



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2017 – 12:21 AM EST

PDB ID : 5WS6
Title : Native XFEL structure of Photosystem II (preflash two-flash dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-12-05
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
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) : rb-20029077

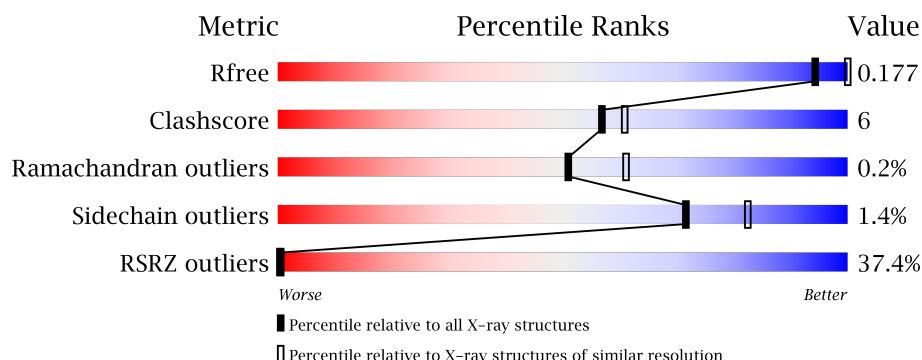
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>24%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>•</div> </div> </div>
1	a	344	<div> <div>33%</div> <div> <div></div> <div>97%</div> <div>•</div> </div> </div>
2	B	505	<div> <div>30%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
2	b	505	<div> <div>34%</div> <div> <div></div> <div>98%</div> <div>•</div> </div> </div>
3	C	455	<div> <div>38%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	A	402	-	-	-	X
22	CL	a	402	-	-	-	X
24	CLA	A	404	X	-	-	-
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	601	X	-	-	X
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	X
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	X
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	X
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	350	X	-	-	-
24	CLA	a	403	X	-	-	-
24	CLA	a	404	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	X
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	X
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	B	617	-	-	-	X
26	BCR	B	618	-	-	-	X
26	BCR	T	101	-	-	-	X
26	BCR	b	618	-	-	-	X
26	BCR	t	102	-	-	-	X
27	SQD	A	411	-	-	-	X
27	SQD	A	413	-	-	-	X
27	SQD	B	620	-	-	-	X
27	SQD	a	411	-	-	-	X
27	SQD	b	620	-	-	-	X
27	SQD	f	101	-	-	-	X
28	GOL	B	626	-	-	-	X
28	GOL	B	627	-	-	-	X
28	GOL	V	202	-	-	-	X
28	GOL	a	410	-	-	-	X
28	GOL	a	416	-	-	-	X
28	GOL	c	502	-	-	-	X
28	GOL	v	202	-	-	-	X
31	PL9	A	416[A]	-	-	-	X
31	PL9	A	416[B]	-	-	-	X
31	PL9	D	405	-	-	-	X
31	PL9	a	414[A]	-	-	-	X
31	PL9	a	414[B]	-	-	-	X
31	PL9	d	405	-	-	-	X
32	UNL	D	408	-	-	-	X
32	UNL	D	409	-	-	-	X
32	UNL	I	102	-	-	-	X
32	UNL	K	101	-	-	-	X
32	UNL	d	409	-	-	-	X
32	UNL	d	410	-	-	-	X
32	UNL	i	101	-	-	-	X
32	UNL	j	102	-	-	-	X
33	LMG	A	418	-	-	-	X
33	LMG	B	621	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	LMG	C	520	-	-	-	X
33	LMG	C	521	-	-	-	X
33	LMG	J	101	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	a	417	-	-	-	X
33	LMG	c	522	-	-	-	X
33	LMG	z	101	-	-	-	X
34	LMT	A	359	-	-	-	X
34	LMT	B	622	-	-	-	X
34	LMT	B	630	-	-	-	X
34	LMT	E	102	-	-	-	X
34	LMT	I	101	-	-	-	X
34	LMT	M	101	-	-	-	X
34	LMT	M	103	-	-	-	X
34	LMT	a	359	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	b	622	-	-	-	X
34	LMT	b	630	-	-	-	X
34	LMT	e	101	-	-	-	X
34	LMT	m	102	-	-	-	X
34	LMT	t	101	-	-	-	X
35	HTG	B	623	-	-	-	X
35	HTG	B	624	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	410	-	-	-	X
35	HTG	V	204	-	-	-	X
35	HTG	b	623	-	-	-	X
35	HTG	b	624	-	-	-	X
35	HTG	b	625	-	-	-	X
35	HTG	c	526	-	-	-	X
35	HTG	h	101	-	-	-	X
36	DGD	C	518	-	-	-	X
36	DGD	H	102	-	-	-	X
36	DGD	h	103	-	-	-	X
38	LHG	D	357	-	-	-	X
38	LHG	D	406	-	-	-	X
38	LHG	D	407	-	-	-	X
38	LHG	E	101	-	-	-	X
38	LHG	L	101	-	-	-	X
38	LHG	a	419	-	-	-	X
38	LHG	d	406	-	-	-	X
38	LHG	d	407	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	LHG	d	408	-	-	-	X
38	LHG	l	101	-	-	-	X
39	HEM	e	102	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II D1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	29	0
			2850	1865	467	502	16			
1	a	334	Total	C	N	O	S	0	29	0
			2852	1867	466	503	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	10	0
			3542	2315	590	624	13			
3	c	455	Total	C	N	O	S	0	10	0
			3577	2340	595	629	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2748	1819	450	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2739	1814	449	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		

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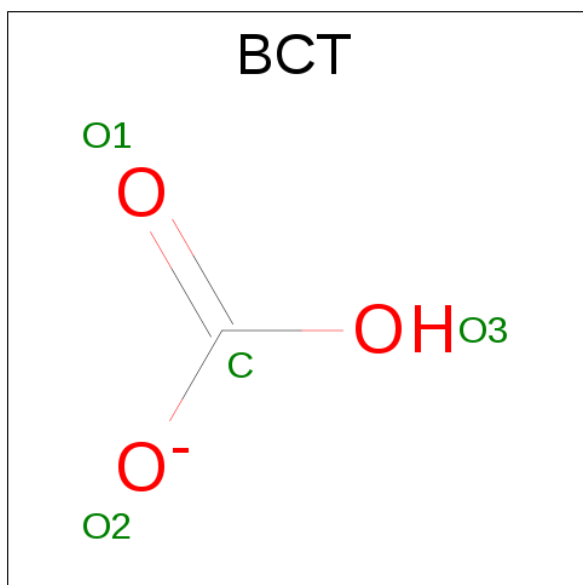
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	1
			2	2		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

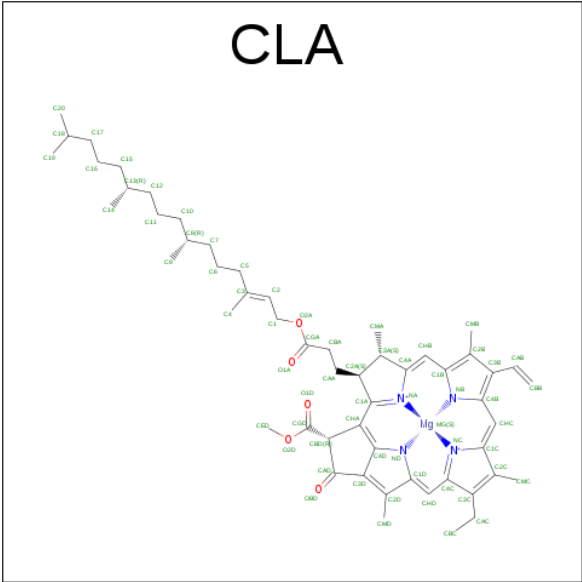
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	1
			8	2	6		
23	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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

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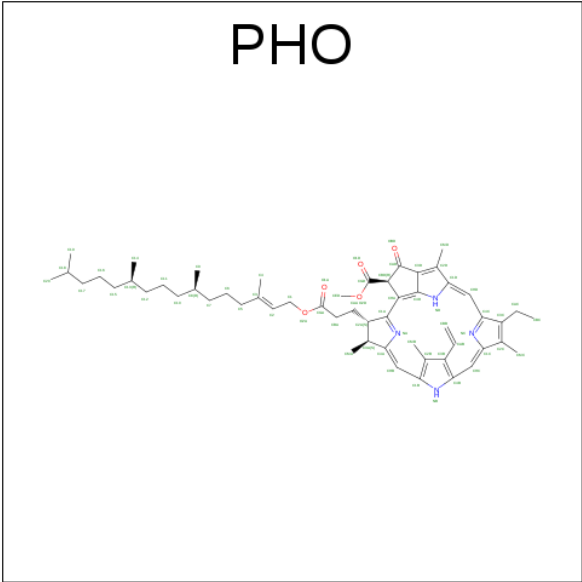
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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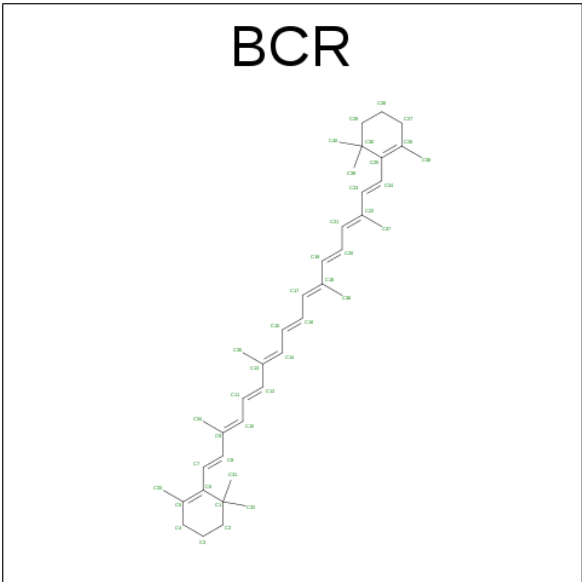
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



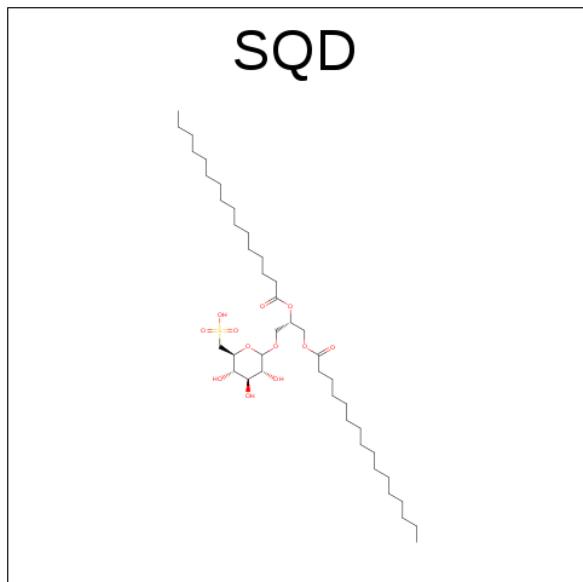
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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	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	Y	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
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	y	1	Total C 40 40	0	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



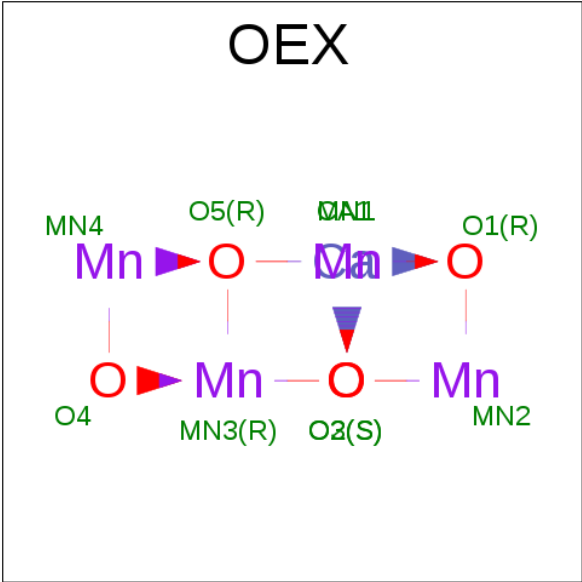
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0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

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



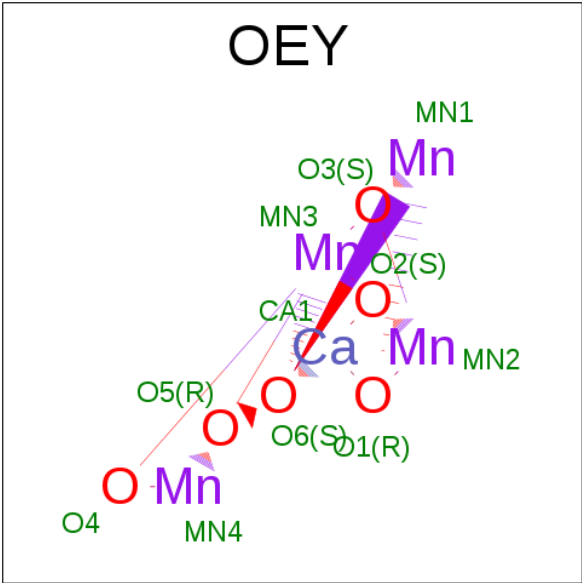
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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



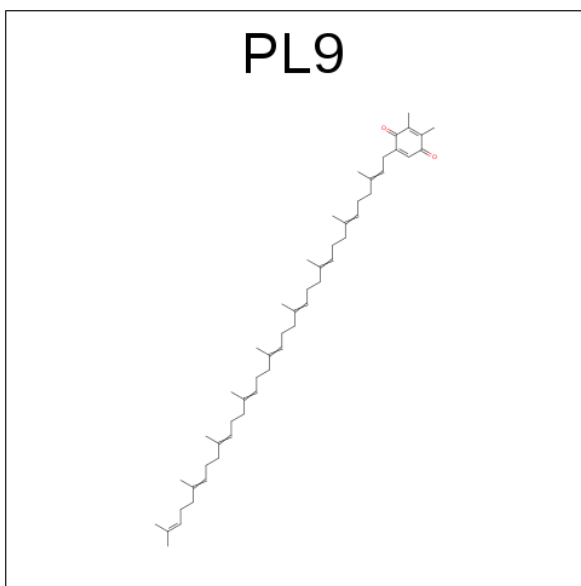
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 31 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
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	0
			55	53	2		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	0
			55	53	2		

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

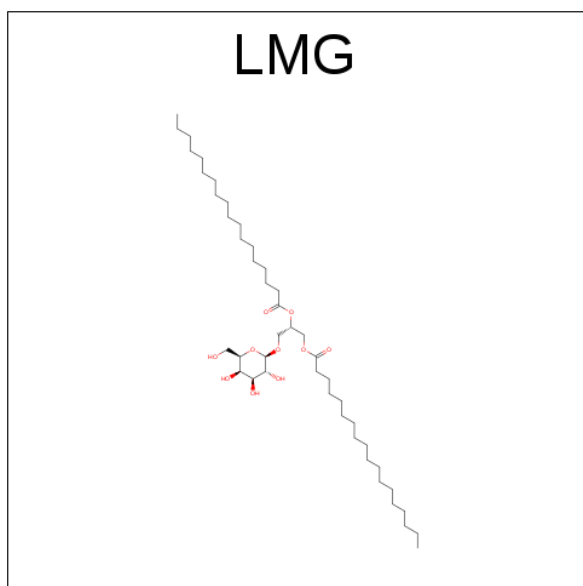
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	K	1	Total	C	O	0	0
			34	29	5		
32	B	1	Total	C	O	0	0
			33	28	5		

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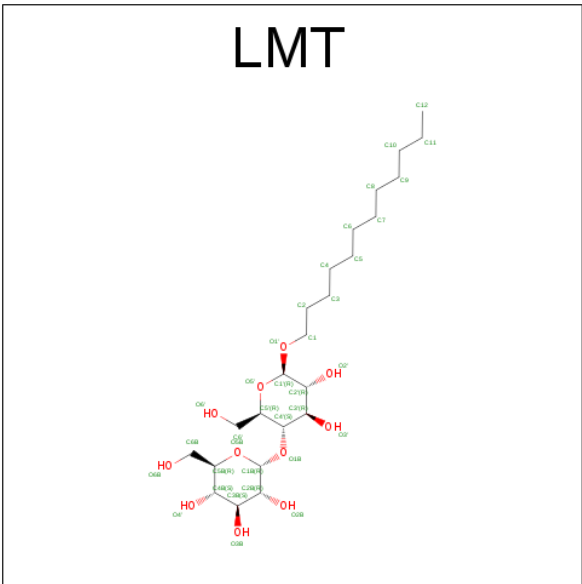
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	I	1	Total	C	O	0	0
			40	35	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	a	1	Total	C	O	0	0
			30	25	5		
32	x	1	Total	C	O	0	0
			18	16	2		
32	A	1	Total	C	O	0	0
			28	23	5		
32	j	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
			18	16	2		
32	d	2	Total	C	O	0	0
			53	47	6		
32	m	1	Total	C		0	0
			10	10			
32	b	1	Total	C	O	0	0
			33	28	5		
32	M	1	Total	C		0	0
			10	10			

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



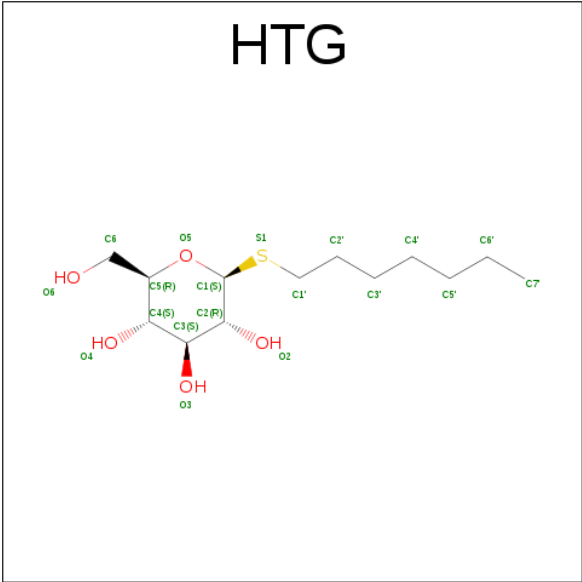
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			51	41	10		
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			35	24	11		
34	B	1	Total	C	O	0	0
			25	19	6		
34	E	1	Total	C	O	0	0
			35	24	11		
34	I	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	M	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	b	1	Total	C	O	0	0
			25	19	6		
34	e	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 35 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



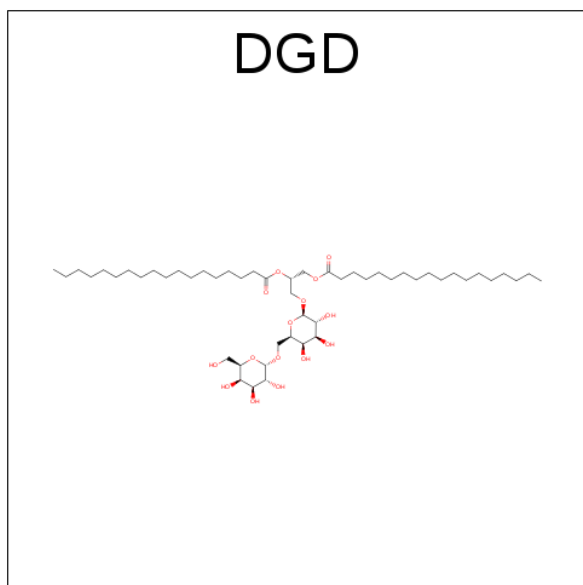
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O		0	0
			11	6	5			
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

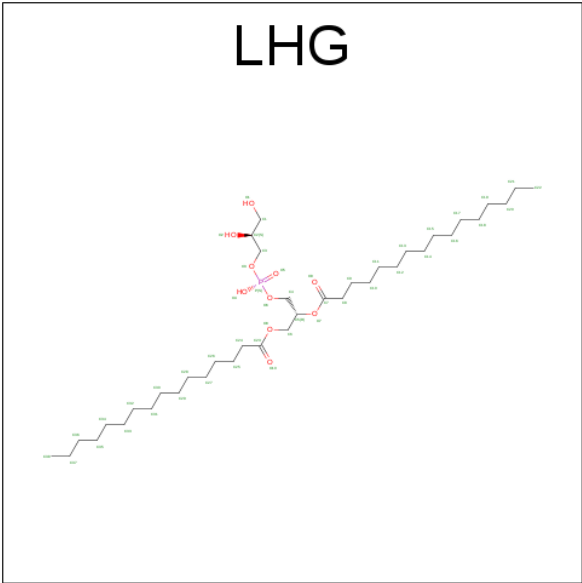


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	b	1	Total Ca 1 1	0	0
37	C	1	Total Ca 1 1	0	0
37	V	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0
37	v	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	D	1	Total C O P 49 38 10 1	0	0
38	E	1	Total C O P 42 31 10 1	0	0

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

- # HEM

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

- 

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	J	1	Total Mg 1 1	0	0
40	j	1	Total Mg 1 1	0	0

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	125	Total O 130 130	0	5
41	B	164	Total O 164 164	0	0
41	C	147	Total O 147 147	0	0
41	D	112	Total O 112 112	0	0
41	E	14	Total O 14 14	0	0
41	F	4	Total O 4 4	0	0
41	H	20	Total O 20 20	0	0
41	I	6	Total O 6 6	0	0
41	J	4	Total O 4 4	0	0
41	K	7	Total O 7 7	0	0
41	L	4	Total O 4 4	0	0
41	M	7	Total O 7 7	0	0
41	O	74	Total O 74 74	0	0
41	T	8	Total O 8 8	0	0
41	U	33	Total O 33 33	0	0
41	V	65	Total O 65 65	0	0
41	X	2	Total O 2 2	0	0
41	Y	1	Total O 1 1	0	0

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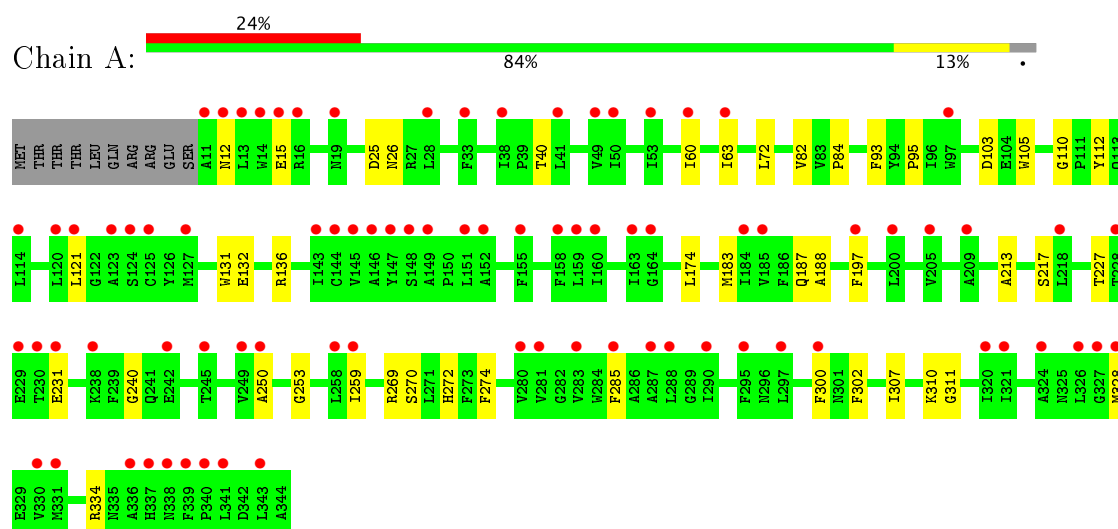
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	a	128	Total 133	O 133	0	5
41	b	185	Total 185	O 185	0	0
41	c	122	Total 122	O 122	0	0
41	d	109	Total 109	O 109	0	0
41	e	7	Total 7	O 7	0	0
41	f	3	Total 3	O 3	0	0
41	h	14	Total 14	O 14	0	0
41	i	3	Total 3	O 3	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	6	Total 6	O 6	0	0
41	m	11	Total 11	O 11	0	0
41	o	78	Total 78	O 78	0	0
41	t	5	Total 5	O 5	0	0
41	u	47	Total 47	O 47	0	0
41	v	49	Total 49	O 49	0	0
41	x	4	Total 4	O 4	0	0
41	y	1	Total 1	O 1	0	0

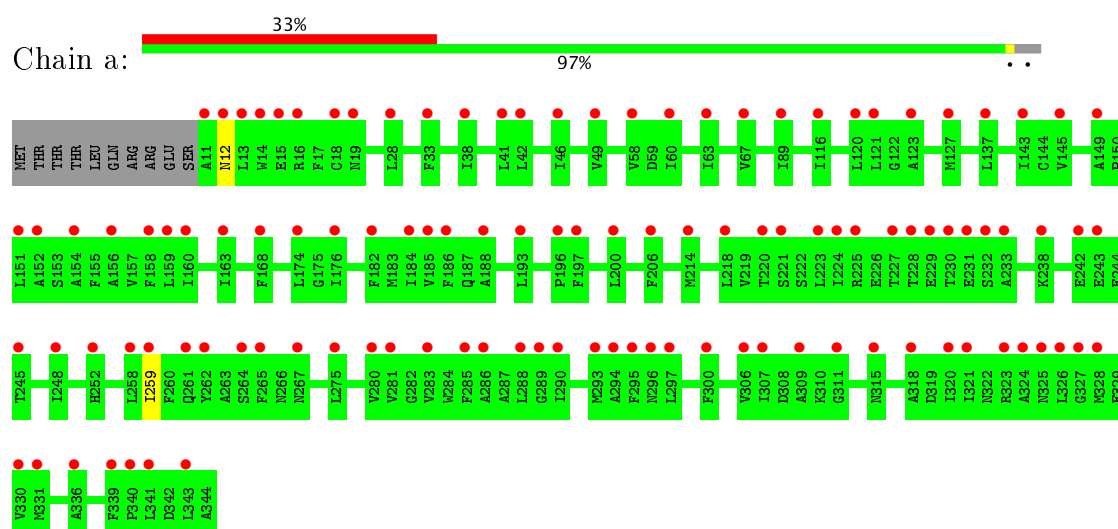
3 Residue-property plots [i](#)

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

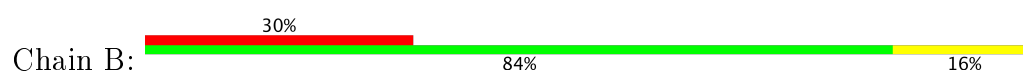
• Molecule 1: Photosystem II D1 protein

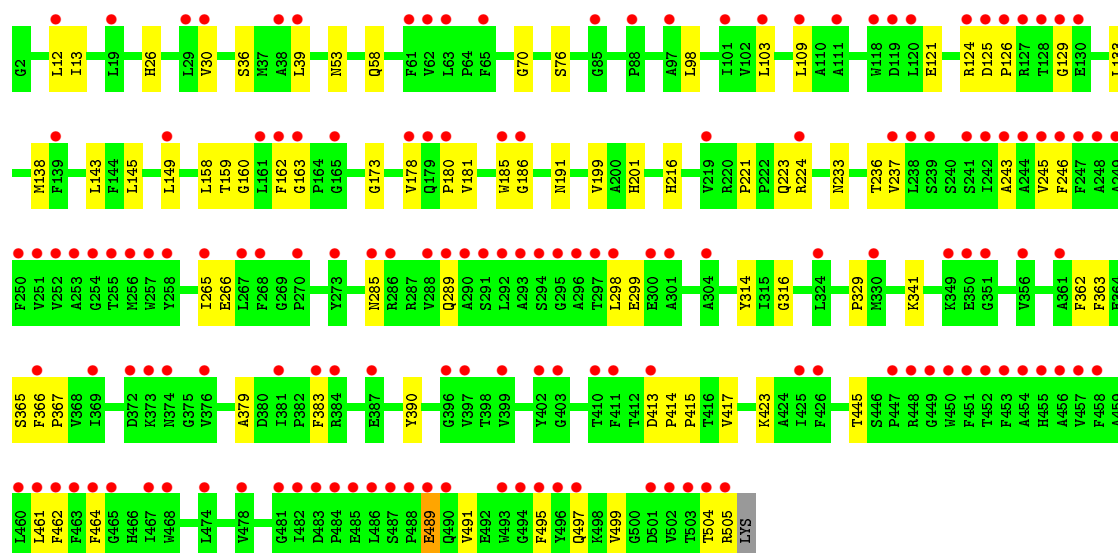


• Molecule 1: Photosystem II D1 protein

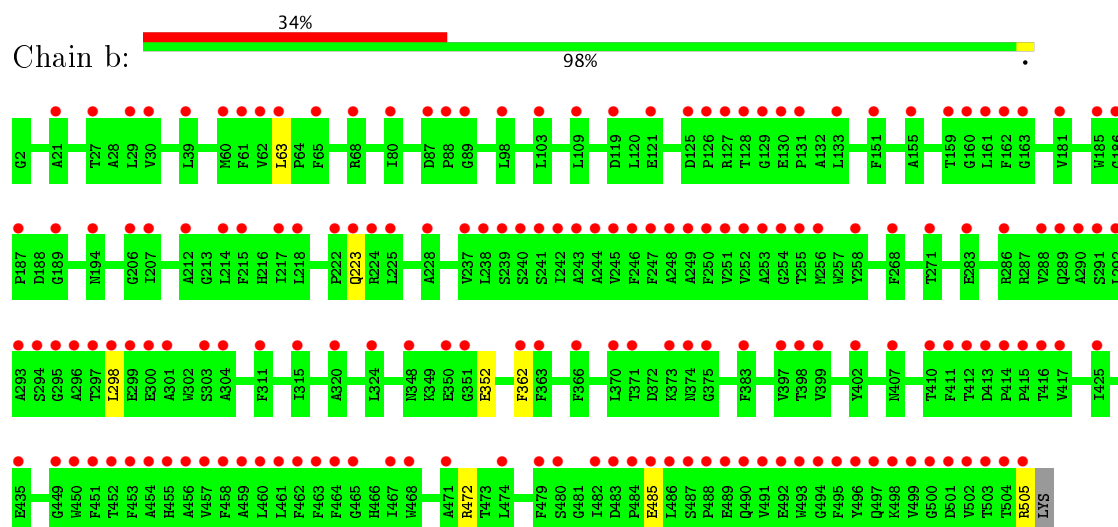


• Molecule 2: Photosystem II CP47 reaction center protein

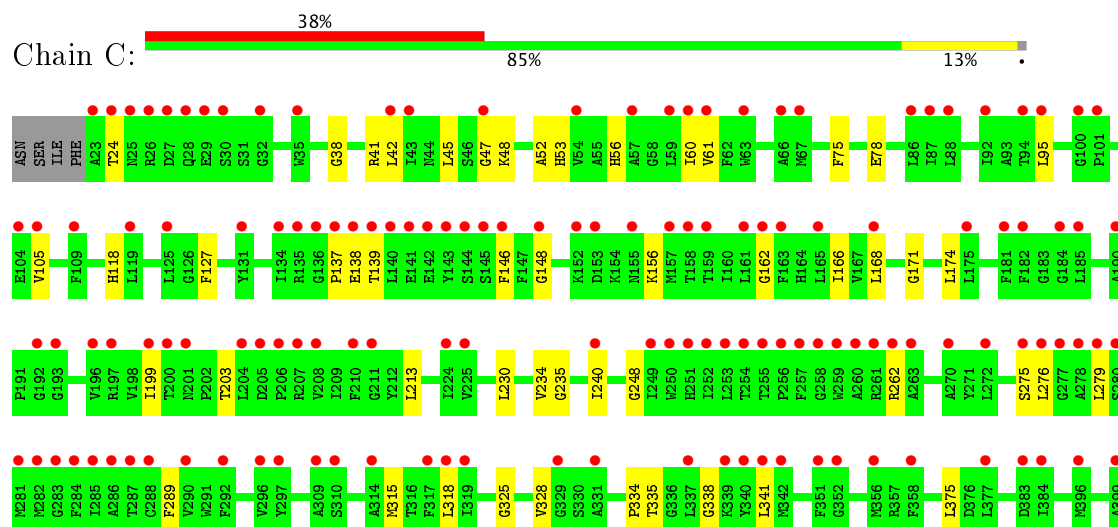


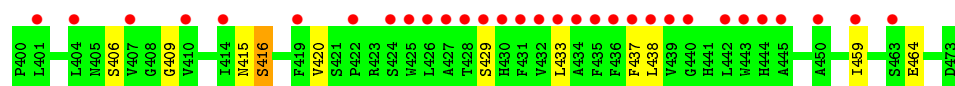


• Molecule 2: Photosystem II CP47 reaction center protein

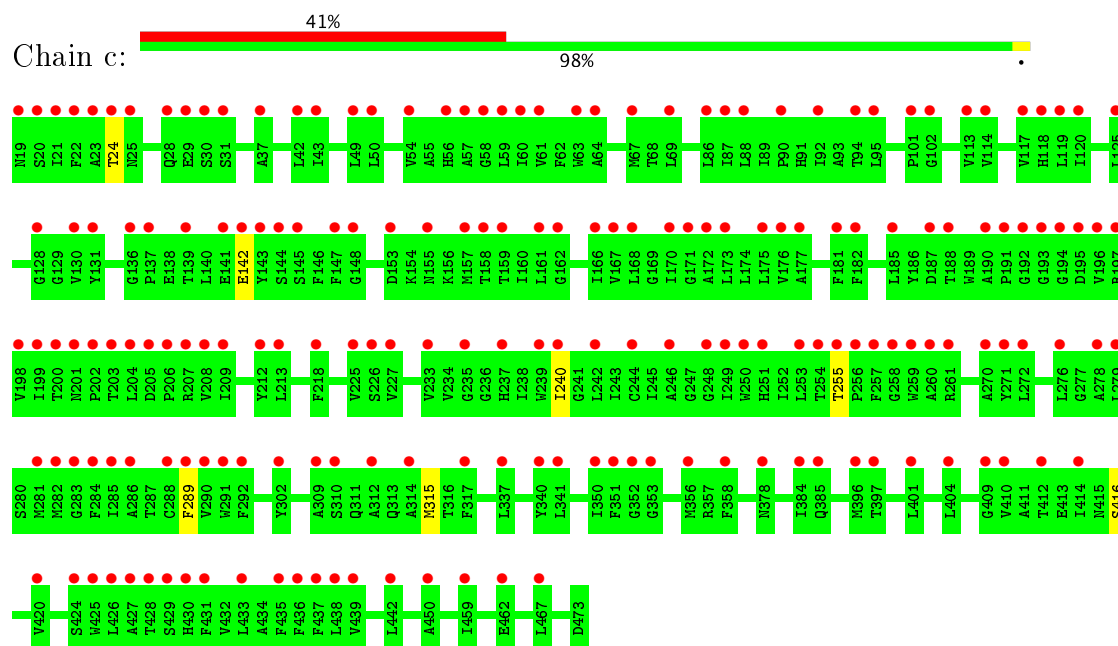


• Molecule 3: Photosystem II CP43 chlorophyll protein

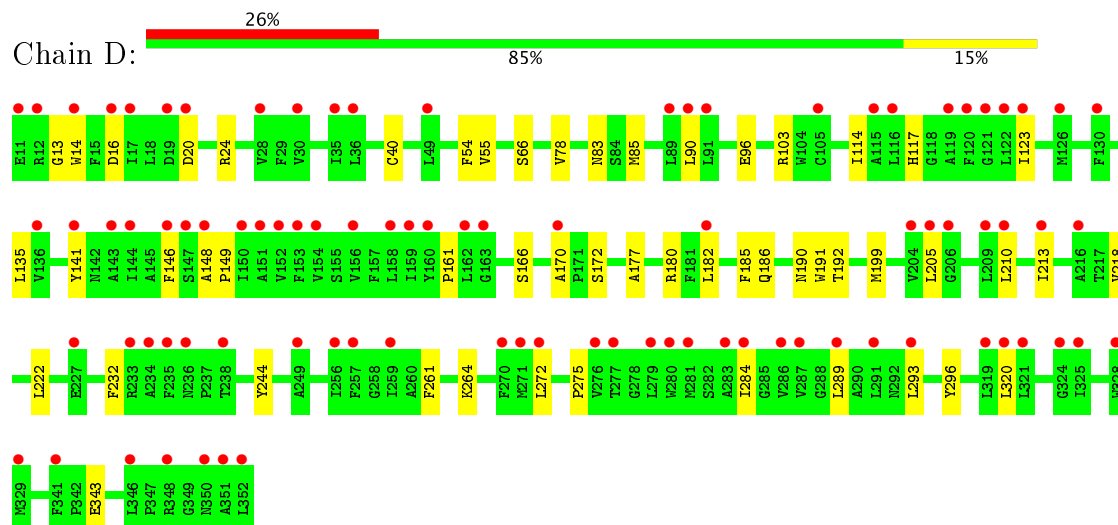




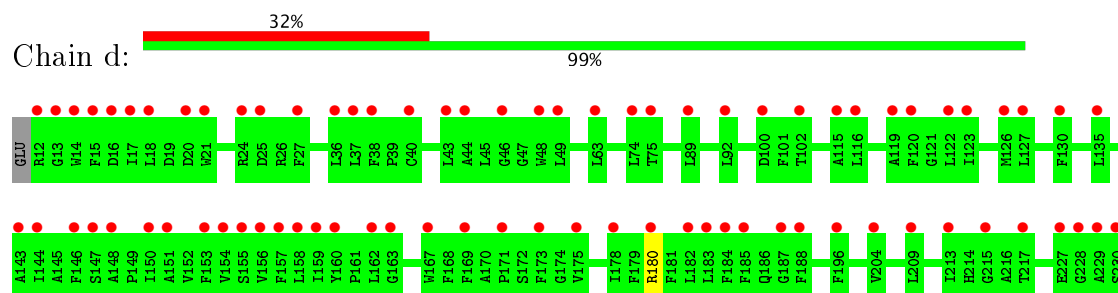
• Molecule 3: Photosystem II CP43 chlorophyll protein

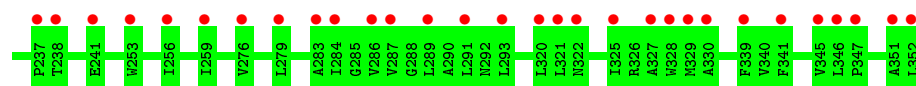


• Molecule 4: Photosystem II D2 protein

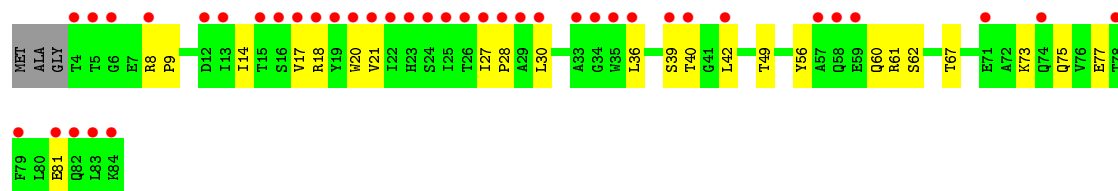


• Molecule 4: Photosystem II D2 protein

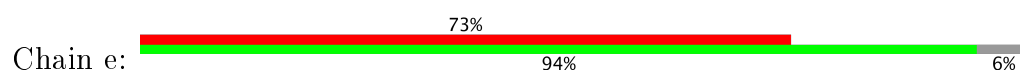




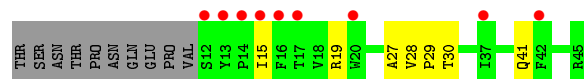
• Molecule 5: Cytochrome b559 subunit alpha



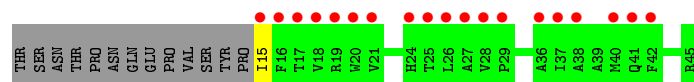
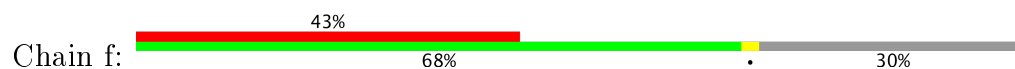
• Molecule 5: Cytochrome b559 subunit alpha



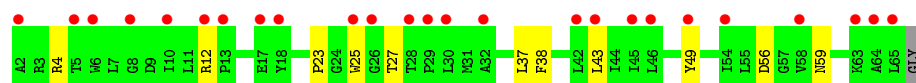
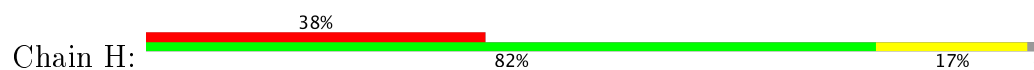
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta

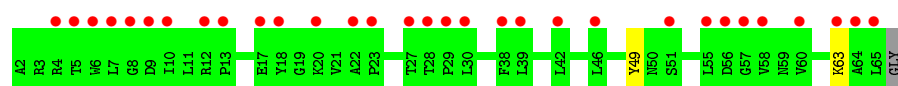


• Molecule 7: Photosystem II reaction center protein H

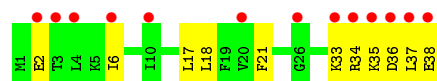


• Molecule 7: Photosystem II reaction center protein H

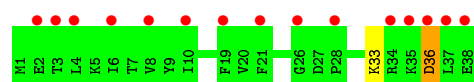




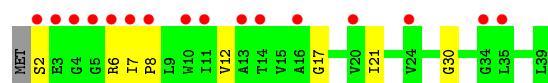
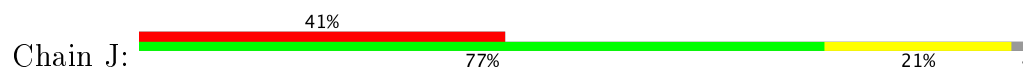
- Molecule 8: Photosystem II reaction center protein I



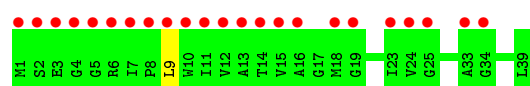
- Molecule 8: Photosystem II reaction center protein I



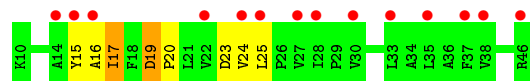
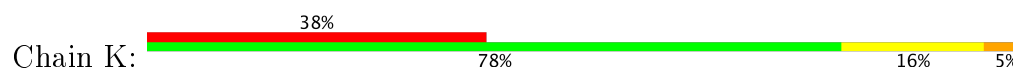
- Molecule 9: Photosystem II reaction center protein J



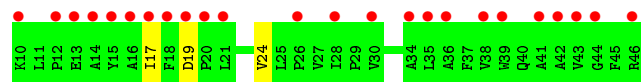
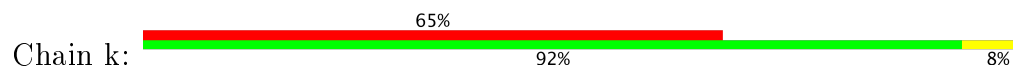
- Molecule 9: Photosystem II reaction center protein J



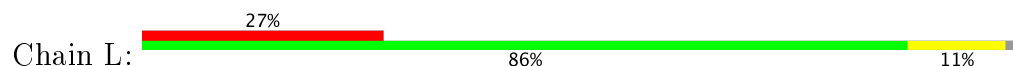
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

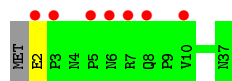


- Molecule 11: Photosystem II reaction center protein L

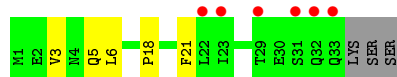
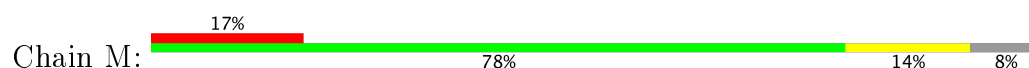




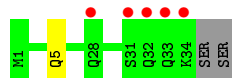
- Molecule 11: Photosystem II reaction center protein L



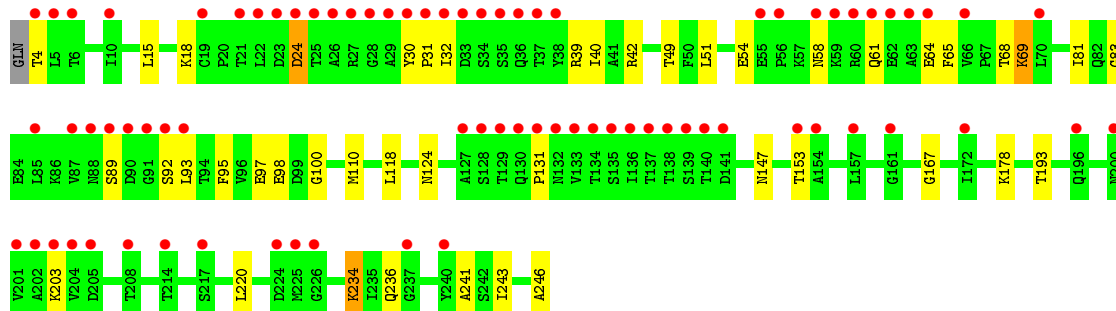
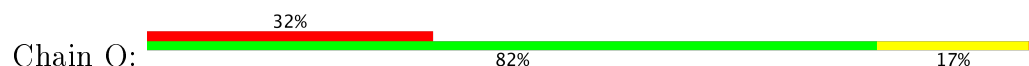
- Molecule 12: Photosystem II reaction center protein M



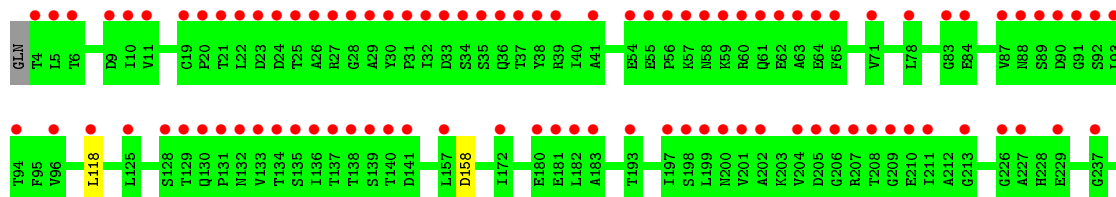
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

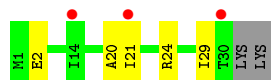
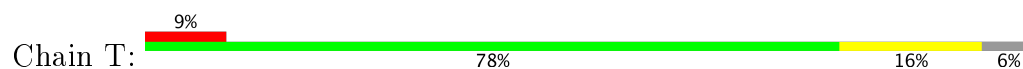


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

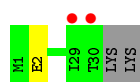




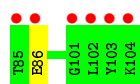
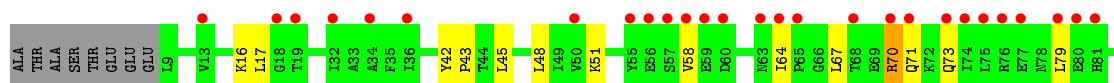
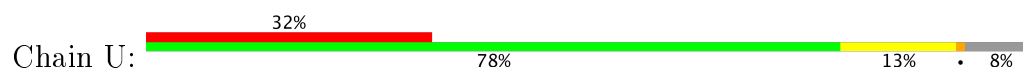
- Molecule 14: Photosystem II reaction center protein T



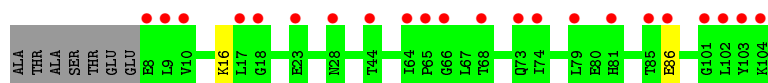
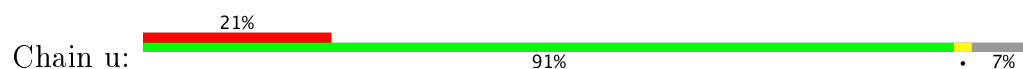
- Molecule 14: Photosystem II reaction center protein T



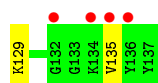
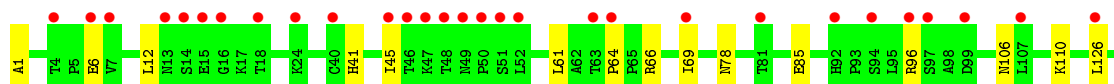
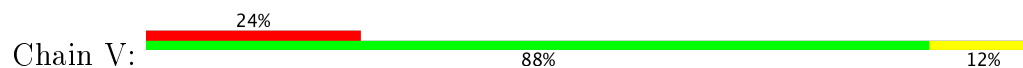
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

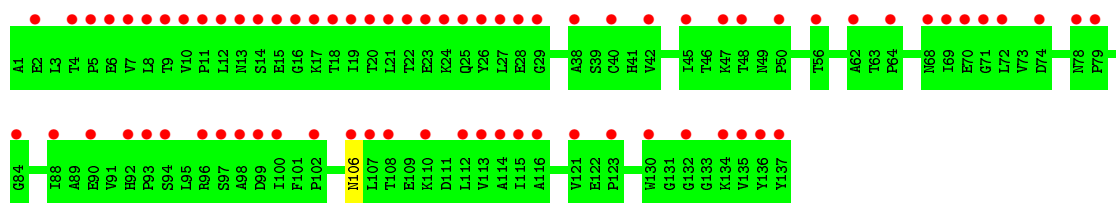


- Molecule 16: Cytochrome c-550

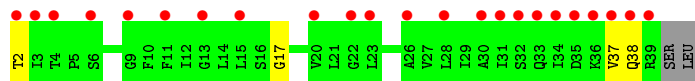
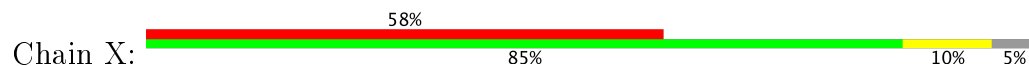


- Molecule 16: Cytochrome c-550

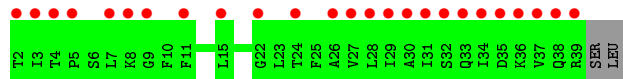




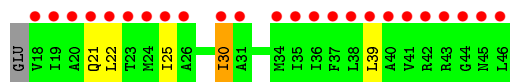
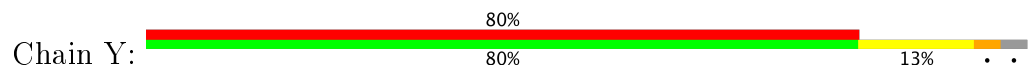
• Molecule 17: Photosystem II reaction center protein X



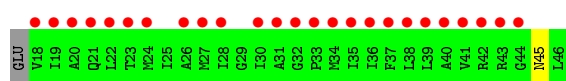
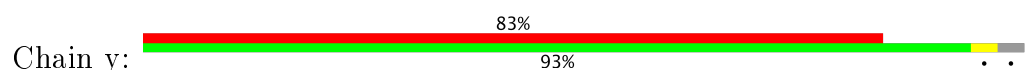
• Molecule 17: Photosystem II reaction center protein X



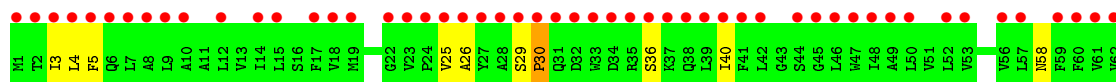
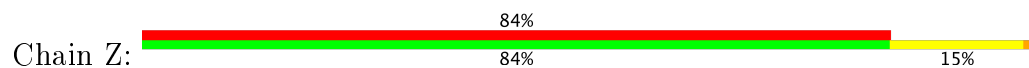
• Molecule 18: Photosystem II reaction center protein Ycf12



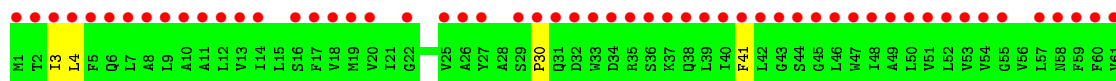
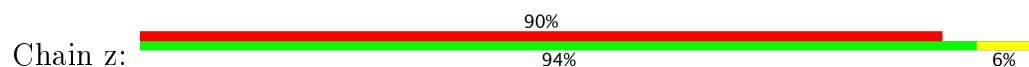
• Molecule 18: Photosystem II reaction center protein Ycf12



• Molecule 19: Photosystem II reaction center protein Z

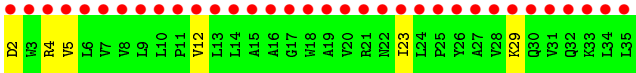
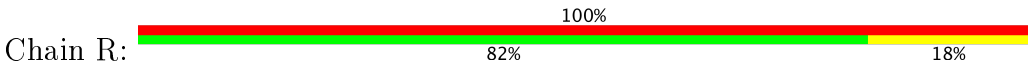


• Molecule 19: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.96Å 230.22Å 286.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 47.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 100.0 (47.05-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.129 , 0.175 0.136 , 0.177	Depositor DCC
R_{free} test set	17092 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	53280	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, OEY, LMG, FE2, BCT, HEM, FME, UNL, HTG, 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	0.50	0/2952	0.59	0/4019
1	a	0.43	0/2957	0.55	0/4027
2	B	0.43	0/4171	0.54	0/5683
2	b	0.41	0/4138	0.53	0/5640
3	C	0.42	0/3667	0.53	0/4992
3	c	0.38	0/3703	0.50	0/5041
4	D	0.46	0/2847	0.56	0/3878
4	d	0.43	0/2838	0.53	0/3866
5	E	0.36	0/687	0.50	0/936
5	e	0.35	0/667	0.47	0/908
6	F	0.42	0/284	0.50	0/387
6	f	0.38	0/257	0.53	0/349
7	H	0.37	0/530	0.57	0/723
7	h	0.33	0/519	0.50	0/708
8	I	0.37	0/311	0.48	0/419
8	i	0.34	0/311	0.49	0/419
9	J	0.34	0/278	0.46	0/376
9	j	0.32	0/283	0.46	0/383
10	K	0.37	0/303	0.51	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.43	0/311	0.47	0/423
11	l	0.41	0/311	0.49	0/423
12	M	0.45	0/261	0.61	0/357
12	m	0.42	0/262	0.59	0/357
13	O	0.39	0/1935	0.56	0/2623
13	o	0.39	0/1910	0.57	1/2589 (0.0%)
14	T	0.49	0/257	0.55	0/349
14	t	0.47	0/257	0.51	0/349
15	U	0.38	0/776	0.54	0/1052
15	u	0.37	0/785	0.54	0/1064
16	V	0.38	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.34	0/1085	0.48	0/1473
17	X	0.33	0/284	0.46	0/384
17	x	0.31	0/284	0.45	0/384
18	Y	0.29	0/216	0.44	0/289
18	y	0.30	0/216	0.47	0/289
19	Z	0.31	0/490	0.44	0/669
19	z	0.29	0/490	0.39	0/669
20	R	0.28	0/279	0.39	0/383
All	All	0.41	0/43500	0.53	1/59185 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2850	0	2705	36	0
1	a	2852	0	2708	0	0
2	B	4007	0	3879	71	0
2	b	3986	0	3855	0	0
3	C	3542	0	3462	61	0
3	c	3577	0	3498	0	0
4	D	2748	0	2650	47	0
4	d	2739	0	2644	0	0
5	E	665	0	653	22	0
5	e	648	0	634	0	0
6	F	275	0	282	7	0
6	f	250	0	261	0	0
7	H	514	0	542	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	506	0	529	0	0
8	I	314	0	328	8	0
8	i	314	0	328	0	0
9	J	272	0	279	8	0
9	j	277	0	284	0	0
10	K	293	0	305	8	0
10	k	293	0	305	0	0
11	L	301	0	315	5	0
11	l	301	0	315	0	0
12	M	265	0	286	5	0
12	m	269	0	288	0	0
13	O	1889	0	1871	28	0
13	o	1873	0	1852	0	0
14	T	258	0	261	5	0
14	t	258	0	261	0	0
15	U	765	0	767	9	0
15	u	774	0	773	0	0
16	V	1064	0	1073	12	0
16	v	1064	0	1073	0	0
17	X	281	0	312	6	0
17	x	281	0	312	0	0
18	Y	215	0	246	7	0
18	y	215	0	246	0	0
19	Z	479	0	516	6	0
19	z	479	0	516	0	0
20	R	273	0	305	6	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	19	0
24	B	1040	0	1152	69	0
24	C	845	0	936	92	0
24	D	130	0	144	12	0
24	a	260	0	288	0	0
24	b	1040	0	1152	0	0
24	c	845	0	936	0	0
24	d	130	0	144	0	0
25	A	128	0	148	6	0
25	a	128	0	148	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	40	0	56	2	0
26	B	120	0	168	13	0
26	C	80	0	112	7	0
26	D	40	0	56	5	0
26	H	40	0	56	3	0
26	K	40	0	56	1	0
26	T	40	0	56	6	0
26	Y	40	0	56	4	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	y	40	0	56	0	0
27	A	108	0	156	8	0
27	B	54	0	78	3	0
27	F	43	0	53	1	0
27	a	108	0	156	0	0
27	b	54	0	78	0	0
27	f	43	0	53	0	0
28	A	6	0	8	0	0
28	B	12	0	16	1	0
28	C	6	0	8	0	0
28	V	6	0	8	0	0
28	a	12	0	16	0	0
28	b	6	0	8	0	0
28	c	6	0	8	0	0
28	v	6	0	8	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	11	0	0	0	0
30	a	11	0	0	0	0
31	A	110	0	160	9	0
31	D	55	0	80	5	0
31	a	110	0	160	0	0
31	d	55	0	80	0	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	1	0
32	I	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	53	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
32	x	18	0	0	0	0
33	A	51	0	72	1	0
33	B	51	0	72	2	0
33	C	102	0	144	5	0
33	J	51	0	72	6	0
33	Z	37	0	44	6	0
33	a	51	0	72	0	0
33	b	51	0	72	0	0
33	c	102	0	144	0	0
33	j	51	0	72	0	0
33	z	39	0	48	0	0
34	A	35	0	46	4	0
34	B	60	0	81	3	0
34	E	35	0	46	1	0
34	I	35	0	46	1	0
34	M	70	0	92	3	0
34	a	70	0	92	0	0
34	b	50	0	70	0	0
34	e	35	0	46	0	0
34	m	35	0	46	0	0
34	t	26	0	35	0	0
35	B	76	0	104	9	0
35	C	38	0	52	2	0
35	D	16	0	17	2	0
35	V	11	0	10	0	0
35	b	76	0	104	0	0
35	c	38	0	52	0	0
35	h	16	0	17	0	0
36	C	186	0	246	10	0
36	H	62	0	82	2	0
36	c	186	0	246	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0
37	V	1	0	0	0	0
37	b	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
37	v	1	0	0	0	0
38	D	147	0	222	14	0
38	E	42	0	57	6	0
38	L	49	0	74	2	0
38	a	42	0	57	0	0
38	d	147	0	222	0	0
38	l	49	0	74	0	0
39	E	43	0	30	2	0
39	V	43	0	30	0	0
39	e	43	0	30	0	0
39	v	43	0	30	0	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	A	130	0	0	1	0
41	B	164	0	0	4	0
41	C	147	0	0	4	0
41	D	112	0	0	1	0
41	E	14	0	0	1	0
41	F	4	0	0	0	0
41	H	20	0	0	0	0
41	I	6	0	0	1	0
41	J	4	0	0	0	0
41	K	7	0	0	0	0
41	L	4	0	0	0	0
41	M	7	0	0	0	0
41	O	74	0	0	2	0
41	T	8	0	0	0	0
41	U	33	0	0	1	0
41	V	65	0	0	1	0
41	X	2	0	0	0	0
41	Y	1	0	0	0	0
41	a	133	0	0	0	0
41	b	185	0	0	0	0
41	c	122	0	0	0	0
41	d	109	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	e	7	0	0	0	0
41	f	3	0	0	0	0
41	h	14	0	0	0	0
41	i	3	0	0	0	0
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	6	0	0	0	0
41	m	11	0	0	0	0
41	o	78	0	0	0	0
41	t	5	0	0	0	0
41	u	47	0	0	0	0
41	v	49	0	0	0	0
41	x	4	0	0	0	0
41	y	1	0	0	0	0
All	All	53280	0	52671	514	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.

The worst 5 of 514 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)
24:C:514:CLA:HBB1	26:C:515:BCR:H24C	1.35	1.05
24:B:604:CLA:H42	24:B:605:CLA:H2	1.47	0.95
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.59	0.89
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.54	0.88
5:E:67:THR:H	5:E:75:GLN:HE22	2.55	0.83

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	359/344 (104%)	355 (99%)	3 (1%)	1 (0%)	44	53
1	a	360/344 (105%)	355 (99%)	4 (1%)	1 (0%)	44	53
2	B	510/505 (101%)	506 (99%)	4 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	38	44
3	c	463/455 (102%)	449 (97%)	12 (3%)	2 (0%)	38	44
4	D	343/342 (100%)	333 (97%)	10 (3%)	0	100	100
4	d	342/342 (100%)	336 (98%)	6 (2%)	0	100	100
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	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	11	9
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	3
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	27 (100%)	0	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	8
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	8
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5316/5384 (99%)	5202 (98%)	104 (2%)	10 (0%)	51	61

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER

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	295/279 (106%)	295 (100%)	0	100	100
1	a	296/279 (106%)	295 (100%)	1 (0%)	94	97
2	B	410/403 (102%)	405 (99%)	5 (1%)	75	86
2	b	406/403 (101%)	398 (98%)	8 (2%)	60	73
3	C	360/356 (101%)	357 (99%)	3 (1%)	85	91
3	c	364/356 (102%)	358 (98%)	6 (2%)	68	79
4	D	280/277 (101%)	279 (100%)	1 (0%)	93	96
4	d	279/277 (101%)	278 (100%)	1 (0%)	93	96
5	E	73/73 (100%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	36	46
7	H	55/54 (102%)	51 (93%)	4 (7%)	16	18
7	h	54/54 (100%)	53 (98%)	1 (2%)	62	75
8	I	34/34 (100%)	33 (97%)	1 (3%)	48	60
8	i	34/34 (100%)	32 (94%)	2 (6%)	23	26
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	38	48
10	K	30/30 (100%)	28 (93%)	2 (7%)	19	21
10	k	30/30 (100%)	27 (90%)	3 (10%)	9	8
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	34 (97%)	1 (3%)	48	60
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	43	54
13	O	211/207 (102%)	205 (97%)	6 (3%)	49	61
13	o	208/207 (100%)	207 (100%)	1 (0%)	91	95
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	25 (96%)	1 (4%)	38	48
15	U	83/89 (93%)	81 (98%)	2 (2%)	54	67
15	u	84/89 (94%)	82 (98%)	2 (2%)	54	67
16	V	117/117 (100%)	116 (99%)	1 (1%)	82	90
16	v	117/117 (100%)	116 (99%)	1 (1%)	82	90
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	32	40
18	y	22/23 (96%)	21 (96%)	1 (4%)	32	40
19	Z	52/52 (100%)	50 (96%)	2 (4%)	38	48
19	z	52/52 (100%)	49 (94%)	3 (6%)	23	27
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4416/4403 (100%)	4353 (99%)	63 (1%)	71	82

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	12	ASN
2	b	485	GLU
16	v	106	ASN
2	b	63	LEU
2	b	298	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
15	U	81	HIS
2	b	223	GLN
13	o	130	GLN
19	Z	58	ASN
2	b	53	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	9,9,10	0.57	0	7,9,11	1.22	1 (14%)
12	FME	M	1	12	9,9,10	0.62	0	7,9,11	1.47	1 (14%)
14	FME	T	1	14	9,9,10	0.63	0	7,9,11	1.36	1 (14%)
8	FME	i	1	8	9,9,10	0.60	0	7,9,11	1.50	2 (28%)
12	FME	m	1	12	9,9,10	0.72	0	7,9,11	1.26	0
14	FME	t	1	14	9,9,10	0.62	0	7,9,11	1.46	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-3.22	117.64	125.15
12	M	1	FME	O-C-CA	-2.51	119.30	125.15
8	I	1	FME	O-C-CA	-2.47	119.39	125.15
8	i	1	FME	O-C-CA	-2.44	119.46	125.15
14	T	1	FME	O-C-CA	-2.22	119.97	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 227 ligands modelled in this entry, 18 are unknown and 18 are monoatomic - leaving 191 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$
34	LMT	A	359	-	36,36,36	0.55	1 (2%)	47,47,47	0.90	1 (2%)
23	BCT	A	403[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
23	BCT	A	403[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	404	1	56,73,73	1.94	12 (21%)	65,113,113	2.38	22 (33%)
24	CLA	A	405	41	56,73,73	1.91	10 (17%)	65,113,113	2.32	23 (35%)
24	CLA	A	406	41	56,73,73	1.90	12 (21%)	65,113,113	2.15	23 (35%)
25	PHO	A	407	-	67,69,69	2.04	17 (25%)	87,99,99	1.98	24 (27%)
25	PHO	A	408	-	67,69,69	2.07	15 (22%)	87,99,99	2.12	25 (28%)
24	CLA	A	409	1	56,73,73	1.90	12 (21%)	65,113,113	2.27	23 (35%)
26	BCR	A	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.63	11 (19%)
27	SQD	A	411	-	53,54,54	0.91	3 (5%)	63,65,65	1.97	16 (25%)
28	GOL	A	412	-	5,5,5	0.38	0	5,5,5	0.30	0
27	SQD	A	413	-	53,54,54	0.99	3 (5%)	63,65,65	1.27	7 (11%)
29	OEX	A	414[A]	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
30	OEY	A	415[B]	1,3,41	1,17,17	1.13	0	0,39,39	0.00	-
31	PL9	A	416[A]	-	55,55,55	0.62	1 (1%)	69,69,69	1.94	23 (33%)
31	PL9	A	416[B]	-	55,55,55	0.62	1 (1%)	69,69,69	1.81	18 (26%)
33	LMG	A	418	-	51,51,55	0.89	2 (3%)	59,59,63	1.22	5 (8%)
24	CLA	B	601	41	56,73,73	1.96	11 (19%)	65,113,113	2.18	22 (33%)
24	CLA	B	602	2	56,73,73	1.92	12 (21%)	65,113,113	2.19	23 (35%)
24	CLA	B	603	2	56,73,73	1.90	12 (21%)	65,113,113	2.50	25 (38%)
24	CLA	B	604	2	56,73,73	1.88	11 (19%)	65,113,113	2.40	19 (29%)
24	CLA	B	605	2	56,73,73	1.86	11 (19%)	65,113,113	2.35	20 (30%)
24	CLA	B	606	2	56,73,73	1.81	10 (17%)	65,113,113	2.33	22 (33%)
24	CLA	B	607	41	56,73,73	1.87	12 (21%)	65,113,113	2.32	20 (30%)
24	CLA	B	608	2	56,73,73	1.90	10 (17%)	65,113,113	2.32	22 (33%)
24	CLA	B	609	2	56,73,73	1.87	11 (19%)	65,113,113	2.25	18 (27%)
24	CLA	B	610	41	56,73,73	1.96	11 (19%)	65,113,113	2.27	23 (35%)
24	CLA	B	611	2	56,73,73	1.84	11 (19%)	65,113,113	2.38	22 (33%)
24	CLA	B	612	2	56,73,73	1.90	12 (21%)	65,113,113	2.46	21 (32%)
24	CLA	B	613	2	56,73,73	1.94	12 (21%)	65,113,113	2.37	23 (35%)
24	CLA	B	614	2	56,73,73	1.86	12 (21%)	65,113,113	2.40	22 (33%)
24	CLA	B	615	2	56,73,73	1.83	10 (17%)	65,113,113	2.20	21 (32%)
24	CLA	B	616	2	56,73,73	1.90	11 (19%)	65,113,113	2.16	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	B	617	-	41,41,41	0.99	2 (4%)	56,56,56	1.53	10 (17%)
26	BCR	B	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.56	14 (25%)
26	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.48	14 (25%)
27	SQD	B	620	-	53,54,54	1.00	3 (5%)	63,65,65	1.55	11 (17%)
33	LMG	B	621	-	51,51,55	0.89	2 (3%)	59,59,63	1.13	3 (5%)
34	LMT	B	622	-	36,36,36	0.42	0	47,47,47	1.12	4 (8%)
35	HTG	B	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.41	4 (17%)
35	HTG	B	624	-	19,19,19	0.88	1 (5%)	23,24,24	1.59	1 (4%)
35	HTG	B	625	-	19,19,19	0.97	1 (5%)	23,24,24	1.83	2 (8%)
28	GOL	B	626	-	5,5,5	0.36	0	5,5,5	0.44	0
28	GOL	B	627	-	5,5,5	0.44	0	5,5,5	0.38	0
35	HTG	B	628	-	19,19,19	0.95	2 (10%)	23,24,24	1.46	3 (13%)
34	LMT	B	630	-	25,25,36	0.43	0	30,30,47	0.73	1 (3%)
24	CLA	C	502	3	56,73,73	1.89	12 (21%)	65,113,113	2.23	21 (32%)
24	CLA	C	503	3	56,73,73	1.90	11 (19%)	65,113,113	2.22	18 (27%)
24	CLA	C	504	3	56,73,73	1.85	12 (21%)	65,113,113	2.09	16 (24%)
24	CLA	C	505	41	56,73,73	1.89	12 (21%)	65,113,113	2.33	25 (38%)
24	CLA	C	506	3	56,73,73	1.87	12 (21%)	65,113,113	2.29	18 (27%)
24	CLA	C	507	3	56,73,73	1.87	12 (21%)	65,113,113	2.31	23 (35%)
24	CLA	C	508	41	56,73,73	1.88	12 (21%)	65,113,113	2.28	19 (29%)
24	CLA	C	509	3	56,73,73	1.99	12 (21%)	65,113,113	2.41	21 (32%)
24	CLA	C	510	3	56,73,73	2.01	12 (21%)	65,113,113	2.26	20 (30%)
24	CLA	C	511	3	56,73,73	1.91	12 (21%)	65,113,113	2.27	22 (33%)
24	CLA	C	512	3	56,73,73	1.96	12 (21%)	65,113,113	2.22	18 (27%)
24	CLA	C	513	3	56,73,73	1.92	12 (21%)	65,113,113	2.29	21 (32%)
24	CLA	C	514	3	56,73,73	1.92	12 (21%)	65,113,113	2.18	18 (27%)
26	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.49	8 (14%)
26	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.62	12 (21%)
36	DGD	C	517	-	63,63,67	0.80	2 (3%)	77,77,81	1.19	5 (6%)
36	DGD	C	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	6 (7%)
36	DGD	C	519	-	63,63,67	0.81	3 (4%)	77,77,81	0.96	4 (5%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.16	4 (6%)
33	LMG	C	521	-	51,51,55	0.99	3 (5%)	59,59,63	1.21	4 (6%)
35	HTG	C	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.60	2 (8%)
35	HTG	C	523	-	19,19,19	1.03	2 (10%)	23,24,24	1.91	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	C	525	-	5,5,5	0.40	0	5,5,5	0.12	0
38	LHG	D	357	-	48,48,48	0.87	2 (4%)	49,54,54	1.26	5 (10%)
24	CLA	D	402	4	56,73,73	1.86	12 (21%)	65,113,113	2.31	23 (35%)
24	CLA	D	403	4	56,73,73	1.89	11 (19%)	65,113,113	2.16	22 (33%)
26	BCR	D	404	-	41,41,41	1.02	1 (2%)	56,56,56	1.84	18 (32%)
31	PL9	D	405	-	55,55,55	0.65	2 (3%)	69,69,69	1.69	19 (27%)
38	LHG	D	406	-	48,48,48	0.87	3 (6%)	49,54,54	1.03	3 (6%)
38	LHG	D	407	-	48,48,48	0.89	2 (4%)	49,54,54	1.03	3 (6%)
35	HTG	D	410	-	16,16,19	1.06	2 (12%)	20,21,24	1.63	1 (5%)
38	LHG	E	101	-	41,41,48	1.00	2 (4%)	42,47,54	1.16	4 (9%)
34	LMT	E	102	-	36,36,36	0.47	0	47,47,47	0.87	0
39	HEM	E	103	5,6	28,50,50	0.89	1 (3%)	17,82,82	2.33	3 (17%)
27	SQD	F	101	-	42,43,54	1.13	3 (7%)	52,54,65	1.76	8 (15%)
26	BCR	H	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.47	10 (17%)
36	DGD	H	102	-	63,63,67	0.81	3 (4%)	77,77,81	0.96	4 (5%)
34	LMT	I	101	-	36,36,36	0.48	0	47,47,47	1.14	3 (6%)
33	LMG	J	101	40	51,51,55	0.87	2 (3%)	59,59,63	0.92	3 (5%)
26	BCR	K	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.61	12 (21%)
38	LHG	L	101	-	48,48,48	0.89	2 (4%)	49,54,54	1.12	4 (8%)
34	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.12	3 (6%)
34	LMT	M	103	-	36,36,36	0.42	0	47,47,47	0.99	3 (6%)
26	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.74	13 (23%)
28	GOL	V	202	-	5,5,5	0.33	0	5,5,5	0.35	0
39	HEM	V	203	16	28,50,50	0.97	3 (10%)	17,82,82	1.52	3 (17%)
35	HTG	V	204	-	11,11,19	0.23	0	13,15,24	1.07	1 (7%)
26	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.74	14 (25%)
33	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.53	7 (15%)
24	CLA	a	350	41	56,73,73	1.92	11 (19%)	65,113,113	2.18	18 (27%)
34	LMT	a	359	-	36,36,36	0.50	1 (2%)	47,47,47	0.94	2 (4%)
24	CLA	a	403	1	56,73,73	1.92	12 (21%)	65,113,113	2.44	25 (38%)
24	CLA	a	404	41	56,73,73	1.90	12 (21%)	65,113,113	2.14	20 (30%)
25	PHO	a	405	-	67,69,69	2.01	17 (25%)	87,99,99	2.03	25 (28%)
25	PHO	a	406	-	67,69,69	2.15	15 (22%)	87,99,99	2.00	25 (28%)
24	CLA	a	407	1	56,73,73	1.88	12 (21%)	65,113,113	2.35	24 (36%)
26	BCR	a	408	-	41,41,41	0.95	1 (2%)	56,56,56	1.55	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	a	409	-	53,54,54	0.93	3 (5%)	63,65,65	1.92	14 (22%)
28	GOL	a	410	-	5,5,5	0.34	0	5,5,5	0.34	0
27	SQD	a	411	-	53,54,54	1.02	3 (5%)	63,65,65	1.40	10 (15%)
29	OEX	a	412[A]	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
30	OXY	a	413[B]	1,3,41	1,17,17	4.21	1 (100%)	0,39,39	0.00	-
31	PL9	a	414[A]	-	55,55,55	0.61	1 (1%)	69,69,69	1.91	20 (28%)
31	PL9	a	414[B]	-	55,55,55	0.62	1 (1%)	69,69,69	1.82	19 (27%)
28	GOL	a	416	-	5,5,5	0.30	0	5,5,5	0.64	0
33	LMG	a	417	-	51,51,55	0.91	2 (3%)	59,59,63	1.20	6 (10%)
34	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.88	0
38	LHG	a	419	-	41,41,48	1.02	2 (4%)	42,47,54	0.94	2 (4%)
23	BCT	a	420[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
23	BCT	a	420[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	b	601	41	56,73,73	1.96	12 (21%)	65,113,113	2.21	19 (29%)
24	CLA	b	602	2	56,73,73	1.95	12 (21%)	65,113,113	2.17	24 (36%)
24	CLA	b	603	2	56,73,73	1.95	12 (21%)	65,113,113	2.37	21 (32%)
24	CLA	b	604	2	56,73,73	1.85	11 (19%)	65,113,113	2.32	20 (30%)
24	CLA	b	605	2	56,73,73	1.84	12 (21%)	65,113,113	2.28	18 (27%)
24	CLA	b	606	2	56,73,73	1.84	11 (19%)	65,113,113	2.26	22 (33%)
24	CLA	b	607	41	56,73,73	1.85	11 (19%)	65,113,113	2.26	20 (30%)
24	CLA	b	608	2	56,73,73	1.92	12 (21%)	65,113,113	2.24	22 (33%)
24	CLA	b	609	2	56,73,73	1.90	12 (21%)	65,113,113	2.28	20 (30%)
24	CLA	b	610	41	56,73,73	1.94	12 (21%)	65,113,113	2.33	21 (32%)
24	CLA	b	611	2	56,73,73	1.86	12 (21%)	65,113,113	2.20	17 (26%)
24	CLA	b	612	2	56,73,73	1.90	12 (21%)	65,113,113	2.35	22 (33%)
24	CLA	b	613	2	56,73,73	1.96	11 (19%)	65,113,113	2.27	19 (29%)
24	CLA	b	614	2	56,73,73	1.89	12 (21%)	65,113,113	2.31	19 (29%)
24	CLA	b	615	2	56,73,73	1.88	11 (19%)	65,113,113	2.16	20 (30%)
24	CLA	b	616	2	56,73,73	1.87	11 (19%)	65,113,113	2.27	22 (33%)
26	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.55	11 (19%)
26	BCR	b	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	16 (28%)
26	BCR	b	619	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	12 (21%)
27	SQD	b	620	-	53,54,54	1.00	3 (5%)	63,65,65	1.60	11 (17%)
33	LMG	b	621	-	51,51,55	0.85	2 (3%)	59,59,63	1.31	6 (10%)
34	LMT	b	622	-	25,25,36	0.45	0	30,30,47	0.74	0
35	HTG	b	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.58	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	b	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.61	1 (4%)
35	HTG	b	625	-	19,19,19	1.07	2 (10%)	23,24,24	2.01	2 (8%)
28	GOL	b	627	-	5,5,5	0.30	0	5,5,5	0.36	0
35	HTG	b	628	-	19,19,19	0.89	2 (10%)	23,24,24	1.36	3 (13%)
34	LMT	b	630	-	25,25,36	0.51	1 (4%)	30,30,47	0.89	0
28	GOL	c	502	-	5,5,5	0.38	0	5,5,5	0.32	0
24	CLA	c	503	3	56,73,73	1.91	12 (21%)	65,113,113	2.14	20 (30%)
24	CLA	c	504	3	56,73,73	1.86	11 (19%)	65,113,113	2.23	20 (30%)
24	CLA	c	505	3	56,73,73	1.86	12 (21%)	65,113,113	2.19	17 (26%)
24	CLA	c	506	41	56,73,73	1.96	12 (21%)	65,113,113	2.16	23 (35%)
24	CLA	c	507	3	56,73,73	1.89	12 (21%)	65,113,113	2.32	18 (27%)
24	CLA	c	508	3	56,73,73	1.94	11 (19%)	65,113,113	2.21	23 (35%)
24	CLA	c	509	41	56,73,73	1.88	11 (19%)	65,113,113	2.18	17 (26%)
24	CLA	c	510	3	56,73,73	1.99	12 (21%)	65,113,113	2.34	19 (29%)
24	CLA	c	511	3	56,73,73	1.94	12 (21%)	65,113,113	2.26	21 (32%)
24	CLA	c	512	3	56,73,73	1.90	12 (21%)	65,113,113	2.28	21 (32%)
24	CLA	c	513	3	56,73,73	1.93	12 (21%)	65,113,113	2.15	20 (30%)
24	CLA	c	514	3	56,73,73	1.90	12 (21%)	65,113,113	2.27	22 (33%)
24	CLA	c	515	3	56,73,73	1.92	12 (21%)	65,113,113	2.19	20 (30%)
26	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.76	12 (21%)
26	BCR	c	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	11 (19%)
36	DGD	c	518	-	63,63,67	0.82	2 (3%)	77,77,81	1.13	5 (6%)
36	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	4 (5%)
36	DGD	c	520	-	63,63,67	0.81	2 (3%)	77,77,81	1.12	3 (3%)
33	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)
33	LMG	c	522	-	51,51,55	0.95	2 (3%)	59,59,63	1.16	6 (10%)
35	HTG	c	523	-	19,19,19	0.95	1 (5%)	23,24,24	1.55	1 (4%)
35	HTG	c	526	-	19,19,19	1.01	2 (10%)	23,24,24	1.66	3 (13%)
24	CLA	d	402	4	56,73,73	1.88	12 (21%)	65,113,113	2.36	23 (35%)
24	CLA	d	403	4	56,73,73	1.91	11 (19%)	65,113,113	2.09	24 (36%)
26	BCR	d	404	-	41,41,41	1.12	2 (4%)	56,56,56	1.83	14 (25%)
31	PL9	d	405	-	55,55,55	0.60	1 (1%)	69,69,69	1.67	17 (24%)
38	LHG	d	406	-	48,48,48	0.88	3 (6%)	49,54,54	1.13	5 (10%)
38	LHG	d	407	-	48,48,48	0.87	2 (4%)	49,54,54	0.94	3 (6%)
38	LHG	d	408	-	48,48,48	0.89	2 (4%)	49,54,54	1.16	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMT	e	101	-	36,36,36	0.47	0	47,47,47	0.84	2 (4%)
39	HEM	e	102	5,6	28,50,50	0.88	1 (3%)	17,82,82	1.84	3 (17%)
27	SQD	f	101	-	42,43,54	1.14	3 (7%)	52,54,65	1.56	10 (19%)
35	HTG	h	101	-	16,16,19	1.13	2 (12%)	20,21,24	1.87	2 (10%)
26	BCR	h	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	11 (19%)
36	DGD	h	103	-	63,63,67	0.84	3 (4%)	77,77,81	0.99	3 (3%)
33	LMG	j	101	40	51,51,55	0.87	2 (3%)	59,59,63	1.16	5 (8%)
26	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	10 (17%)
38	LHG	l	101	-	48,48,48	0.89	2 (4%)	49,54,54	1.14	3 (6%)
34	LMT	m	102	-	36,36,36	0.43	0	47,47,47	0.92	1 (2%)
34	LMT	t	101	-	26,26,36	0.55	1 (3%)	31,31,47	1.17	2 (6%)
26	BCR	t	102	-	41,41,41	0.99	1 (2%)	56,56,56	1.70	15 (26%)
28	GOL	v	202	-	5,5,5	0.34	0	5,5,5	0.28	0
39	HEM	v	203	16	28,50,50	0.95	3 (10%)	17,82,82	1.53	2 (11%)
26	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	11 (19%)
33	LMG	z	101	-	39,39,55	1.06	2 (5%)	47,47,63	1.13	4 (8%)

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
34	LMT	A	359	-	-	0/21/61/61	0/2/2/2
23	BCT	A	403[A]	21	-	0/0/0/0	0/0/0/0
23	BCT	A	403[B]	21	-	0/0/0/0	0/0/0/0
24	CLA	A	404	1	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	405	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	406	41	3/3/20/25	0/37/135/135	0/0/9/9
25	PHO	A	407	-	-	0/53/103/103	0/1/6/6
25	PHO	A	408	-	-	0/53/103/103	0/1/6/6
24	CLA	A	409	1	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
27	SQD	A	411	-	-	0/49/69/69	0/1/1/1
28	GOL	A	412	-	-	0/4/4/4	0/0/0/0
27	SQD	A	413	-	-	0/49/69/69	0/1/1/1
29	OEX	A	414[A]	1,3,41	-	0/0/68/68	0/0/6/6
30	OXY	A	415[B]	1,3,41	-	0/0/86/86	0/0/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PL9	A	416[A]	-	-	0/53/73/73	0/1/1/1
31	PL9	A	416[B]	-	-	0/53/73/73	0/1/1/1
33	LMG	A	418	-	-	0/46/66/70	0/1/1/1
24	CLA	B	601	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	602	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	2	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
27	SQD	B	620	-	-	0/49/69/69	0/1/1/1
33	LMG	B	621	-	-	0/46/66/70	0/1/1/1
34	LMT	B	622	-	-	0/21/61/61	0/2/2/2
35	HTG	B	623	-	-	0/10/30/30	0/1/1/1
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
35	HTG	B	625	-	-	0/10/30/30	0/1/1/1
28	GOL	B	626	-	-	0/4/4/4	0/0/0/0
28	GOL	B	627	-	-	0/4/4/4	0/0/0/0
35	HTG	B	628	-	-	0/10/30/30	0/1/1/1
34	LMT	B	630	-	-	0/17/37/61	0/1/1/2
24	CLA	C	502	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	3	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	507	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	514	3	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2
36	DGD	C	518	-	-	0/51/91/95	0/2/2/2
36	DGD	C	519	-	-	0/51/91/95	0/2/2/2
33	LMG	C	520	-	-	0/46/66/70	0/1/1/1
33	LMG	C	521	-	-	0/46/66/70	0/1/1/1
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
35	HTG	C	523	-	-	0/10/30/30	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	0/0/0/0
38	LHG	D	357	-	-	0/53/53/53	0/0/0/0
24	CLA	D	402	4	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	D	403	4	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	404	-	-	0/29/63/63	0/2/2/2
31	PL9	D	405	-	-	0/53/73/73	0/1/1/1
38	LHG	D	406	-	-	0/53/53/53	0/0/0/0
38	LHG	D	407	-	-	0/53/53/53	0/0/0/0
35	HTG	D	410	-	-	0/7/27/30	0/1/1/1
38	LHG	E	101	-	-	0/46/46/53	0/0/0/0
34	LMT	E	102	-	-	0/21/61/61	0/2/2/2
39	HEM	E	103	5,6	-	0/6/54/54	0/0/8/8
27	SQD	F	101	-	-	2/38/58/69	0/1/1/1
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
34	LMT	I	101	-	-	0/21/61/61	0/2/2/2
33	LMG	J	101	40	-	0/46/66/70	0/1/1/1
26	BCR	K	102	-	-	0/29/63/63	0/2/2/2
38	LHG	L	101	-	-	0/53/53/53	0/0/0/0
34	LMT	M	101	-	-	0/21/61/61	0/2/2/2
34	LMT	M	103	-	-	0/21/61/61	0/2/2/2
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
28	GOL	V	202	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	HEM	V	203	16	-	0/6/54/54	0/0/8/8
35	HTG	V	204	-	-	0/2/19/30	0/1/1/1
26	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	2/31/51/70	0/1/1/1
24	CLA	a	350	41	3/3/20/25	0/37/135/135	0/0/9/9
34	LMT	a	359	-	-	0/21/61/61	0/2/2/2
24	CLA	a	403	1	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	a	404	41	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	a	405	-	-	0/53/103/103	0/1/6/6
25	PHO	a	406	-	-	0/53/103/103	0/1/6/6
24	CLA	a	407	1	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	a	408	-	-	0/29/63/63	0/2/2/2
27	SQD	a	409	-	-	0/49/69/69	0/1/1/1
28	GOL	a	410	-	-	0/4/4/4	0/0/0/0
27	SQD	a	411	-	-	0/49/69/69	0/1/1/1
29	OEX	a	412[A]	1,3,41	-	0/0/68/68	0/0/6/6
30	OXY	a	413[B]	1,3,41	-	0/0/86/86	0/0/7/7
31	PL9	a	414[A]	-	-	0/53/73/73	0/1/1/1
31	PL9	a	414[B]	-	-	0/53/73/73	0/1/1/1
28	GOL	a	416	-	-	0/4/4/4	0/0/0/0
33	LMG	a	417	-	-	0/46/66/70	0/1/1/1
34	LMT	a	418	-	-	0/21/61/61	0/2/2/2
38	LHG	a	419	-	-	0/46/46/53	0/0/0/0
23	BCT	a	420[A]	21	-	0/0/0/0	0/0/0/0
23	BCT	a	420[B]	21	-	0/0/0/0	0/0/0/0
24	CLA	b	601	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	602	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	603	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	604	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	2	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	614	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	2	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
27	SQD	b	620	-	-	0/49/69/69	0/1/1/1
33	LMG	b	621	-	-	0/46/66/70	0/1/1/1
34	LMT	b	622	-	-	0/17/37/61	0/1/1/2
35	HTG	b	623	-	-	0/10/30/30	0/1/1/1
35	HTG	b	624	-	-	0/10/30/30	0/1/1/1
35	HTG	b	625	-	-	0/10/30/30	0/1/1/1
28	GOL	b	627	-	-	0/4/4/4	0/0/0/0
35	HTG	b	628	-	-	0/10/30/30	0/1/1/1
34	LMT	b	630	-	-	0/17/37/61	0/1/1/2
28	GOL	c	502	-	-	0/4/4/4	0/0/0/0
24	CLA	c	503	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	505	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	3	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	509	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	514	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	515	3	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
26	BCR	c	517	-	-	0/29/63/63	0/2/2/2
36	DGD	c	518	-	-	0/51/91/95	0/2/2/2
36	DGD	c	519	-	-	0/51/91/95	0/2/2/2
36	DGD	c	520	-	-	0/51/91/95	0/2/2/2
33	LMG	c	521	-	-	0/46/66/70	0/1/1/1
33	LMG	c	522	-	-	0/46/66/70	0/1/1/1
35	HTG	c	523	-	-	0/10/30/30	0/1/1/1
35	HTG	c	526	-	-	0/10/30/30	0/1/1/1
24	CLA	d	402	4	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	403	4	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	d	404	-	-	0/29/63/63	0/2/2/2
31	PL9	d	405	-	-	0/53/73/73	0/1/1/1
38	LHG	d	406	-	-	0/53/53/53	0/0/0/0
38	LHG	d	407	-	-	0/53/53/53	0/0/0/0
38	LHG	d	408	-	-	0/53/53/53	0/0/0/0
34	LMT	e	101	-	-	0/21/61/61	0/2/2/2
39	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
27	SQD	f	101	-	-	2/38/58/69	0/1/1/1
35	HTG	h	101	-	-	0/7/27/30	0/1/1/1
26	BCR	h	102	-	-	0/29/63/63	0/2/2/2
36	DGD	h	103	-	-	0/51/91/95	0/2/2/2
33	LMG	j	101	40	-	0/46/66/70	0/1/1/1
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
38	LHG	l	101	-	-	0/53/53/53	0/0/0/0
34	LMT	m	102	-	-	0/21/61/61	0/2/2/2
34	LMT	t	101	-	-	0/17/38/61	0/1/1/2
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
28	GOL	v	202	-	-	0/4/4/4	0/0/0/0
39	HEM	v	203	16	-	0/6/54/54	0/0/8/8
26	BCR	y	101	-	-	0/29/63/63	0/2/2/2
33	LMG	z	101	-	-	0/34/54/70	0/1/1/1

The worst 5 of 1034 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	404	BCR	C23-C22	-5.30	1.34	1.45
26	K	102	BCR	C23-C22	-5.21	1.34	1.45
26	B	619	BCR	C23-C22	-5.17	1.34	1.45
26	k	101	BCR	C23-C22	-5.06	1.34	1.45
26	C	516	BCR	C23-C22	-5.06	1.34	1.45

The worst 5 of 2226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	CHD-C4C-C3C	-6.95	114.44	124.92
24	B	615	CLA	CHD-C4C-C3C	-6.91	114.51	124.92
24	B	605	CLA	CHD-C4C-C3C	-6.83	114.62	124.92
24	B	606	CLA	CHD-C4C-C3C	-6.74	114.77	124.92
24	c	507	CLA	C1C-NC-C4C	-6.56	103.28	107.06

5 of 191 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C8-O7-C10-O9
33	Z	101	LMG	C8-O7-C10-C11
27	f	101	SQD	C45-O47-C7-O49
27	F	101	SQD	C45-O47-C7-O49
27	f	101	SQD	C45-O47-C7-C8

There are no ring outliers.

81 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	359	LMT	4	0
24	A	404	CLA	10	0
24	A	405	CLA	3	0
24	A	406	CLA	5	0
25	A	407	PHO	2	0
25	A	408	PHO	4	0
24	A	409	CLA	3	0
26	A	410	BCR	2	0
27	A	411	SQD	6	0
27	A	413	SQD	2	0
31	A	416[A]	PL9	4	0
31	A	416[B]	PL9	5	0
33	A	418	LMG	1	0
24	B	601	CLA	3	0
24	B	602	CLA	7	0
24	B	603	CLA	3	0
24	B	604	CLA	4	0
24	B	605	CLA	10	0
24	B	606	CLA	7	0
24	B	607	CLA	1	0
24	B	609	CLA	7	0
24	B	610	CLA	2	0
24	B	611	CLA	2	0
24	B	612	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	613	CLA	7	0
24	B	614	CLA	8	0
24	B	615	CLA	4	0
24	B	616	CLA	6	0
26	B	617	BCR	3	0
26	B	618	BCR	4	0
26	B	619	BCR	6	0
27	B	620	SQD	3	0
33	B	621	LMG	2	0
34	B	622	LMT	3	0
35	B	623	HTG	5	0
35	B	624	HTG	3	0
35	B	625	HTG	1	0
28	B	627	GOL	1	0
24	C	502	CLA	7	0
24	C	503	CLA	8	0
24	C	504	CLA	10	0
24	C	505	CLA	6	0
24	C	506	CLA	8	0
24	C	507	CLA	15	0
24	C	508	CLA	6	0
24	C	509	CLA	8	0
24	C	510	CLA	8	0
24	C	511	CLA	8	0
24	C	512	CLA	12	0
24	C	513	CLA	8	0
24	C	514	CLA	11	0
26	C	515	BCR	4	0
26	C	516	BCR	3	0
36	C	517	DGD	2	0
36	C	518	DGD	2	0
36	C	519	DGD	6	0
33	C	521	LMG	5	0
35	C	522	HTG	2	0
38	D	357	LHG	2	0
24	D	402	CLA	7	0
24	D	403	CLA	5	0
26	D	404	BCR	5	0
31	D	405	PL9	5	0
38	D	406	LHG	5	0
38	D	407	LHG	7	0
35	D	410	HTG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	E	101	LHG	6	0
34	E	102	LMT	1	0
39	E	103	HEM	2	0
27	F	101	SQD	1	0
26	H	101	BCR	3	0
36	H	102	DGD	2	0
34	I	101	LMT	1	0
33	J	101	LMG	6	0
26	K	102	BCR	1	0
38	L	101	LHG	2	0
34	M	101	LMT	1	0
34	M	103	LMT	2	0
26	T	101	BCR	6	0
26	Y	101	BCR	4	0
33	Z	101	LMG	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 [i](#)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	1.54	82 (24%) 1 1	40, 48, 69, 120	1 (0%)
1	a	334/344 (97%)	1.80	113 (33%) 0 0	41, 52, 84, 120	0
2	B	504/505 (99%)	1.68	151 (29%) 1 0	41, 53, 83, 128	0
2	b	504/505 (99%)	1.86	172 (34%) 0 0	44, 57, 97, 149	0
3	C	451/455 (99%)	1.87	171 (37%) 0 0	43, 59, 81, 142	0
3	c	455/455 (100%)	2.02	188 (41%) 0 0	48, 67, 90, 129	0
4	D	342/342 (100%)	1.48	90 (26%) 1 1	38, 49, 68, 139	0
4	d	341/342 (99%)	1.66	108 (31%) 0 0	43, 55, 78, 147	0
5	E	81/84 (96%)	2.39	40 (49%) 0 0	53, 70, 100, 151	0
5	e	79/84 (94%)	3.56	61 (77%) 0 0	62, 78, 122, 140	0
6	F	34/44 (77%)	1.51	9 (26%) 1 1	52, 63, 90, 117	0
6	f	31/44 (70%)	2.78	19 (61%) 0 0	62, 68, 100, 140	0
7	H	64/65 (98%)	1.99	25 (39%) 0 0	49, 62, 81, 129	0
7	h	64/65 (98%)	2.26	31 (48%) 0 0	58, 69, 95, 147	0
8	I	37/38 (97%)	2.06	13 (35%) 0 0	55, 62, 127, 147	0
8	i	37/38 (97%)	2.07	15 (40%) 0 0	57, 66, 123, 138	0
9	J	38/39 (97%)	2.17	16 (42%) 0 0	51, 71, 129, 175	0
9	j	39/39 (100%)	2.88	23 (58%) 0 0	56, 80, 149, 175	0
10	K	37/37 (100%)	1.77	14 (37%) 0 0	60, 67, 89, 101	0
10	k	37/37 (100%)	2.45	24 (64%) 0 0	70, 77, 101, 117	0
11	L	36/37 (97%)	1.90	10 (27%) 1 1	41, 47, 109, 162	0
11	l	36/37 (97%)	1.51	7 (19%) 1 2	43, 48, 103, 152	0
12	M	32/36 (88%)	1.41	6 (18%) 1 2	43, 49, 74, 134	0
12	m	33/36 (91%)	1.59	5 (15%) 2 4	43, 50, 86, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	1.94	77 (31%) 0 0	40, 63, 115, 176	0
13	o	243/244 (99%)	2.07	100 (41%) 0 0	44, 65, 121, 161	0
14	T	29/32 (90%)	1.23	3 (10%) 7 11	42, 49, 81, 115	0
14	t	29/32 (90%)	1.18	2 (6%) 18 25	43, 50, 81, 130	0
15	U	96/104 (92%)	1.84	33 (34%) 0 0	47, 60, 90, 101	0
15	u	97/104 (93%)	1.38	22 (22%) 1 1	51, 62, 84, 121	0
16	V	137/137 (100%)	1.57	33 (24%) 1 1	46, 57, 82, 112	0
16	v	137/137 (100%)	2.43	74 (54%) 0 0	52, 71, 104, 137	0
17	X	38/40 (95%)	2.51	23 (60%) 0 0	59, 71, 96, 126	0
17	x	38/40 (95%)	3.16	25 (65%) 0 0	65, 78, 117, 154	0
18	Y	29/30 (96%)	4.46	24 (82%) 0 0	73, 87, 140, 155	0
18	y	29/30 (96%)	4.10	25 (86%) 0 0	79, 97, 126, 136	0
19	Z	62/62 (100%)	3.99	52 (83%) 0 0	67, 84, 131, 173	0
19	z	62/62 (100%)	4.84	56 (90%) 0 0	83, 99, 148, 185	0
20	R	34/34 (100%)	6.60	34 (100%) 0 0	97, 125, 149, 154	0
All	All	5283/5384 (98%)	1.98	1976 (37%) 0 0	38, 59, 104, 185	1 (0%)

The worst 5 of 1976 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	15.0
6	f	15	ILE	12.4
11	L	2	GLU	12.3
19	z	33	TRP	12.3
18	Y	19	ILE	11.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	FME	M	1	10/11	0.85	0.24	-	34,56,91,100	0
12	FME	m	1	10/11	0.89	0.18	-	47,60,91,103	0
8	FME	I	1	10/11	0.80	0.25	-	46,65,76,76	0
14	FME	t	1	10/11	0.89	0.17	-	43,51,75,84	0
8	FME	i	1	10/11	0.81	0.28	-	59,64,77,78	0
14	FME	T	1	10/11	0.86	0.19	-	44,50,74,88	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	UNL	K	101	34/-	0.28	0.61	10.03	83,119,134,150	0
32	UNL	j	102	10/-	0.52	0.59	9.94	87,106,117,118	0
34	LMT	B	630	25/35	0.43	0.47	8.47	54,89,147,148	0
28	GOL	v	202	6/6	0.71	0.78	8.46	75,86,94,96	0
32	UNL	d	410	36/-	0.44	0.59	7.81	73,100,136,140	0
32	UNL	d	409	17/-	0.80	0.66	7.49	68,83,111,114	0
35	HTG	B	624	19/19	0.57	0.35	7.25	71,103,114,115	0
34	LMT	a	359	35/35	0.31	0.49	6.47	65,144,151,154	0
35	HTG	D	410	16/19	0.21	0.51	6.19	82,121,136,138	0
34	LMT	A	359	35/35	0.30	0.52	6.06	73,134,144,148	0
34	LMT	b	630	25/35	0.50	0.43	5.83	57,81,151,153	0
32	UNL	D	408	17/-	0.83	0.58	5.56	66,85,107,110	0
28	GOL	a	416	6/6	0.65	0.35	5.45	55,82,84,86	0
38	LHG	D	357	49/49	0.75	0.49	5.21	49,64,86,102	0
34	LMT	M	103	35/35	0.44	0.37	5.07	68,146,169,171	0
28	GOL	V	202	6/6	0.78	0.74	5.03	64,74,85,92	0
35	HTG	b	624	19/19	0.47	0.43	4.51	114,128,145,170	0
35	HTG	b	623	19/19	0.47	0.41	4.50	68,88,130,131	0
28	GOL	a	410	6/6	0.73	0.31	4.38	79,81,90,95	0
27	SQD	A	413	54/54	0.52	0.42	4.37	63,91,128,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	GOL	c	502	6/6	0.91	0.54	4.30	68,70,71,75	0
38	LHG	D	407	49/49	0.79	0.42	4.15	53,61,120,125	0
28	GOL	B	626	6/6	0.94	0.32	4.14	85,88,90,95	0
31	PL9	A	416[A]	55/55	0.72	0.39	4.13	66,93,107,111	55
34	LMT	e	101	35/35	0.30	0.67	4.03	121,166,181,186	0
34	LMT	E	102	35/35	0.55	0.46	4.02	119,145,171,173	0
33	LMG	c	522	51/55	0.20	0.54	3.99	80,127,154,158	0
27	SQD	b	620	54/54	0.39	0.44	3.98	68,93,144,152	0
31	PL9	A	416[B]	55/55	0.72	0.39	3.89	66,93,108,113	55
33	LMG	a	417	51/55	0.41	0.52	3.86	76,100,122,129	0
38	LHG	D	406	49/49	0.83	0.40	3.84	47,57,76,93	0
32	UNL	D	409	40/-	0.58	0.43	3.76	67,93,136,140	0
31	PL9	a	414[A]	55/55	0.65	0.43	3.76	97,107,120,124	55
31	PL9	a	414[B]	55/55	0.65	0.43	3.75	97,107,120,124	55
27	SQD	a	411	54/54	0.49	0.43	3.67	72,95,139,149	0
35	HTG	B	623	19/19	0.60	0.35	3.64	70,88,128,128	0
33	LMG	C	521	51/55	0.28	0.46	3.49	68,121,155,157	0
26	BCR	B	618	40/40	0.83	0.34	3.42	44,57,70,77	0
38	LHG	d	407	49/49	0.78	0.36	3.38	48,59,73,85	0
22	CL	a	402	1/1	0.98	0.40	3.35	51,51,51,51	0
36	DGD	H	102	62/66	0.64	0.48	3.31	46,63,76,78	0
26	BCR	b	618	40/40	0.84	0.35	3.26	44,60,73,75	0
28	GOL	B	627	6/6	0.88	0.34	3.15	58,77,85,87	0
26	BCR	t	102	40/40	0.88	0.32	3.12	45,60,76,80	0
34	LMT	t	101	26/35	0.67	0.28	3.06	71,110,152,153	0
32	UNL	i	101	40/-	0.19	0.45	3.03	77,109,164,165	0
38	LHG	L	101	49/49	0.78	0.36	2.99	45,55,67,96	0
34	LMT	B	622	35/35	0.22	0.45	2.91	78,125,142,144	0
38	LHG	d	408	49/49	0.80	0.34	2.88	53,68,121,125	0
36	DGD	h	103	62/66	0.47	0.51	2.76	52,66,78,86	0
27	SQD	B	620	54/54	0.48	0.42	2.75	65,93,132,134	0
26	BCR	B	617	40/40	0.89	0.29	2.70	44,52,59,65	0
33	LMG	A	418	51/55	0.46	0.50	2.69	61,97,118,121	0
38	LHG	l	101	49/49	0.70	0.32	2.66	50,60,74,91	0
34	LMT	b	622	25/35	0.04	0.59	2.64	88,117,159,160	0
33	LMG	B	621	51/55	0.60	0.42	2.61	53,72,94,108	0
24	CLA	B	605	65/65	0.74	0.33	2.54	39,48,65,68	0
27	SQD	A	411	54/54	0.64	0.41	2.52	55,86,123,126	0
22	CL	A	402	1/1	0.98	0.33	2.48	44,44,44,44	0
38	LHG	d	406	49/49	0.79	0.38	2.47	50,66,90,106	0
26	BCR	T	101	40/40	0.84	0.33	2.46	46,57,68,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	B	601	65/65	0.78	0.30	2.45	53,77,112,132	0
36	DGD	C	518	62/66	0.67	0.37	2.43	48,67,127,131	0
31	PL9	D	405	55/55	0.92	0.34	2.41	37,49,62,78	0
35	HTG	C	523	19/19	0.48	0.54	2.40	84,153,166,186	0
35	HTG	b	625	19/19	0.15	0.45	2.34	91,138,154,196	0
32	UNL	I	102	40/-	0.47	0.39	2.32	66,113,156,158	0
33	LMG	J	101	51/55	0.76	0.30	2.22	48,73,119,126	0
38	LHG	E	101	42/49	0.36	0.45	2.10	72,118,132,132	0
31	PL9	d	405	55/55	0.89	0.29	2.09	41,50,66,85	0
24	CLA	b	608	65/65	0.76	0.40	2.00	46,58,81,84	0
33	LMG	b	621	51/55	0.62	0.36	1.97	53,74,105,124	0
25	PHO	a	405	64/64	0.89	0.31	1.95	41,49,56,64	0
24	CLA	C	505	65/65	0.69	0.40	1.88	42,56,103,113	0
34	LMT	I	101	35/35	0.21	0.49	1.86	110,145,160,162	0
24	CLA	b	605	65/65	0.79	0.34	1.84	43,52,70,74	0
35	HTG	V	204	11/19	0.83	0.44	1.84	104,117,122,125	0
36	DGD	c	518	62/66	0.73	0.37	1.82	49,67,95,103	0
24	CLA	c	505	65/65	0.68	0.41	1.82	58,67,77,83	0
38	LHG	a	419	42/49	0.25	0.51	1.80	78,141,167,179	0
36	DGD	C	517	62/66	0.73	0.40	1.79	43,63,104,106	0
24	CLA	B	608	65/65	0.77	0.35	1.75	41,54,68,71	0
24	CLA	C	504	65/65	0.70	0.40	1.71	47,58,76,85	0
28	GOL	C	525	6/6	0.83	0.40	1.68	66,73,76,78	0
27	SQD	a	409	54/54	0.74	0.30	1.64	63,85,127,131	0
35	HTG	c	526	19/19	0.12	0.58	1.64	114,161,170,200	0
25	PHO	A	407	64/64	0.86	0.31	1.61	35,45,54,58	0
24	CLA	b	610	65/65	0.79	0.34	1.60	47,58,73,75	0
36	DGD	C	519	62/66	0.78	0.28	1.57	43,60,94,116	0
34	LMT	a	418	35/35	0.35	0.50	1.55	113,136,151,151	0
24	CLA	b	603	65/65	0.74	0.38	1.55	46,56,85,92	0
24	CLA	C	506	65/65	0.75	0.36	1.50	49,57,92,100	0
24	CLA	B	604	65/65	0.80	0.38	1.48	34,46,123,127	0
24	CLA	b	607	65/65	0.81	0.30	1.47	35,49,77,87	0
35	HTG	b	628	19/19	0.50	0.31	1.45	61,82,106,112	0
28	GOL	b	627	6/6	0.74	0.29	1.45	97,106,113,116	0
32	UNL	X	101	18/-	0.75	0.27	1.39	57,76,100,100	0
33	LMG	c	521	51/55	0.62	0.39	1.37	68,101,145,156	0
36	DGD	c	519	62/66	0.73	0.34	1.37	56,73,136,145	0
24	CLA	B	609	65/65	0.63	0.30	1.34	47,57,73,80	0
24	CLA	B	614	65/65	0.80	0.25	1.34	38,49,103,113	0
24	CLA	B	610	65/65	0.84	0.31	1.34	43,53,64,80	0
32	UNL	x	101	18/-	0.69	0.27	1.33	70,85,105,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CL	A	347	1/1	0.98	0.37	1.31	49,49,49,49	0
35	HTG	h	101	16/19	0.24	0.51	1.28	98,133,140,163	0
24	CLA	c	510	65/65	0.76	0.30	1.27	53,63,141,145	0
36	DGD	c	520	62/66	0.84	0.28	1.27	55,64,100,116	0
27	SQD	f	101	43/54	0.25	0.51	1.25	118,136,170,175	0
24	CLA	B	603	65/65	0.83	0.34	1.23	42,52,69,76	0
24	CLA	b	612	65/65	0.78	0.34	1.20	43,54,64,75	0
24	CLA	B	607	65/65	0.81	0.30	1.18	32,45,71,78	0
24	CLA	B	611	65/65	0.76	0.34	1.17	37,47,63,73	0
25	PHO	A	408	64/64	0.86	0.27	1.16	37,49,57,60	0
34	LMT	m	102	35/35	0.19	0.45	1.16	63,95,117,121	0
24	CLA	C	511	65/65	0.81	0.42	1.15	49,61,74,88	0
24	CLA	a	350	65/65	0.76	0.27	1.15	36,46,63,77	0
33	LMG	C	520	51/55	0.65	0.42	1.13	56,90,127,140	0
24	CLA	c	512	65/65	0.71	0.39	1.07	50,65,81,92	0
24	CLA	b	602	65/65	0.61	0.38	1.04	51,62,79,88	0
24	CLA	c	507	65/65	0.71	0.30	1.04	49,61,91,95	0
24	CLA	B	602	65/65	0.71	0.34	1.04	45,55,80,84	0
26	BCR	C	516	40/40	0.88	0.30	1.04	53,62,72,81	0
24	CLA	C	509	65/65	0.76	0.35	1.03	44,57,115,131	0
24	CLA	B	613	65/65	0.80	0.36	1.02	37,47,94,103	0
26	BCR	b	617	40/40	0.88	0.25	0.98	45,52,63,63	0
33	LMG	Z	101	37/55	0.33	0.45	0.98	77,129,150,151	0
23	BCT	a	420[A]	4/4	0.92	0.22	0.97	58,63,63,68	4
23	BCT	a	420[B]	4/4	0.92	0.22	0.97	54,63,64,72	4
24	CLA	C	503	65/65	0.84	0.37	0.97	47,55,78,95	0
24	CLA	A	404	65/65	0.79	0.27	0.95	36,43,66,80	0
24	CLA	a	403	65/65	0.81	0.29	0.94	36,48,69,86	0
24	CLA	c	503	65/65	0.82	0.32	0.92	56,66,79,86	0
24	CLA	c	511	65/65	0.80	0.32	0.90	51,69,82,89	0
24	CLA	C	510	65/65	0.87	0.34	0.89	49,60,81,91	0
24	CLA	B	612	65/65	0.78	0.32	0.86	35,47,57,74	0
24	CLA	B	606	65/65	0.76	0.25	0.86	41,52,104,114	0
24	CLA	C	502	65/65	0.78	0.33	0.86	48,59,73,83	0
24	CLA	b	604	65/65	0.84	0.36	0.85	37,50,122,128	0
24	CLA	A	406	65/65	0.81	0.24	0.84	36,47,110,116	0
24	CLA	A	405	65/65	0.78	0.26	0.82	34,45,54,63	0
39	HEM	e	102	43/43	0.81	0.42	0.80	67,93,128,137	0
24	CLA	b	609	65/65	0.70	0.30	0.76	50,61,83,99	0
24	CLA	b	614	65/65	0.77	0.25	0.74	41,49,116,120	0
33	LMG	j	101	51/55	0.78	0.27	0.73	60,70,121,138	0
24	CLA	c	506	65/65	0.81	0.34	0.72	51,66,116,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	c	504	65/65	0.78	0.36	0.71	45,65,86,89	0
24	CLA	b	601	65/65	0.73	0.30	0.70	58,85,115,130	0
34	LMT	M	101	35/35	0.29	0.42	0.70	61,99,123,126	0
24	CLA	c	515	65/65	0.65	0.34	0.68	70,91,134,138	0
24	CLA	C	514	65/65	0.61	0.31	0.67	60,81,122,127	0
24	CLA	b	606	65/65	0.75	0.26	0.67	45,58,114,129	0
23	BCT	A	403[B]	4/4	0.88	0.24	0.65	55,61,62,78	4
22	CL	a	347	1/1	0.97	0.29	0.65	53,53,53,53	0
23	BCT	A	403[A]	4/4	0.88	0.24	0.65	58,60,60,69	4
24	CLA	d	402	65/65	0.82	0.29	0.65	39,48,74,86	0
25	PHO	a	406	64/64	0.82	0.28	0.62	41,55,63,65	0
33	LMG	z	101	39/55	0.39	0.42	0.60	84,133,148,153	0
24	CLA	b	613	65/65	0.84	0.33	0.59	42,49,101,106	0
24	CLA	a	404	65/65	0.80	0.27	0.57	42,53,126,133	0
35	HTG	B	628	19/19	0.68	0.25	0.55	65,80,89,95	0
24	CLA	C	508	65/65	0.80	0.30	0.54	49,60,80,82	0
26	BCR	a	408	40/40	0.87	0.23	0.46	42,52,65,68	0
24	CLA	b	611	65/65	0.81	0.28	0.36	41,52,73,82	0
26	BCR	A	410	40/40	0.91	0.22	0.34	42,51,61,62	0
24	CLA	D	402	65/65	0.81	0.24	0.31	31,45,68,82	0
29	OEX	A	414[A]	10/10	0.92	0.24	0.25	44,48,55,59	10
30	OEY	A	415[B]	11/11	0.92	0.23	0.21	43,49,55,56	11
30	OEY	a	413[B]	11/11	0.93	0.24	0.21	50,54,58,74	11
27	SQD	F	101	43/54	0.67	0.33	0.19	81,114,134,137	0
26	BCR	K	102	40/40	0.86	0.23	0.19	56,67,74,81	0
26	BCR	D	404	40/40	0.87	0.22	0.18	46,61,94,95	0
24	CLA	c	513	65/65	0.74	0.24	0.10	57,71,91,97	0
24	CLA	C	507	65/65	0.76	0.27	0.09	53,69,137,141	0
29	OEX	a	412[A]	10/10	0.92	0.24	0.04	50,55,61,74	10
24	CLA	C	513	65/65	0.76	0.24	-0.02	60,73,118,123	0
26	BCR	b	619	40/40	0.88	0.20	-0.05	51,62,81,84	0
24	CLA	c	514	65/65	0.77	0.26	-0.09	59,80,123,128	0
26	BCR	k	101	40/40	0.83	0.26	-0.10	58,73,84,90	0
24	CLA	A	409	65/65	0.87	0.21	-0.10	42,53,136,144	0
24	CLA	b	615	65/65	0.75	0.23	-0.10	46,59,81,86	0
24	CLA	c	509	65/65	0.81	0.25	-0.15	56,70,86,92	0
24	CLA	B	615	65/65	0.80	0.20	-0.16	37,52,74,83	0
24	CLA	d	403	65/65	0.82	0.20	-0.24	46,64,132,137	0
26	BCR	h	102	40/40	0.71	0.24	-0.26	56,70,80,81	0
40	MG	J	103	1/1	0.86	0.18	-0.32	61,61,61,61	0
24	CLA	C	512	65/65	0.72	0.23	-0.34	52,63,79,86	0
24	CLA	c	508	65/65	0.75	0.26	-0.34	60,72,120,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	BCR	H	101	40/40	0.79	0.21	-0.38	50,65,77,82	0
39	HEM	E	103	43/43	0.77	0.26	-0.39	60,70,80,93	0
24	CLA	D	403	65/65	0.85	0.21	-0.40	44,58,139,144	0
24	CLA	b	616	65/65	0.80	0.21	-0.40	50,60,124,127	0
24	CLA	a	407	65/65	0.90	0.19	-0.46	44,57,134,140	0
26	BCR	d	404	40/40	0.84	0.20	-0.61	53,67,96,98	0
26	BCR	B	619	40/40	0.87	0.18	-0.63	45,57,80,87	0
24	CLA	B	616	65/65	0.86	0.19	-0.66	45,58,147,153	0
39	HEM	V	203	43/43	0.84	0.19	-0.69	39,52,58,60	0
26	BCR	c	517	40/40	0.89	0.20	-0.70	56,67,80,81	0
26	BCR	Y	101	40/40	0.89	0.18	-0.92	57,68,74,81	0
26	BCR	C	515	40/40	0.86	0.16	-1.04	63,75,82,85	0
40	MG	j	103	1/1	0.91	0.17	-1.10	64,64,64,64	0
26	BCR	c	516	40/40	0.83	0.22	-1.23	77,86,93,96	0
39	HEM	v	203	43/43	0.86	0.17	-1.27	51,64,72,78	0
28	GOL	A	412	6/6	0.88	0.17	-1.56	80,82,86,98	0
37	CA	O	301	1/1	0.66	0.32	-1.59	119,119,119,119	0
37	CA	c	525	1/1	0.83	0.17	-1.69	92,92,92,92	0
37	CA	o	301	1/1	0.85	0.25	-1.69	108,108,108,108	0
37	CA	C	524	1/1	0.99	0.20	-1.78	72,72,72,72	0
37	CA	c	524	1/1	0.94	0.20	-2.37	78,78,78,78	0
26	BCR	y	101	40/40	0.83	0.16	-2.39	58,74,88,88	0
21	FE2	a	401[B]	1/1	0.99	0.07	-4.31	60,60,60,60	1
21	FE2	a	401[A]	1/1	0.99	0.07	-4.31	60,60,60,60	1
21	FE2	A	401[B]	1/1	0.99	0.05	-8.02	60,60,60,60	1
21	FE2	A	401[A]	1/1	0.99	0.05	-8.02	62,62,62,62	1
32	UNL	c	527	32/-	0.48	0.38	-	93,125,140,143	0
32	UNL	a	415	30/-	0.33	0.41	-	98,115,136,146	0
35	HTG	B	625	19/19	0.28	0.36	-	82,167,178,238	0
32	UNL	b	629	33/-	0.22	0.40	-	72,108,162,162	0
32	UNL	m	101	10/-	0.69	0.55	-	69,78,80,84	0
35	HTG	c	523	19/19	-0.05	0.61	-	118,144,148,169	0
37	CA	v	201	1/1	0.84	0.20	-	123,123,123,123	0
32	UNL	J	102	10/-	0.82	0.49	-	77,81,99,104	0
35	HTG	C	522	19/19	0.39	0.39	-	112,123,133,150	0
32	UNL	B	629	33/-	0.30	0.44	-	57,103,166,173	0
37	CA	V	201	1/1	0.09	0.21	-	141,141,141,141	0
32	UNL	A	417	28/-	0.24	0.44	-	98,110,128,144	0
32	UNL	M	102	10/-	0.82	0.47	-	62,72,86,92	0
37	CA	b	626	1/1	0.80	0.53	-	151,151,151,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.