/65	0.95	0.16	0.28	20,29,37,40	0
25	CLA	C	509	65/65	0.92	0.17	0.23	35,43,55,60	0
25	CLA	B	611	65/65	0.95	0.17	0.23	19,27,39,42	0
24	CL	a	605	1/1	0.97	0.17	0.23	38,38,38,38	1
23	LMG	C	519	51/55	0.77	0.26	0.20	48,64,79,84	0
25	CLA	B	604	65/65	0.93	0.20	0.20	20,32,50,65	0
25	CLA	c	512	65/65	0.91	0.19	0.19	44,57,65,68	0
25	CLA	B	603	65/65	0.95	0.16	0.12	21,31,48,53	0
35	HEM	V	201	43/43	0.97	0.14	0.11	31,38,46,48	0
25	CLA	B	615	65/65	0.93	0.15	0.09	28,36,47,55	0
25	CLA	b	608	65/65	0.94	0.20	0.07	28,40,49,56	0
25	CLA	B	612	65/65	0.94	0.17	0.05	25,31,40,44	0
25	CLA	C	504	65/65	0.92	0.20	0.04	35,49,67,75	0
32	UNL	b	623	13/-	0.88	0.17	0.02	37,44,53,54	0
33	DGD	c	517	62/66	0.93	0.17	0.01	33,45,66,77	0
25	CLA	C	503	65/65	0.91	0.17	0.00	32,44,49,50	0
24	CL	A	604	1/1	0.96	0.15	-0.01	35,35,35,35	0
26	BCR	h	101	40/40	0.87	0.18	-0.01	34,44,52,53	0
25	CLA	C	501	65/65	0.95	0.15	-0.04	21,34,46,51	0
25	CLA	C	506	65/65	0.93	0.13	-0.10	32,41,67,71	0
26	BCR	H	101	40/40	0.88	0.17	-0.11	32,37,53,54	0
25	CLA	b	614	65/65	0.93	0.16	-0.13	25,38,57,65	0
32	UNL	M	102	16/-	0.92	0.16	-0.17	28,43,53,56	0
35	HEM	E	102	43/43	0.94	0.18	-0.17	42,53,68,74	0
25	CLA	B	602	65/65	0.94	0.16	-0.20	21,34,47,50	0
25	CLA	C	511	65/65	0.90	0.18	-0.20	42,58,67,70	0
25	CLA	A	606	65/65	0.95	0.16	-0.20	19,29,35,47	0
35	HEM	e	101	43/43	0.94	0.15	-0.28	49,57,69,72	0
25	CLA	b	602	65/65	0.95	0.14	-0.31	29,41,55,60	0
25	CLA	b	611	65/65	0.94	0.17	-0.32	23,36,45,48	0
25	CLA	D	403	65/65	0.95	0.14	-0.32	23,30,39,49	0
31	BCT	a	618	4/4	0.90	0.13	-0.33	36,38,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UNL	C	520	15/-	0.91	0.14	-0.36	31,42,47,47	0
25	CLA	D	404	65/65	0.96	0.15	-0.36	18,28,40,43	0
25	CLA	d	401	65/65	0.95	0.15	-0.37	20,30,45,53	0
35	HEM	v	201	43/43	0.95	0.15	-0.40	29,39,47,55	0
25	CLA	B	613	65/65	0.95	0.18	-0.42	21,30,50,60	0
25	CLA	c	511	65/65	0.90	0.15	-0.46	39,54,62,66	0
25	CLA	a	606	65/65	0.95	0.16	-0.46	19,30,40,48	0
31	BCT	A	616	4/4	0.97	0.12	-0.51	28,33,33,38	0
25	CLA	b	615	65/65	0.93	0.14	-0.68	31,39,49,52	0
30	SO4	d	410	5/5	0.95	0.19	-0.76	73,73,83,84	0
24	CL	A	605	1/1	0.99	0.18	-1.10	26,26,26,26	0
21	OEX	A	601	10/10	0.98	0.13	-1.45	34,40,52,57	0
21	OEX	a	601	10/10	0.97	0.11	-2.70	33,37,46,51	0
22	FE	a	602	1/1	0.91	0.08	-3.06	37,37,37,37	0
22	FE	A	602	1/1	0.97	0.06	-6.06	34,34,34,34	0
32	UNL	B	626	9/-	0.83	0.27	-	35,40,44,47	0
30	SO4	A	615	5/5	0.93	0.28	-	49,50,62,64	0
32	UNL	B	625	16/-	0.90	0.15	-	37,42,49,50	0
32	UNL	b	626	9/-	0.90	0.27	-	32,45,53,56	0
30	SO4	O	302	5/5	0.94	0.32	-	65,66,78,80	0
32	UNL	M	101	10/-	0.86	0.22	-	45,49,60,62	0
30	SO4	a	617	5/5	0.91	0.21	-	52,57,70,79	0
32	UNL	I	101	14/-	0.89	0.16	-	32,41,48,49	0
32	UNL	i	101	16/-	0.84	0.23	-	33,42,48,48	0
32	UNL	m	101	10/-	0.85	0.21	-	44,53,58,59	0
30	SO4	O	301	5/5	0.89	0.32	-	51,67,76,82	0
32	UNL	b	625	16/-	0.83	0.18	-	37,43,48,49	0
30	SO4	U	201	5/5	0.94	0.14	-	47,60,63,71	5
30	SO4	o	301	5/5	0.94	0.29	-	62,68,71,91	0
32	UNL	k	101	9/-	0.93	0.26	-	44,52,56,56	0
30	SO4	u	201	5/5	0.95	0.19	-	63,66,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.