wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:05 PM GMT

PDB ID	:	4UB8
Title	:	Native structure of photosystem II (dataset-2) by a femtosecond X-ray laser
Authors	:	Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.
Deposited on	:	2014-08-12
Resolution	:	1.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

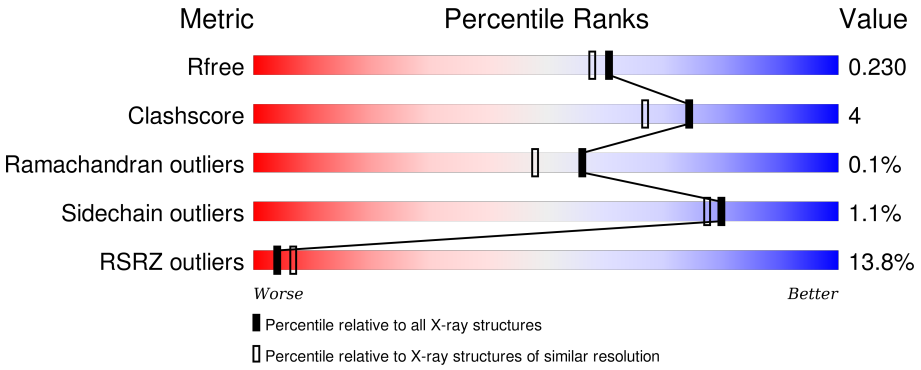
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 <=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	14% 90% 6%
1	a	344	20% 97%
2	B	505	9% 90% 10%
2	b	505	10% 99%
3	C	455	6% 90% 9%

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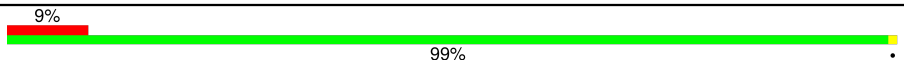
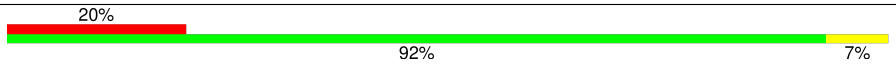
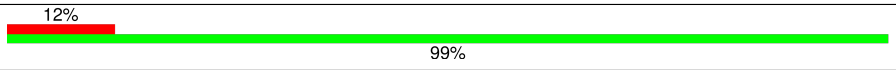
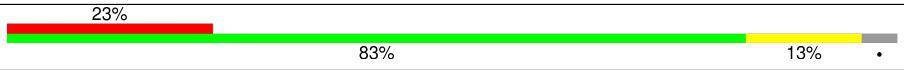
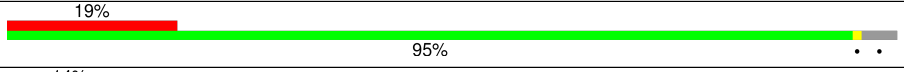
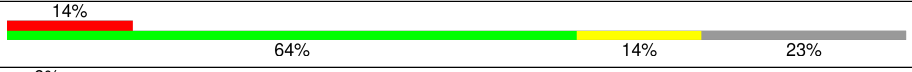
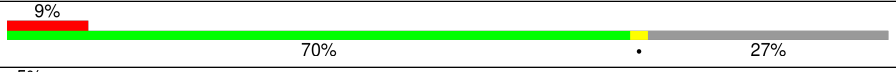
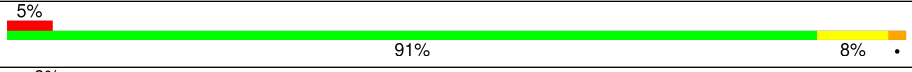
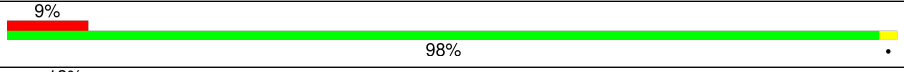
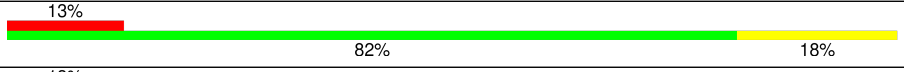
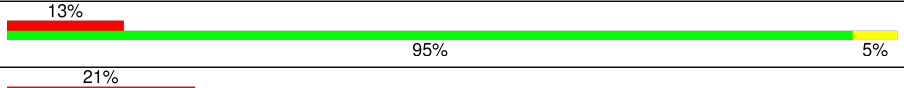
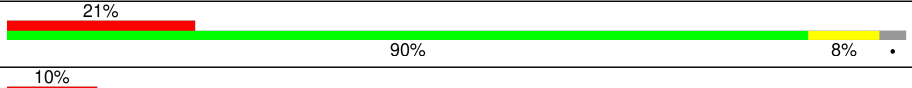
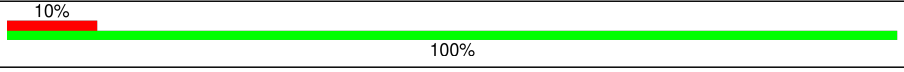
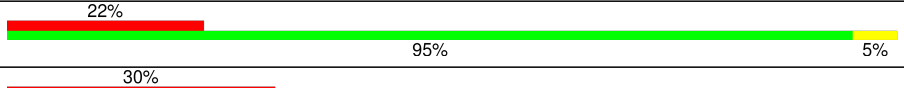
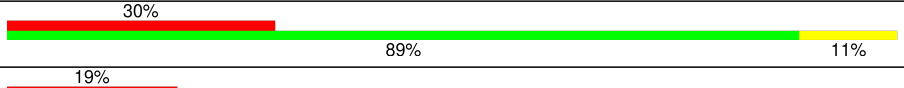
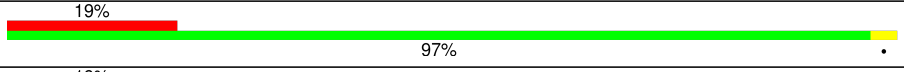
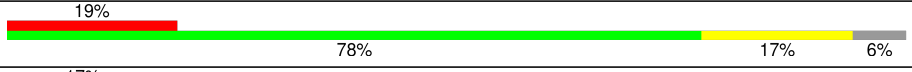
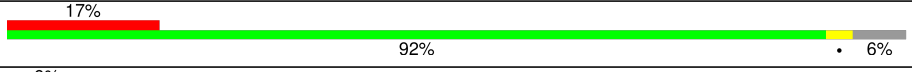
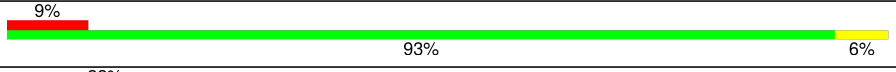
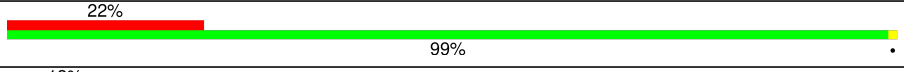
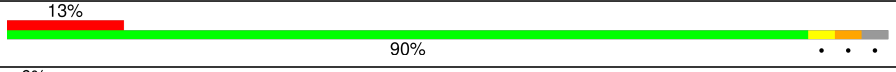
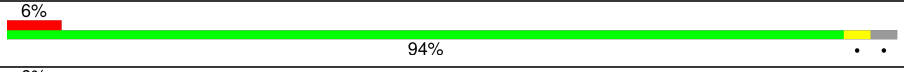
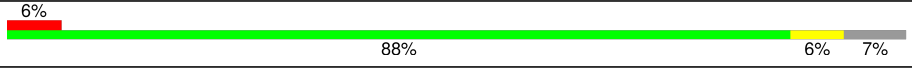
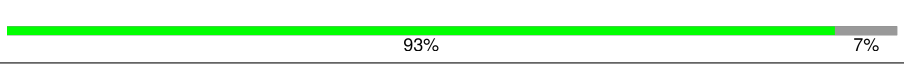
Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	104	
15	u	104	

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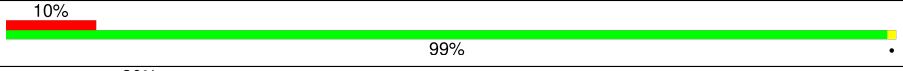
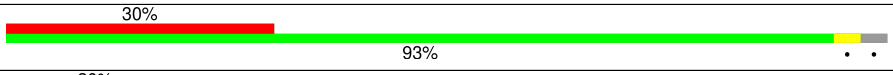
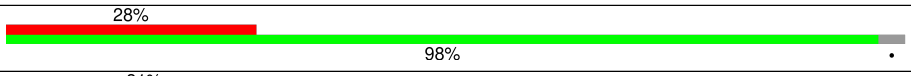
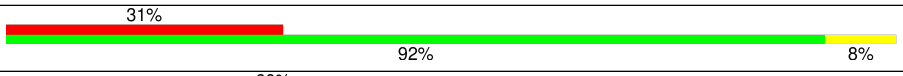
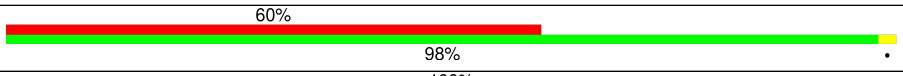
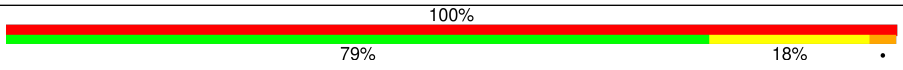
Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
23	BCT	a	418	-	-	-	X
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	602	X	-	-	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	-	-	-
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	B	617	X	-	-	X
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	504	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	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	606	X	-	-	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	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	404	X	-	-	-
26	BCR	B	619	-	-	-	X
26	BCR	b	623	-	-	-	X
26	BCR	d	405	-	-	-	X
27	SQD	A	416	-	-	-	X
27	SQD	a	402	-	-	-	X
27	SQD	l	101	-	-	-	X
28	GOL	A	413	-	-	-	X
28	GOL	A	414	-	-	-	X
28	GOL	B	625	-	-	-	X
28	GOL	B	626	-	-	-	X
28	GOL	B	627	-	-	-	X
28	GOL	B	628	-	-	-	X
28	GOL	B	629	-	-	-	X
28	GOL	C	524	-	-	-	X
28	GOL	F	103	-	-	-	X
28	GOL	V	205	-	-	-	X
28	GOL	V	206	-	-	-	X
28	GOL	V	207	-	-	-	X
28	GOL	V	208	-	-	-	X
28	GOL	a	412	-	-	-	X
28	GOL	a	413	-	-	-	X
28	GOL	b	632	-	-	-	X
28	GOL	b	633	-	-	-	X
28	GOL	c	525	-	-	-	X
28	GOL	c	527	-	-	-	X
28	GOL	f	104	-	-	-	X
28	GOL	t	102	-	-	-	X
28	GOL	v	203	-	-	-	X
29	UNL	C	526	-	-	-	X
29	UNL	D	413	-	-	-	X
29	UNL	I	101	-	-	-	X
29	UNL	J	103	-	-	-	X
29	UNL	X	101	-	-	-	X
29	UNL	d	412	-	-	-	X
29	UNL	d	413	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	UNL	i	101	-	-	-	X
29	UNL	j	103	-	-	-	X
29	UNL	k	101	-	-	-	X
29	UNL	k	102	-	-	-	X
30	LMT	A	417	-	-	-	X
30	LMT	B	634	-	-	-	X
30	LMT	E	102	-	-	-	X
30	LMT	I	102	-	-	-	X
30	LMT	M	101	-	-	-	X
30	LMT	a	401	-	-	-	X
30	LMT	a	417	-	-	-	X
30	LMT	b	602	-	-	-	X
30	LMT	f	102	-	-	-	X
30	LMT	m	103	-	-	-	X
32	PL9	A	419	-	-	-	X
32	PL9	a	416	-	-	-	X
34	LMG	C	501	-	-	-	X
34	LMG	J	101	-	-	-	X
34	LMG	Z	101	-	-	-	X
34	LMG	b	625	-	-	-	X
34	LMG	j	101	-	-	-	X
34	LMG	z	101	-	-	-	X
35	HTG	B	631	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	411	-	-	-	X
35	HTG	V	204	-	-	-	X
35	HTG	b	627	-	-	-	X
35	HTG	c	523	-	-	-	X
36	DGD	D	407	-	-	-	X
36	DGD	d	407	-	-	-	X
39	MG	j	102	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 53958 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2631	1725	431	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2634	1727	431	461	15			

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4023	2642	667	701	13			
2	b	504	Total	C	N	O	S	0	11	0
			4028	2645	668	702	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	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	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 668	C 436	N 107	O 125	0	2	0
5	e	81	Total 662	C 432	N 107	O 123	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 275	C 187	N 45	O 42	S 1	0	0	0
6	f	32	Total 257	C 175	N 43	O 38	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 519	C 346	N 85	O 86	S 2	0	1	0
7	h	65	Total 511	C 341	N 82	O 86	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total 272	C 182	N 42	O 47	S 1	0	0	0
9	j	39	Total 282	C 188	N 43	O 49	S 2	0	0	0

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	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	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	3	0
			1879	1175	315	384	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	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

- 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	0
			1	1		

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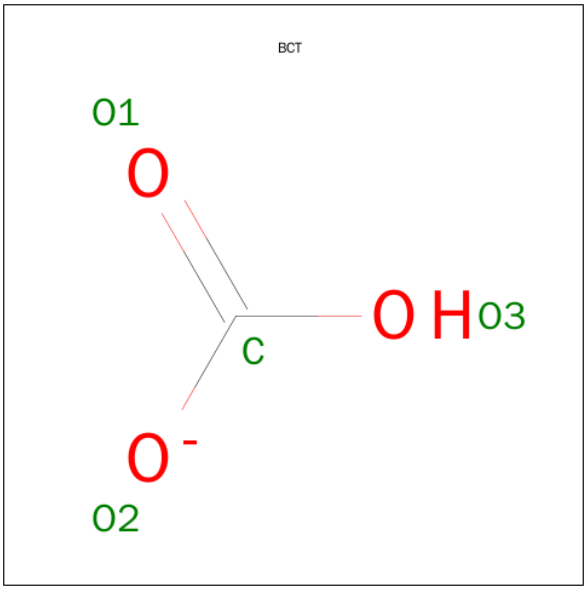
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	a	1	Total Fe 1 1	0	0

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

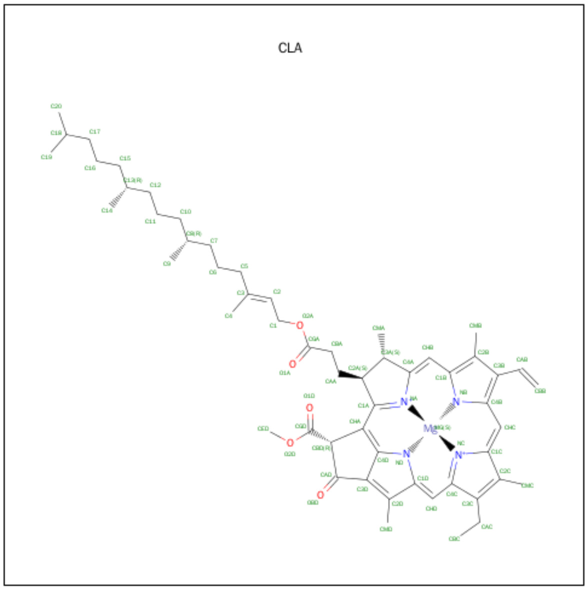
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 2 2	0	0
22	A	2	Total Cl 2 2	0	0
22	V	1	Total Cl 1 1	0	0
22	u	1	Total Cl 1 1	0	0

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



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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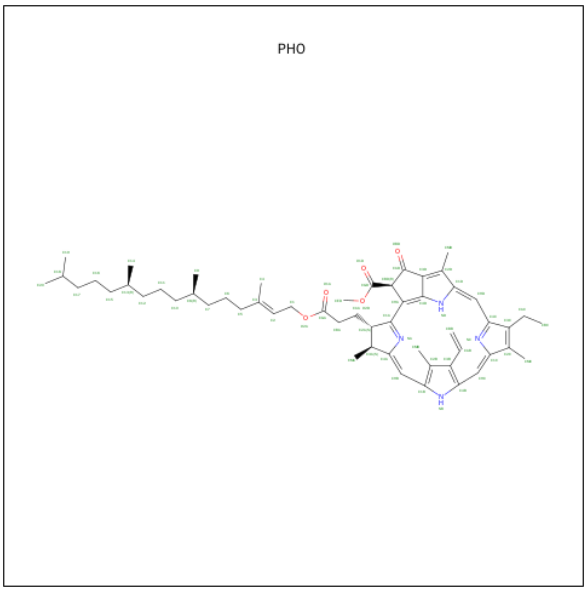
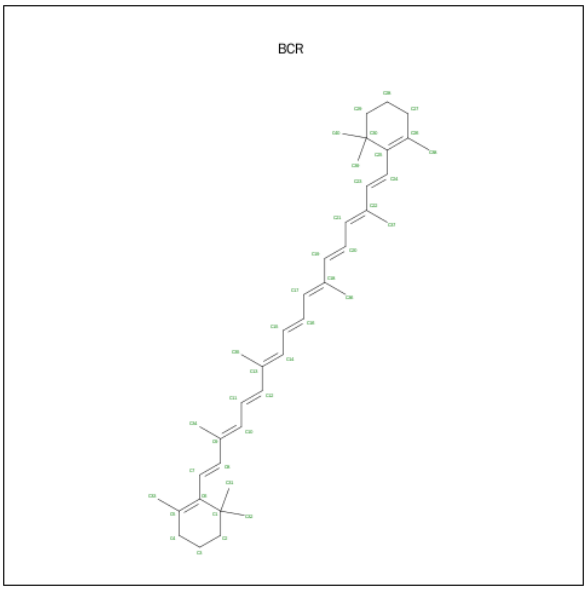
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



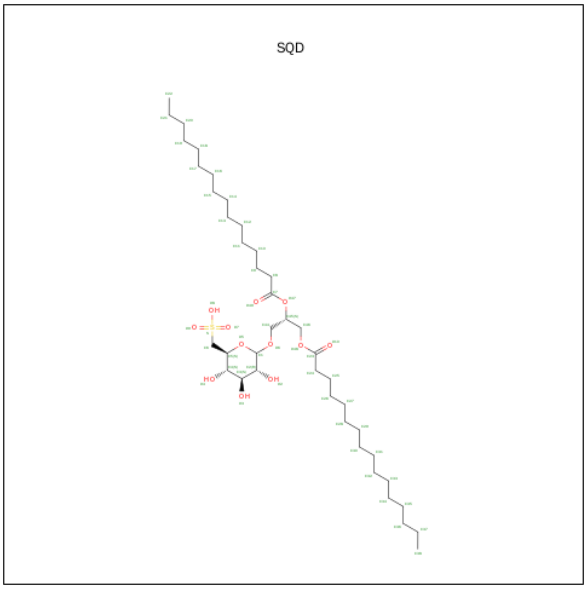
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



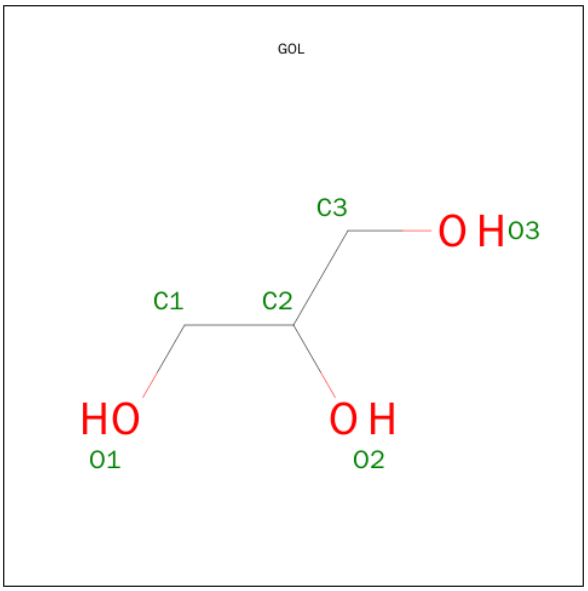
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total 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	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		
27	l	1	Total	C	O	S	0	0
			54	41	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 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	F	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	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	b	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	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	f	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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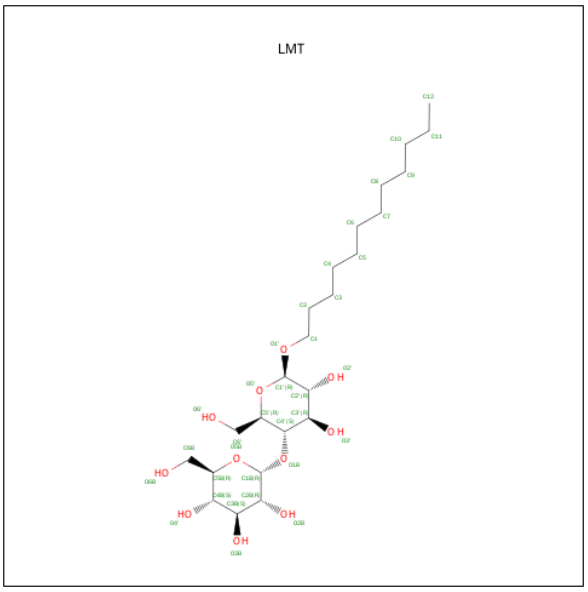
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	v	1	Total C O 6 3 3	0	0
28	v	1	Total C O 6 3 3	0	0

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

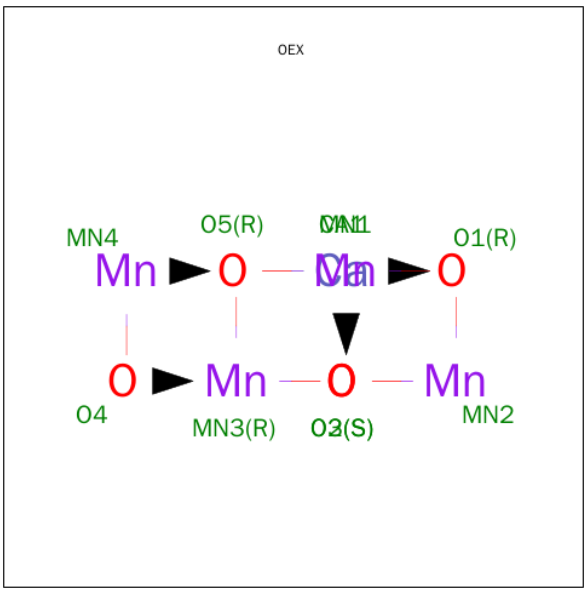
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	J	1	Total C 10 10	0	0
29	i	1	Total C O 40 35 5	0	0
29	D	2	Total C O 57 51 6	0	0
29	k	2	Total C O 42 37 5	0	0
29	B	1	Total C O 33 28 5	0	0
29	I	1	Total C O 40 35 5	0	0
29	C	1	Total C O 34 29 5	0	0
29	a	1	Total C O 30 25 5	0	0
29	x	1	Total C 10 10	0	0
29	A	1	Total C O 28 23 5	0	0
29	j	1	Total C 10 10	0	0
29	X	1	Total C 10 10	0	0
29	d	2	Total C O 53 47 6	0	0
29	m	1	Total C 10 10	0	0
29	b	1	Total C O 33 28 5	0	0
29	M	1	Total C 10 10	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



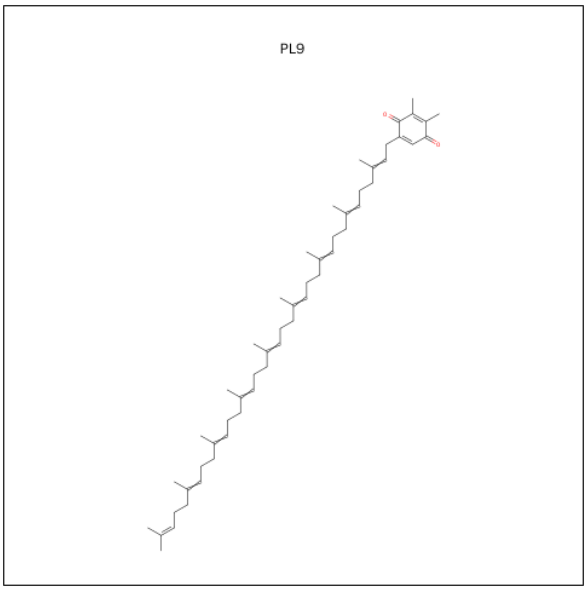
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 33 22 11	0	0
30	B	1	Total C O 25 19 6	0	0
30	D	1	Total C O 35 24 11	0	0
30	E	1	Total C O 35 24 11	0	0
30	I	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	M	1	Total C O 35 24 11	0	0
30	a	1	Total C O 35 24 11	0	0
30	a	1	Total C O 35 24 11	0	0
30	b	1	Total C O 25 19 6	0	0
30	b	1	Total C O 25 19 6	0	0
30	f	1	Total C O 35 24 11	0	0
30	m	1	Total C O 35 24 11	0	0
30	m	1	Total C O 35 24 11	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 32 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: $C_{53}H_{80}O_2$).

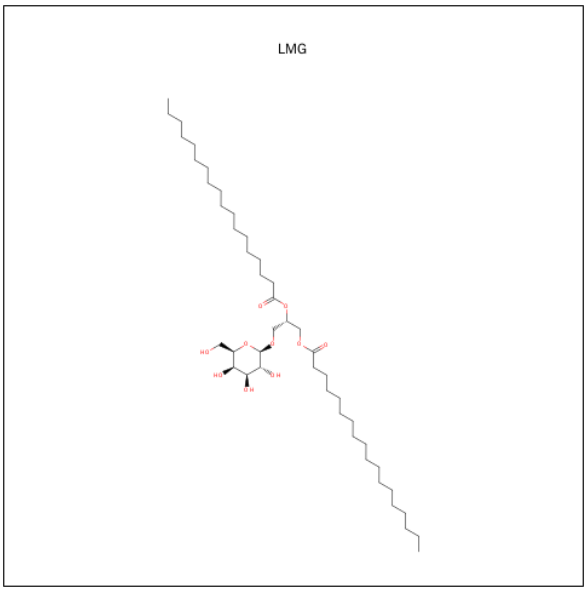


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 55 53 2	0	0
32	D	1	Total C O 55 53 2	0	0
32	a	1	Total C O 55 53 2	0	0
32	d	1	Total C O 55 53 2	0	0

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

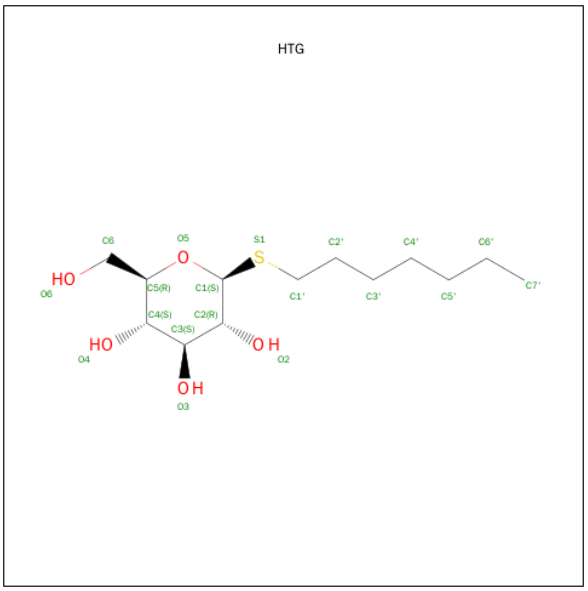
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- 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	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	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	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	b	1	Total	C	O	S	0	0
			19	13	5	1		

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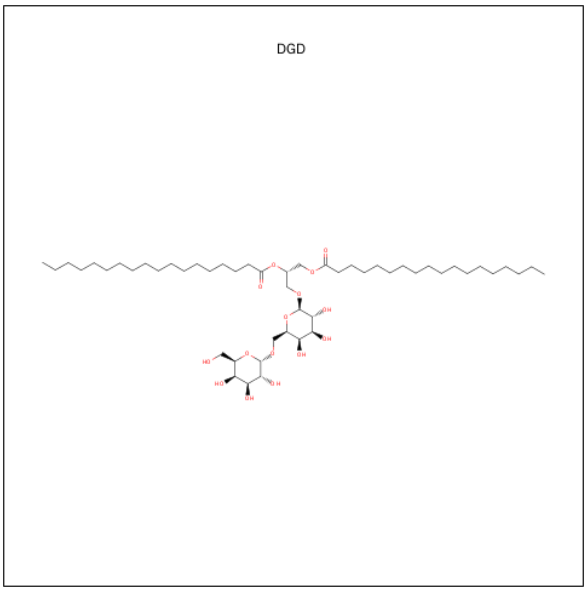
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	c	1	Total C O S 19 13 5 1	0	0
35	c	1	Total C O S 19 13 5 1	0	0
35	d	1	Total C O S 16 10 5 1	0	0

- 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 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

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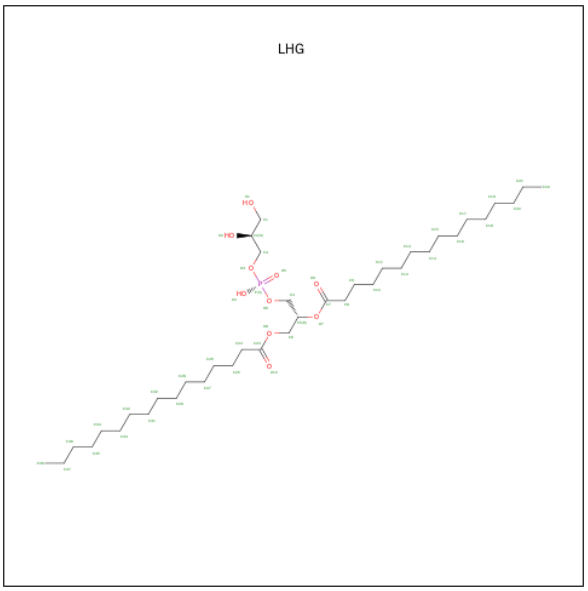
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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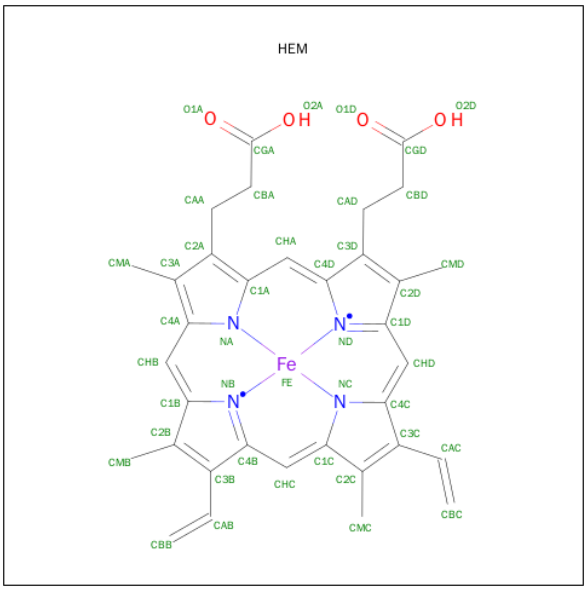
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	146	Total O 149 149	0	3
40	B	277	Total O 280 280	0	3
40	C	206	Total O 209 209	0	3
40	D	157	Total O 161 161	0	4
40	E	28	Total O 28 28	0	0
40	F	7	Total O 7 7	0	0
40	H	39	Total O 40 40	0	1
40	I	8	Total O 8 8	0	0
40	J	12	Total O 12 12	0	0
40	K	6	Total O 6 6	0	0
40	L	12	Total O 12 12	0	0
40	M	15	Total O 15 15	0	0
40	O	164	Total O 165 165	0	1
40	T	12	Total O 13 13	0	1
40	U	75	Total O 76 76	0	1
40	V	111	Total O 111 111	0	0
40	Y	1	Total O 1 1	0	0
40	X	8	Total O 8 8	0	0
40	a	151	Total O 151 151	0	0
40	b	247	Total O 249 249	0	2
40	c	187	Total O 189 189	0	2
40	d	136	Total O 139 139	0	3

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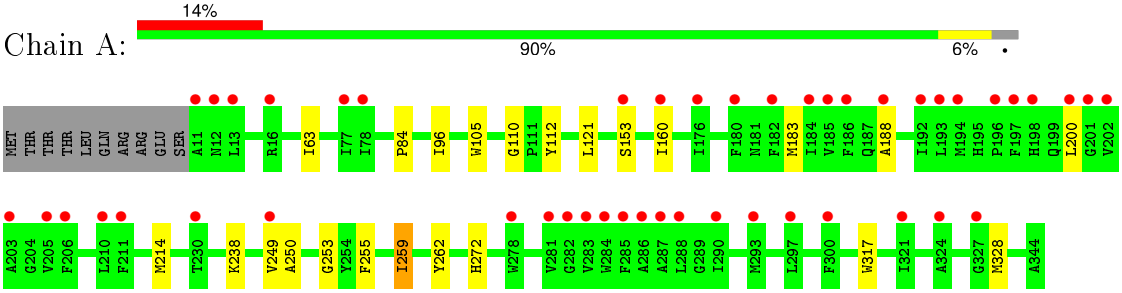
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	e	15	Total O 15 15	0	0
40	f	7	Total O 7 7	0	0
40	h	36	Total O 36 36	0	0
40	i	5	Total O 5 5	0	0
40	j	7	Total O 7 7	0	0
40	k	3	Total O 3 3	0	0
40	l	10	Total O 10 10	0	0
40	m	12	Total O 12 12	0	0
40	o	137	Total O 137 137	0	0
40	t	10	Total O 10 10	0	0
40	u	89	Total O 89 89	0	0
40	v	80	Total O 80 80	0	0
40	y	4	Total O 4 4	0	0
40	x	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

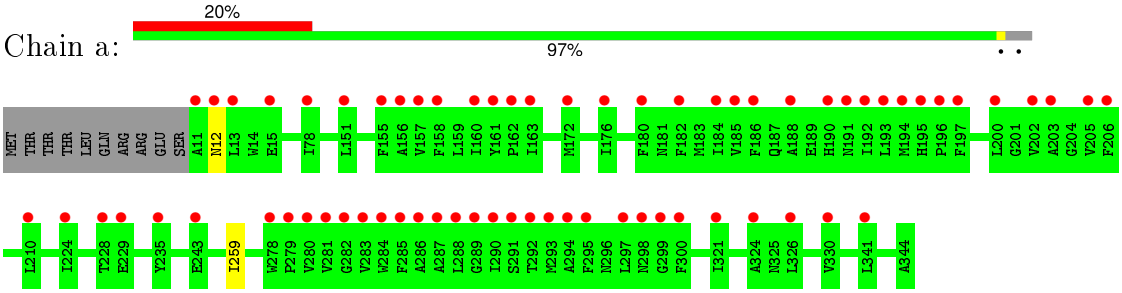
- Molecule 1: Photosystem Q(B) protein

Chain A:



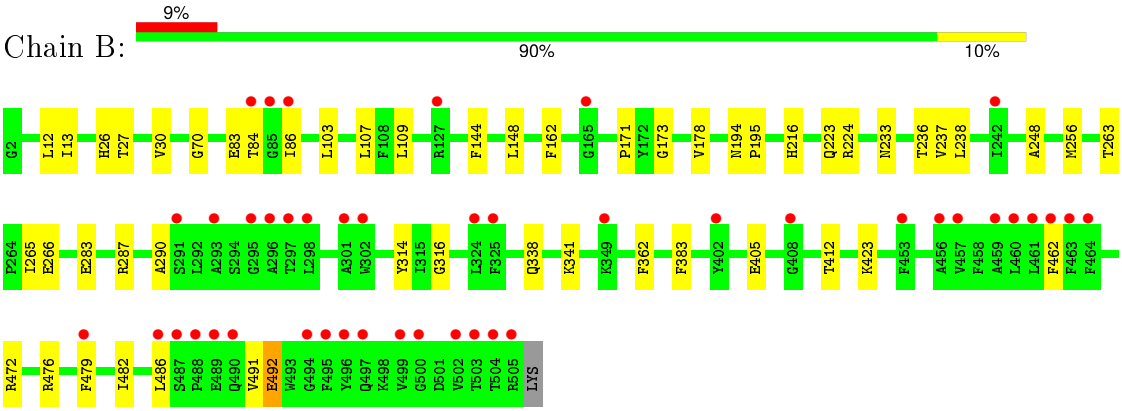
- Molecule 1: Photosystem Q(B) protein

Chain a:



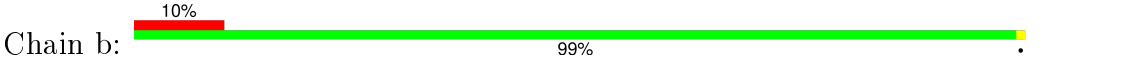
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

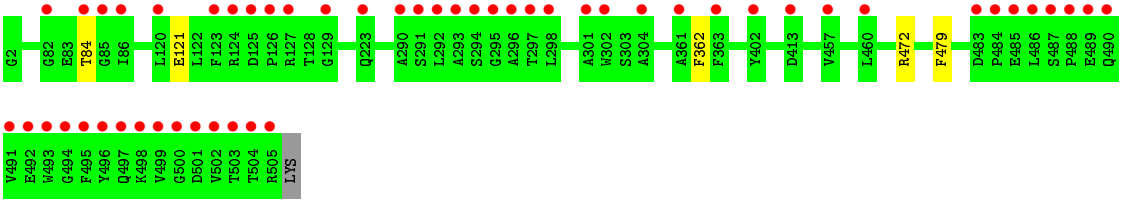
Chain B:



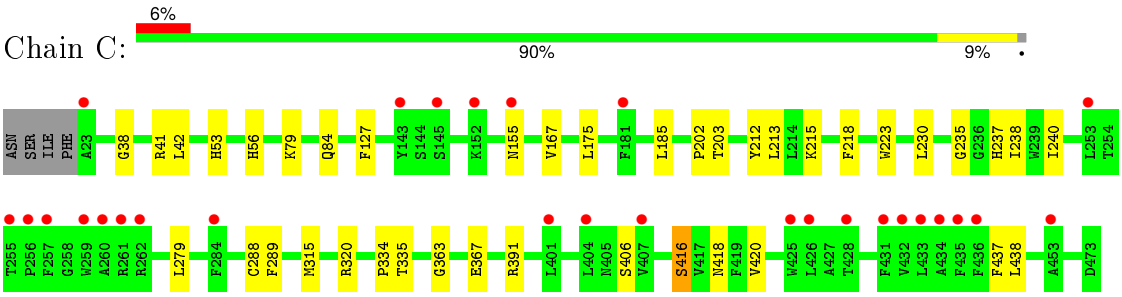
- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

Chain b:

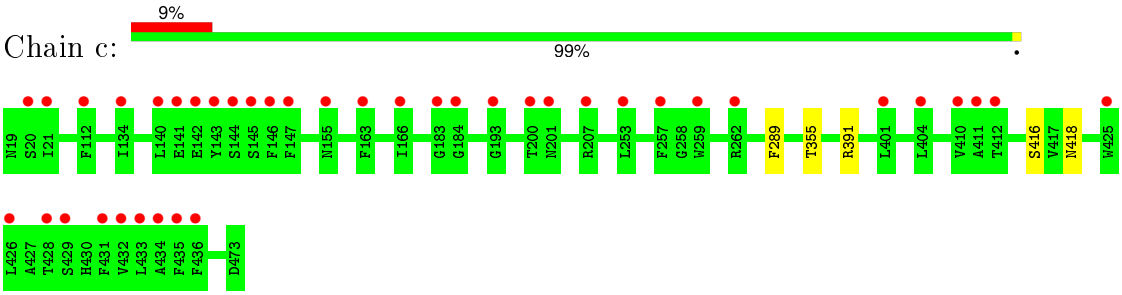




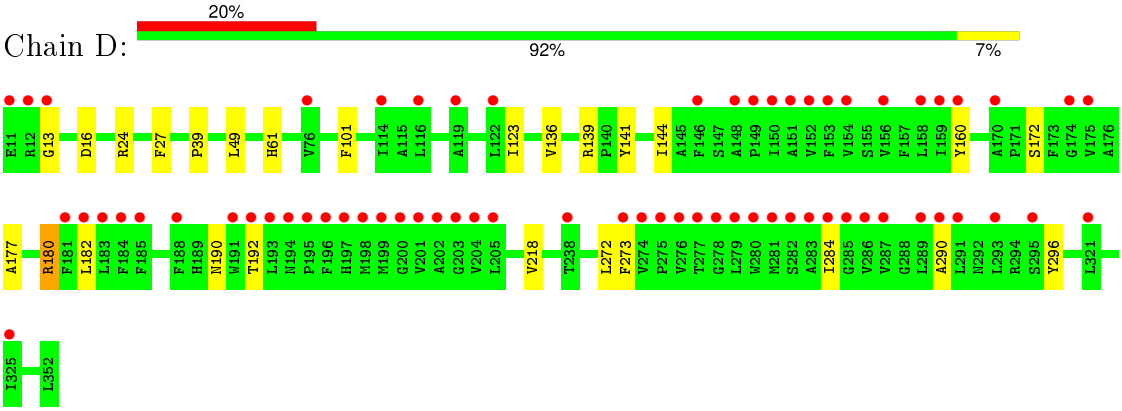
• Molecule 3: Photosystem II 44 kDa reaction center protein



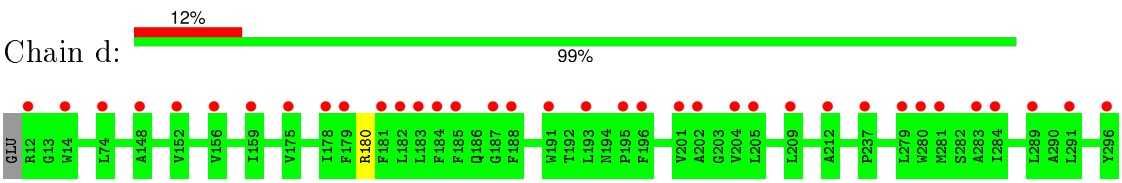
• Molecule 3: Photosystem II 44 kDa reaction center protein

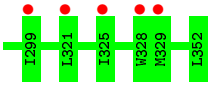


• Molecule 4: Photosystem II D2 protein



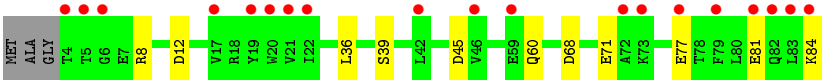
• Molecule 4: Photosystem II D2 protein





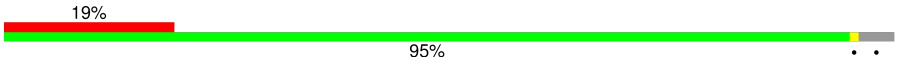
• Molecule 5: Cytochrome b559 subunit alpha

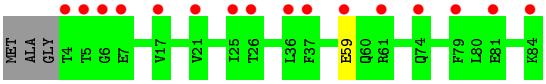
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

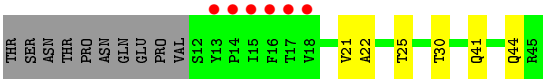
Chain e:





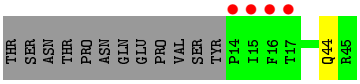
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



• Molecule 6: Cytochrome b559 subunit beta

Chain f:

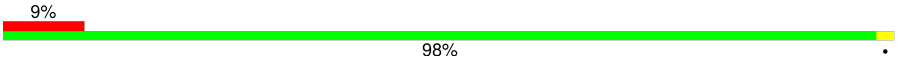


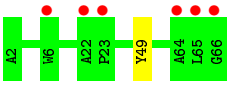
• Molecule 7: Photosystem II reaction center protein H

Chain H:

• Molecule 7: Photosystem II reaction center protein H

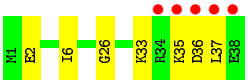
Chain h:





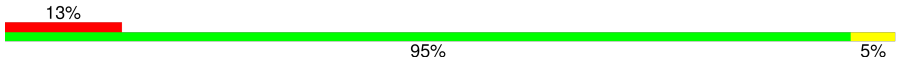
• Molecule 8: Photosystem II reaction center protein I

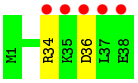
Chain I:



• Molecule 8: Photosystem II reaction center protein I

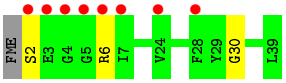
Chain i:





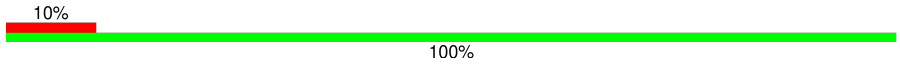
• Molecule 9: Photosystem II reaction center protein J

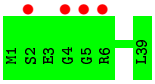
Chain J:



• Molecule 9: Photosystem II reaction center protein J

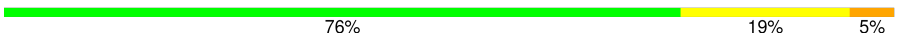
Chain j:

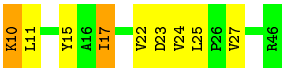




• Molecule 10: Photosystem II reaction center protein K

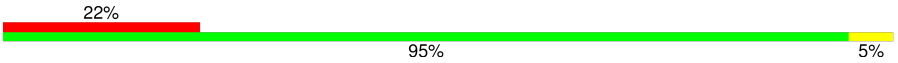
Chain K:

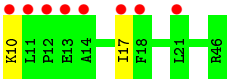




• Molecule 10: Photosystem II reaction center protein K

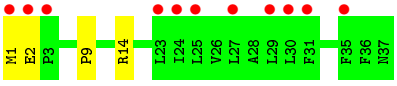
Chain k:





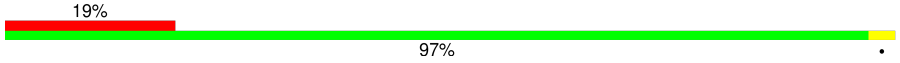
• Molecule 11: Photosystem II reaction center protein L

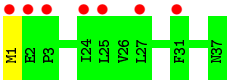
Chain L:



• Molecule 11: Photosystem II reaction center protein L

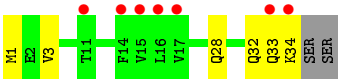
Chain l:





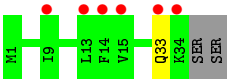
• Molecule 12: Photosystem II reaction center protein M

Chain M:



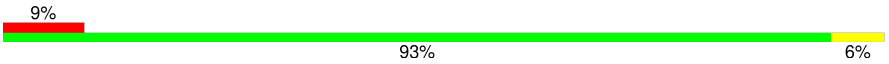
• Molecule 12: Photosystem II reaction center protein M

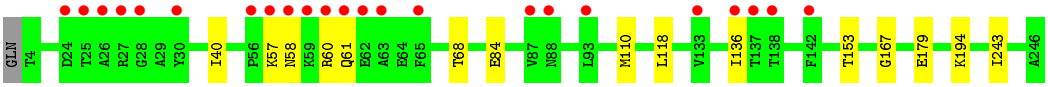
Chain m:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

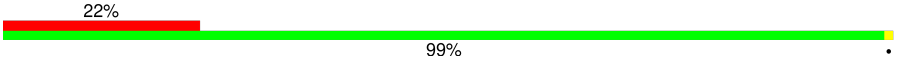
Chain O:

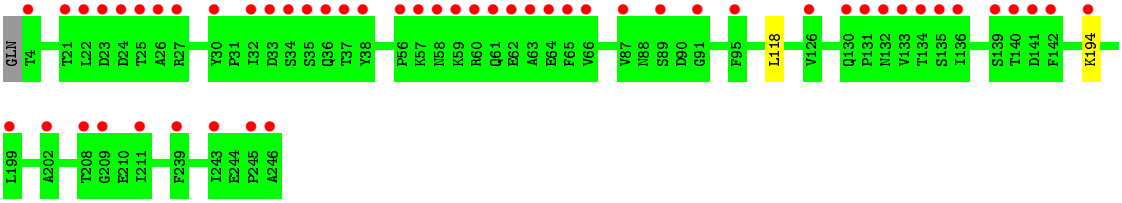




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

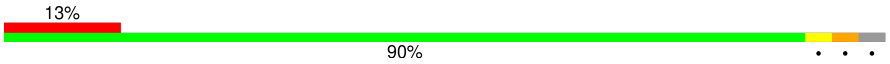
Chain o:

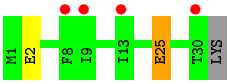




• Molecule 14: Photosystem II reaction center protein T

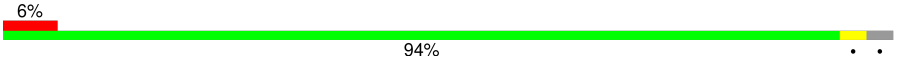
Chain T:

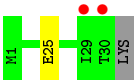




• Molecule 14: Photosystem II reaction center protein T

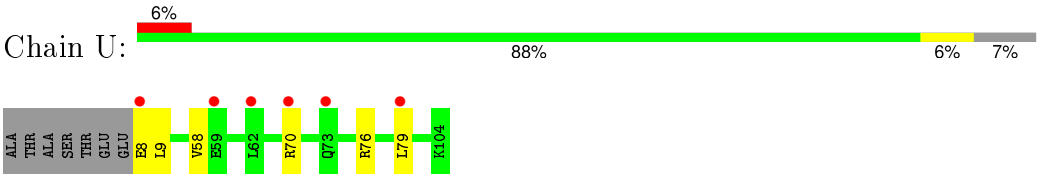
Chain t:





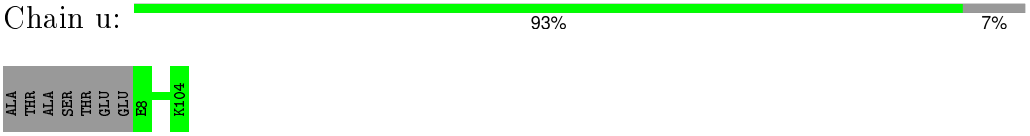
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



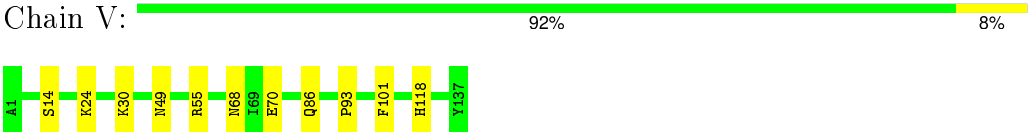
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



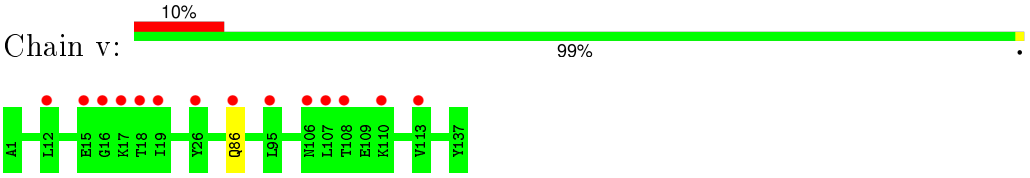
• Molecule 16: Cytochrome c-550

Chain V:



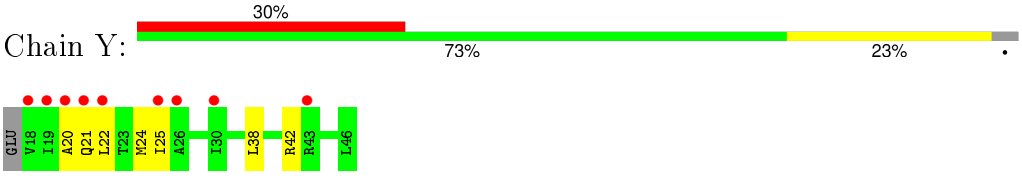
• Molecule 16: Cytochrome c-550

Chain v:



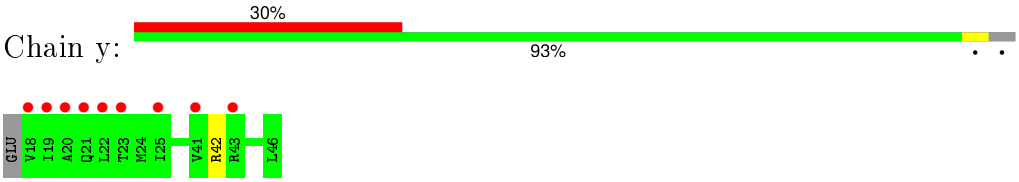
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



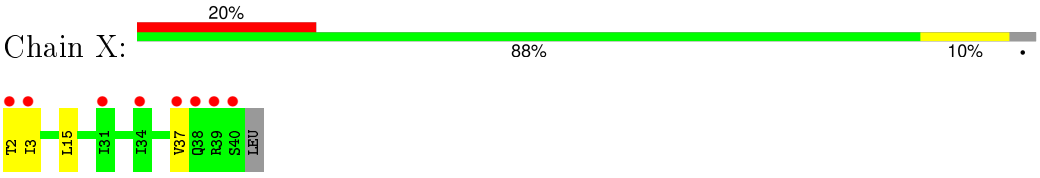
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



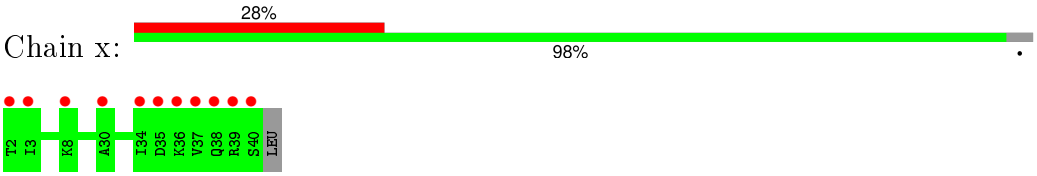
• Molecule 18: Photosystem II reaction center protein X

Chain X:



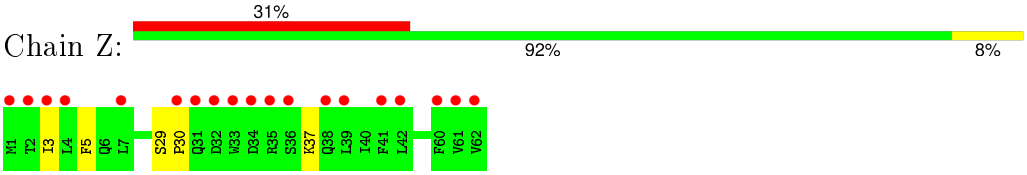
• Molecule 18: Photosystem II reaction center protein X

Chain x:



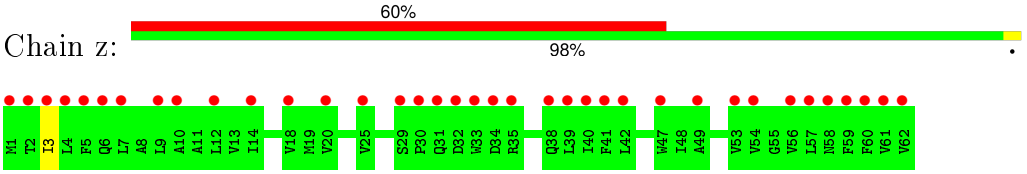
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



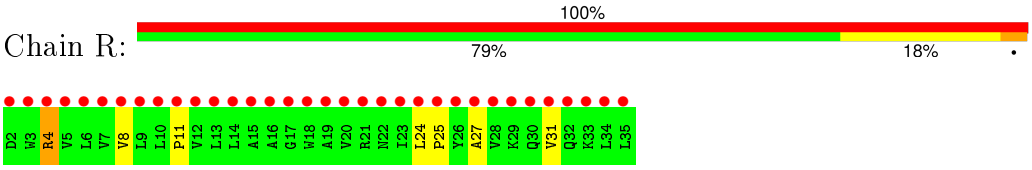
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.81Å 230.00Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.90 – 1.95 61.90 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.90-1.95) 85.6 (61.90-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.188 , 0.225 0.195 , 0.230	Depositor DCC
R_{free} test set	29289 reflections (6.01%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 585991 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	53958	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.53	0/2725	0.59	0/3716
1	a	0.55	0/2731	0.58	0/3724
2	B	0.49	0/4193	0.56	0/5712
2	b	0.47	0/4201	0.55	0/5723
3	C	0.46	0/3634	0.54	0/4947
3	c	0.46	0/3676	0.54	0/5004
4	D	0.53	0/2821	0.56	0/3844
4	d	0.52	0/2818	0.55	0/3840
5	E	0.36	0/693	0.52	0/944
5	e	0.33	0/681	0.52	0/928
6	F	0.39	0/284	0.48	0/387
6	f	0.37	0/265	0.51	0/360
7	H	0.40	0/535	0.53	0/728
7	h	0.35	0/524	0.50	0/713
8	I	0.38	0/311	0.51	0/419
8	i	0.40	0/311	0.50	0/419
9	J	0.37	0/278	0.46	0/376
9	j	0.38	0/278	0.48	0/376
10	K	0.36	0/303	0.48	0/416
10	k	0.36	0/303	0.51	0/416
11	L	0.48	0/319	0.49	0/433
11	l	0.49	0/319	0.50	0/433
12	M	0.43	0/270	0.58	0/368
12	m	0.47	0/262	0.58	0/357
13	O	0.41	0/1926	0.56	0/2611
13	o	0.40	0/1919	0.57	0/2601
14	T	0.54	0/266	0.56	0/362
14	t	0.54	0/266	0.56	0/362
15	U	0.44	0/785	0.55	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.45	0/1096	0.54	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.41	0/1085	0.53	0/1473
17	Y	0.29	0/216	0.46	0/289
17	y	0.28	0/216	0.46	0/289
18	X	0.34	0/298	0.44	0/403
18	x	0.34	0/290	0.48	0/392
19	Z	0.31	0/490	0.43	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.24	0/279	0.38	0/383
All	All	0.46	0/43142	0.55	0/58701

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2631	0	2538	24	0
1	a	2634	0	2543	0	0
2	B	4023	0	3904	52	0
2	b	4028	0	3910	0	0
3	C	3506	0	3439	33	0
3	c	3544	0	3480	0	0
4	D	2726	0	2627	27	0
4	d	2720	0	2626	0	0
5	E	668	0	658	8	0
5	e	662	0	648	0	0
6	F	275	0	282	4	0
6	f	257	0	269	0	0
7	H	519	0	545	8	0
7	h	511	0	532	0	0
8	I	314	0	328	5	0
8	i	314	0	328	0	0
9	J	272	0	279	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	282	0	290	0	0
10	K	293	0	305	8	0
10	k	293	0	305	0	0
11	L	309	0	327	3	0
11	l	309	0	327	0	0
12	M	274	0	299	8	0
12	m	269	0	288	0	0
13	O	1883	0	1865	10	0
13	o	1879	0	1858	0	0
14	T	264	0	267	3	0
14	t	264	0	267	0	0
15	U	774	0	773	3	0
15	u	774	0	773	0	0
16	V	1072	0	1086	9	0
16	v	1064	0	1073	0	0
17	Y	215	0	246	5	0
17	y	215	0	246	0	0
18	X	292	0	328	3	0
18	x	287	0	317	0	0
19	Z	479	0	516	4	0
19	z	479	0	516	0	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	V	1	0	0	1	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	195	0	216	13	0
24	B	1040	0	1152	50	0
24	C	845	0	936	53	0
24	D	195	0	216	11	0
24	a	195	0	216	0	0
24	b	1040	0	1152	0	0
24	c	845	0	936	0	0
24	d	195	0	216	0	0
25	A	128	0	148	2	0
25	a	64	0	74	0	0
25	d	64	0	74	0	0
26	A	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	120	0	168	6	0
26	C	80	0	112	7	0
26	D	40	0	56	4	0
26	H	40	0	56	6	0
26	K	40	0	56	2	0
26	T	40	0	56	5	0
26	Y	40	0	56	2	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	F	43	0	53	5	0
27	a	108	0	155	0	0
27	b	54	0	78	0	0
27	f	43	0	53	0	0
27	l	54	0	78	0	0
28	A	18	0	24	4	0
28	B	42	0	56	4	0
28	C	12	0	16	3	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	1	0
28	V	30	0	40	4	0
28	a	12	0	16	0	0
28	b	30	0	40	0	0
28	c	18	0	24	0	0
28	f	6	0	7	0	0
28	t	6	0	8	0	0
28	v	24	0	32	0	0
29	A	28	0	0	0	0
29	B	33	0	0	0	0
29	C	34	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	M	10	0	0	0	0
29	X	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	30	0	0	0	0
29	b	33	0	0	0	0
29	d	53	0	0	0	0
29	i	40	0	0	0	0
29	j	10	0	0	0	0
29	k	42	0	0	0	0
29	m	10	0	0	0	0
29	x	10	0	0	0	0
30	A	33	0	39	0	0
30	B	25	0	35	1	0
30	D	35	0	46	1	0
30	E	35	0	46	0	0
30	I	35	0	46	2	0
30	M	70	0	92	3	0
30	a	70	0	92	0	0
30	b	50	0	70	0	0
30	f	35	0	46	0	0
30	m	70	0	92	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	55	0	80	4	0
32	D	55	0	80	0	0
32	a	55	0	80	0	0
32	d	55	0	80	0	0
33	B	1	0	0	0	0
33	F	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	f	1	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	11	0
34	J	51	0	72	3	0
34	Z	37	0	44	6	0
34	b	51	0	72	0	0
34	c	153	0	216	0	0
34	j	51	0	72	0	0
34	z	39	0	48	0	0
35	B	95	0	130	1	0
35	C	38	0	52	3	0
35	D	16	0	17	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	O	19	0	26	0	0
35	V	19	0	26	1	0
35	b	76	0	104	0	0
35	c	38	0	52	0	0
35	d	16	0	17	0	0
36	C	186	0	246	10	0
36	D	62	0	82	6	0
36	H	62	0	82	2	0
36	c	186	0	246	0	0
36	d	62	0	82	0	0
36	h	62	0	82	0	0
37	D	147	0	222	12	0
37	E	42	0	57	6	0
37	L	49	0	74	1	0
37	d	147	0	222	0	0
37	e	42	0	57	0	0
37	l	49	0	74	0	0
38	E	43	0	30	0	0
38	V	43	0	30	0	0
38	e	43	0	30	0	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	149	0	0	2	0
40	B	280	0	0	6	0
40	C	209	0	0	4	0
40	D	161	0	0	2	0
40	E	28	0	0	1	0
40	F	7	0	0	0	0
40	H	40	0	0	0	0
40	I	8	0	0	0	0
40	J	12	0	0	1	0
40	K	6	0	0	1	0
40	L	12	0	0	1	0
40	M	15	0	0	0	0
40	O	165	0	0	2	0
40	T	13	0	0	0	0
40	U	76	0	0	2	0
40	V	111	0	0	1	0
40	X	8	0	0	0	0
40	Y	1	0	0	0	0
40	a	151	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	b	249	0	0	0	0
40	c	189	0	0	0	0
40	d	139	0	0	0	0
40	e	15	0	0	0	0
40	f	7	0	0	0	0
40	h	36	0	0	0	0
40	i	5	0	0	0	0
40	j	7	0	0	0	0
40	k	3	0	0	0	0
40	l	10	0	0	0	0
40	m	12	0	0	0	0
40	o	137	0	0	0	0
40	t	10	0	0	0	0
40	u	89	0	0	0	0
40	v	80	0	0	0	0
40	x	5	0	0	0	0
40	y	4	0	0	0	0
All	All	53958	0	52755	346	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 346 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)
1:A:214:MET:HG2	32:A:419:PL9:H102	1.51	0.93
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.30	0.92
24:B:616:CLA:H71	24:B:617:CLA:H192	1.64	0.78
24:C:503:CLA:H193	35:C:522:HTG:H3'1	1.67	0.74
24:C:504:CLA:H61	24:C:514:CLA:H42	27.00	0.74

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	335/344 (97%)	330 (98%)	4 (1%)	1 (0%)	46	35
1	a	336/344 (98%)	331 (98%)	4 (1%)	1 (0%)	46	35
2	B	512/505 (101%)	507 (99%)	5 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	454/455 (100%)	445 (98%)	7 (2%)	2 (0%)	39	27
3	c	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	39	27
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	1
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	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	245/244 (100%)	242 (99%)	3 (1%)	0	100	100
13	o	244/244 (100%)	238 (98%)	6 (2%)	0	100	100
14	T	29/31 (94%)	29 (100%)	0	0	100	100
14	t	29/31 (94%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5279/5382 (98%)	5168 (98%)	104 (2%)	7 (0%)	56	48

5 of 7 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	273/279 (98%)	272 (100%)	1 (0%)	93	93
2	B	412/403 (102%)	407 (99%)	5 (1%)	78	75
2	b	413/403 (102%)	408 (99%)	5 (1%)	78	75
3	C	357/356 (100%)	352 (99%)	5 (1%)	74	70
3	c	362/356 (102%)	358 (99%)	4 (1%)	80	77
4	D	277/277 (100%)	276 (100%)	1 (0%)	93	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	d	277/277 (100%)	276 (100%)	1 (0%)	93 93
5	E	74/73 (101%)	74 (100%)	0	100 100
5	e	72/73 (99%)	71 (99%)	1 (1%)	74 70
6	F	28/38 (74%)	27 (96%)	1 (4%)	42 28
6	f	26/38 (68%)	25 (96%)	1 (4%)	40 25
7	H	55/54 (102%)	52 (94%)	3 (6%)	27 12
7	h	54/54 (100%)	53 (98%)	1 (2%)	65 58
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	33 (97%)	1 (3%)	50 38
9	J	26/26 (100%)	26 (100%)	0	100 100
9	j	26/26 (100%)	26 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20 7
10	k	30/30 (100%)	28 (93%)	2 (7%)	20 7
11	L	36/35 (103%)	35 (97%)	1 (3%)	51 39
11	l	36/35 (103%)	35 (97%)	1 (3%)	51 39
12	M	31/32 (97%)	31 (100%)	0	100 100
12	m	30/32 (94%)	29 (97%)	1 (3%)	45 32
13	O	210/207 (101%)	208 (99%)	2 (1%)	82 80
13	o	209/207 (101%)	207 (99%)	2 (1%)	82 80
14	T	27/27 (100%)	25 (93%)	2 (7%)	17 5
14	t	27/27 (100%)	25 (93%)	2 (7%)	17 5
15	U	84/89 (94%)	83 (99%)	1 (1%)	78 75
15	u	84/89 (94%)	84 (100%)	0	100 100
16	V	118/117 (101%)	117 (99%)	1 (1%)	86 85
16	v	117/117 (100%)	116 (99%)	1 (1%)	84 83
17	Y	22/23 (96%)	22 (100%)	0	100 100
17	y	22/23 (96%)	21 (96%)	1 (4%)	34 18
18	X	33/33 (100%)	33 (100%)	0	100 100
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65 58
19	z	52/52 (100%)	51 (98%)	1 (2%)	65 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	R	29/29 (100%)	28 (97%)	1 (3%)	44 30
All	All	4383/4399 (100%)	4331 (99%)	52 (1%)	80 75

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	V	86	GLN
2	b	362	PHE
14	t	25[B]	GLU
19	Z	3	ILE
1	a	12	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	497	GLN
19	z	6	GLN
13	o	109	GLN
4	D	142	ASN
15	u	81	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.56	0	6,9,11	1.64	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	FME	M	1	12	8,9,10	0.56	0	6,9,11	1.67	2 (33%)
14	FME	T	1	14	8,9,10	0.61	0	6,9,11	1.84	3 (50%)
8	FME	i	1	8	8,9,10	0.56	0	6,9,11	1.43	1 (16%)
9	FME	j	1	9	8,9,10	0.57	0	6,9,11	1.54	2 (33%)
12	FME	m	1	12	8,9,10	0.62	0	6,9,11	1.29	1 (16%)
14	FME	t	1	14	8,9,10	0.79	0	6,9,11	2.35	3 (50%)

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
9	FME	j	1	9	-	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 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O1-CN-N	-3.56	119.63	124.76
14	t	1	FME	O-C-CA	-3.22	116.92	125.44
14	T	1	FME	O-C-CA	-3.01	117.48	125.44
9	j	1	FME	O1-CN-N	-2.84	120.67	124.76
12	M	1	FME	O1-CN-N	-2.64	120.95	124.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 252 ligands modelled in this entry, 19 are unknown and 17 are monoatomic - leaving 216 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	$\#\|Z\| > 2$
23	BCT	A	404	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	405	-	55,73,73	1.98	12 (21%)	61,113,113	2.16	20 (32%)
24	CLA	A	406	40	55,73,73	1.95	11 (20%)	61,113,113	2.12	22 (36%)
25	PHO	A	407	-	67,69,69	2.12	16 (23%)	84,99,99	1.88	20 (23%)
25	PHO	A	408	-	67,69,69	2.04	14 (20%)	84,99,99	1.97	23 (27%)
24	CLA	A	409	-	55,73,73	1.96	12 (21%)	61,113,113	2.06	20 (32%)
26	BCR	A	410	-	41,41,41	0.98	1 (2%)	56,56,56	1.33	5 (8%)
27	SQD	A	411	-	53,54,54	1.35	3 (5%)	61,65,65	1.66	10 (16%)
28	GOL	A	412	-	5,5,5	0.21	0	5,5,5	0.62	0
28	GOL	A	413	-	5,5,5	0.42	0	5,5,5	0.58	0
28	GOL	A	414	-	5,5,5	0.38	0	5,5,5	0.19	0
27	SQD	A	416	-	53,54,54	1.41	3 (5%)	61,65,65	1.20	7 (11%)
30	LMT	A	417	-	34,34,36	0.38	0	45,45,47	1.05	3 (6%)
31	OEX	A	418	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
32	PL9	A	419	-	55,55,55	0.63	1 (1%)	68,69,69	2.01	26 (38%)
24	CLA	B	602	40	55,73,73	1.95	12 (21%)	61,113,113	2.10	18 (29%)
24	CLA	B	603	-	55,73,73	1.94	12 (21%)	61,113,113	2.20	22 (36%)
24	CLA	B	604	-	55,73,73	1.98	12 (21%)	61,113,113	2.25	23 (37%)
24	CLA	B	605	-	55,73,73	1.80	12 (21%)	61,113,113	2.24	19 (31%)
24	CLA	B	606	-	55,73,73	1.87	12 (21%)	61,113,113	2.25	19 (31%)
24	CLA	B	607	-	55,73,73	1.90	12 (21%)	61,113,113	2.27	21 (34%)
24	CLA	B	608	40	55,73,73	1.94	12 (21%)	61,113,113	2.14	22 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	609	-	55,73,73	1.98	12 (21%)	61,113,113	2.09	17 (27%)
24	CLA	B	610	-	55,73,73	1.88	11 (20%)	61,113,113	2.09	19 (31%)
24	CLA	B	611	40	55,73,73	1.92	12 (21%)	61,113,113	2.15	21 (34%)
24	CLA	B	612	-	55,73,73	1.94	12 (21%)	61,113,113	2.11	19 (31%)
24	CLA	B	613	-	55,73,73	1.93	12 (21%)	61,113,113	2.09	16 (26%)
24	CLA	B	614	-	55,73,73	1.94	12 (21%)	61,113,113	2.05	18 (29%)
24	CLA	B	615	-	55,73,73	1.86	11 (20%)	61,113,113	2.26	21 (34%)
24	CLA	B	616	-	55,73,73	1.87	12 (21%)	61,113,113	2.05	20 (32%)
24	CLA	B	617	-	55,73,73	1.96	12 (21%)	61,113,113	2.24	19 (31%)
26	BCR	B	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.26	5 (8%)
26	BCR	B	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.01	3 (5%)
26	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.48	11 (19%)
34	LMG	B	621	-	51,51,55	0.88	2 (3%)	59,59,63	1.03	4 (6%)
35	HTG	B	622	-	19,19,19	1.12	1 (5%)	22,24,24	1.63	3 (13%)
35	HTG	B	623	-	19,19,19	0.82	1 (5%)	22,24,24	1.43	1 (4%)
35	HTG	B	624	-	19,19,19	0.99	1 (5%)	22,24,24	2.17	3 (13%)
28	GOL	B	625	-	5,5,5	0.29	0	5,5,5	0.59	0
28	GOL	B	626	-	5,5,5	0.28	0	5,5,5	0.47	0
28	GOL	B	627	-	5,5,5	0.30	0	5,5,5	0.65	0
28	GOL	B	628	-	5,5,5	0.39	0	5,5,5	0.23	0
28	GOL	B	629	-	5,5,5	0.29	0	5,5,5	0.36	0
35	HTG	B	630	-	19,19,19	0.91	1 (5%)	22,24,24	1.61	1 (4%)
35	HTG	B	631	-	19,19,19	0.96	2 (10%)	22,24,24	1.75	2 (9%)
28	GOL	B	633	-	5,5,5	0.26	0	5,5,5	0.63	0
30	LMT	B	634	-	25,25,36	0.47	0	30,30,47	0.74	0
28	GOL	B	635	-	5,5,5	0.36	0	5,5,5	0.29	0
34	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.12	3 (5%)
24	CLA	C	502	-	55,73,73	1.91	12 (21%)	61,113,113	2.13	18 (29%)
24	CLA	C	503	-	55,73,73	1.94	12 (21%)	61,113,113	2.15	20 (32%)
24	CLA	C	504	-	55,73,73	1.96	12 (21%)	61,113,113	2.02	19 (31%)
24	CLA	C	505	40	55,73,73	1.93	12 (21%)	61,113,113	2.18	16 (26%)
24	CLA	C	506	-	55,73,73	1.95	12 (21%)	61,113,113	2.14	17 (27%)
24	CLA	C	507	-	55,73,73	1.91	12 (21%)	61,113,113	2.18	17 (27%)
24	CLA	C	508	40	55,73,73	1.93	12 (21%)	61,113,113	2.12	19 (31%)
24	CLA	C	509	-	55,73,73	1.97	12 (21%)	61,113,113	2.20	19 (31%)
24	CLA	C	510	-	55,73,73	1.98	12 (21%)	61,113,113	2.22	19 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	511	-	55,73,73	1.97	12 (21%)	61,113,113	2.12	16 (26%)
24	CLA	C	512	3	55,73,73	1.89	12 (21%)	61,113,113	1.98	13 (21%)
24	CLA	C	513	-	55,73,73	1.92	12 (21%)	61,113,113	2.19	21 (34%)
24	CLA	C	514	-	55,73,73	1.92	12 (21%)	61,113,113	2.10	19 (31%)
26	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.40	5 (8%)
26	BCR	C	516	-	41,41,41	0.98	1 (2%)	56,56,56	1.41	9 (16%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.06	5 (6%)
36	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	5 (6%)
36	DGD	C	519	-	63,63,67	0.79	2 (3%)	77,77,81	0.91	4 (5%)
34	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.10	4 (6%)
34	LMG	C	521	-	51,51,55	0.93	2 (3%)	59,59,63	1.15	4 (6%)
35	HTG	C	522	-	19,19,19	0.94	2 (10%)	22,24,24	1.57	2 (9%)
35	HTG	C	523	-	19,19,19	0.95	1 (5%)	22,24,24	1.96	4 (18%)
28	GOL	C	524	-	5,5,5	0.30	0	5,5,5	0.89	0
28	GOL	C	525	-	5,5,5	0.27	0	5,5,5	0.68	0
24	CLA	D	401	40	55,73,73	1.97	12 (21%)	61,113,113	2.21	22 (36%)
30	LMT	D	402	-	36,36,36	0.46	0	47,47,47	1.03	3 (6%)
24	CLA	D	403	-	55,73,73	1.93	12 (21%)	61,113,113	2.15	20 (32%)
24	CLA	D	404	-	55,73,73	1.92	12 (21%)	61,113,113	2.12	18 (29%)
26	BCR	D	405	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	12 (21%)
32	PL9	D	406	-	55,55,55	0.79	2 (3%)	68,69,69	1.64	19 (27%)
36	DGD	D	407	-	63,63,67	0.93	3 (4%)	77,77,81	1.31	9 (11%)
37	LHG	D	408	-	48,48,48	0.83	2 (4%)	49,54,54	1.11	5 (10%)
37	LHG	D	409	-	48,48,48	0.83	2 (4%)	49,54,54	1.08	5 (10%)
37	LHG	D	410	-	48,48,48	0.90	2 (4%)	49,54,54	0.97	3 (6%)
35	HTG	D	411	-	16,16,19	1.08	2 (12%)	19,21,24	1.14	2 (10%)
37	LHG	E	101	-	41,41,48	0.98	2 (4%)	42,47,54	1.10	3 (7%)
30	LMT	E	102	-	36,36,36	0.45	0	47,47,47	0.78	0
38	HEM	E	103	5,6	30,50,50	2.27	7 (23%)	24,82,82	2.49	12 (50%)
27	SQD	F	101	-	42,43,54	1.41	3 (7%)	50,54,65	1.75	9 (18%)
28	GOL	F	103	33	5,5,5	0.35	0	5,5,5	0.32	0
26	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.28	5 (8%)
36	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.91	4 (5%)
30	LMT	I	102	-	36,36,36	0.44	0	47,47,47	1.21	5 (10%)
34	LMG	J	101	39	51,51,55	0.81	2 (3%)	59,59,63	1.01	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	K	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.47	12 (21%)
37	LHG	L	101	-	48,48,48	0.86	2 (4%)	49,54,54	1.17	4 (8%)
30	LMT	M	101	-	36,36,36	0.56	1 (2%)	47,47,47	0.87	0
30	LMT	M	102	-	36,36,36	0.39	0	47,47,47	0.89	0
28	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.33	0
35	HTG	O	303	-	19,19,19	1.00	1 (5%)	22,24,24	1.09	1 (4%)
28	GOL	T	101	-	5,5,5	0.44	0	5,5,5	0.29	0
26	BCR	T	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.41	10 (17%)
28	GOL	T	103	-	5,5,5	0.38	0	5,5,5	0.22	0
28	GOL	V	201	-	5,5,5	0.33	0	5,5,5	0.45	0
38	HEM	V	203	16	30,50,50	2.20	7 (23%)	24,82,82	2.46	10 (41%)
35	HTG	V	204	-	19,19,19	0.93	2 (10%)	22,24,24	1.47	3 (13%)
28	GOL	V	205	-	5,5,5	0.33	0	5,5,5	0.30	0
28	GOL	V	206	-	5,5,5	0.33	0	5,5,5	0.43	0
28	GOL	V	207	-	5,5,5	0.34	0	5,5,5	0.48	0
28	GOL	V	208	-	5,5,5	0.34	0	5,5,5	0.24	0
26	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.52	8 (14%)
34	LMG	Z	101	-	37,37,55	0.93	2 (5%)	45,45,63	1.44	6 (13%)
30	LMT	a	401	-	36,36,36	0.44	0	47,47,47	0.99	2 (4%)
27	SQD	a	402	-	53,54,54	1.39	3 (5%)	61,65,65	1.22	6 (9%)
24	CLA	a	406	-	55,73,73	1.92	12 (21%)	61,113,113	2.14	19 (31%)
24	CLA	a	407	40	55,73,73	1.91	12 (21%)	61,113,113	2.10	20 (32%)
25	PHO	a	408	-	67,69,69	2.11	15 (22%)	84,99,99	1.93	18 (21%)
24	CLA	a	409	-	55,73,73	1.90	13 (23%)	61,113,113	2.20	19 (31%)
26	BCR	a	410	-	41,41,41	1.11	1 (2%)	56,56,56	1.35	9 (16%)
27	SQD	a	411	-	53,54,54	1.30	3 (5%)	61,65,65	1.68	11 (18%)
28	GOL	a	412	-	5,5,5	0.32	0	5,5,5	0.50	0
28	GOL	a	413	-	5,5,5	0.40	0	5,5,5	0.30	0
31	OEX	a	415	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
32	PL9	a	416	-	55,55,55	0.63	2 (3%)	68,69,69	1.97	20 (29%)
30	LMT	a	417	-	36,36,36	0.43	0	47,47,47	0.86	1 (2%)
23	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
27	SQD	b	601	-	53,54,54	1.32	3 (5%)	61,65,65	1.81	10 (16%)
30	LMT	b	602	-	25,25,36	0.45	0	30,30,47	1.27	3 (10%)
35	HTG	b	603	-	19,19,19	1.00	1 (5%)	22,24,24	1.58	1 (4%)
35	HTG	b	604	-	19,19,19	0.95	2 (10%)	22,24,24	1.31	2 (9%)
24	CLA	b	606	40	55,73,73	1.96	11 (20%)	61,113,113	2.10	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	607	-	55,73,73	1.98	12 (21%)	61,113,113	2.22	20 (32%)
24	CLA	b	608	-	55,73,73	1.95	12 (21%)	61,113,113	2.35	21 (34%)
24	CLA	b	609	-	55,73,73	1.94	12 (21%)	61,113,113	2.23	17 (27%)
24	CLA	b	610	-	55,73,73	1.85	12 (21%)	61,113,113	2.20	20 (32%)
24	CLA	b	611	-	55,73,73	1.91	12 (21%)	61,113,113	2.15	21 (34%)
24	CLA	b	612	40	55,73,73	1.87	11 (20%)	61,113,113	2.25	22 (36%)
24	CLA	b	613	-	55,73,73	1.94	12 (21%)	61,113,113	2.14	24 (39%)
24	CLA	b	614	-	55,73,73	1.94	12 (21%)	61,113,113	2.15	21 (34%)
24	CLA	b	615	40	55,73,73	1.98	12 (21%)	61,113,113	2.06	18 (29%)
24	CLA	b	616	-	55,73,73	1.91	12 (21%)	61,113,113	2.22	20 (32%)
24	CLA	b	617	-	55,73,73	1.93	12 (21%)	61,113,113	2.06	17 (27%)
24	CLA	b	618	-	55,73,73	1.96	12 (21%)	61,113,113	2.10	17 (27%)
24	CLA	b	619	-	55,73,73	1.92	12 (21%)	61,113,113	2.28	23 (37%)
24	CLA	b	620	-	55,73,73	1.94	12 (21%)	61,113,113	2.11	17 (27%)
24	CLA	b	621	-	55,73,73	1.95	12 (21%)	61,113,113	2.20	17 (27%)
26	BCR	b	622	-	41,41,41	1.10	1 (2%)	56,56,56	1.40	7 (12%)
26	BCR	b	623	-	41,41,41	1.04	1 (2%)	56,56,56	1.14	4 (7%)
26	BCR	b	624	-	41,41,41	0.95	1 (2%)	56,56,56	1.26	7 (12%)
34	LMG	b	625	-	51,51,55	0.87	2 (3%)	59,59,63	1.03	2 (3%)
30	LMT	b	626	-	25,25,36	0.48	0	30,30,47	0.66	0
35	HTG	b	627	-	19,19,19	0.80	1 (5%)	22,24,24	1.50	3 (13%)
35	HTG	b	628	-	19,19,19	1.03	2 (10%)	22,24,24	2.18	3 (13%)
28	GOL	b	629	-	5,5,5	0.36	0	5,5,5	0.27	0
28	GOL	b	630	-	5,5,5	0.30	0	5,5,5	0.17	0
28	GOL	b	631	-	5,5,5	0.31	0	5,5,5	0.48	0
28	GOL	b	632	-	5,5,5	0.41	0	5,5,5	0.57	0
28	GOL	b	633	-	5,5,5	0.35	0	5,5,5	0.36	0
34	LMG	c	501	-	51,51,55	0.85	2 (3%)	59,59,63	1.27	6 (10%)
24	CLA	c	503	-	55,73,73	1.94	12 (21%)	61,113,113	2.21	19 (31%)
24	CLA	c	504	-	55,73,73	1.87	12 (21%)	61,113,113	2.12	16 (26%)
24	CLA	c	505	-	55,73,73	1.87	12 (21%)	61,113,113	2.10	19 (31%)
24	CLA	c	506	40	55,73,73	1.94	12 (21%)	61,113,113	2.16	21 (34%)
24	CLA	c	507	-	55,73,73	1.85	12 (21%)	61,113,113	2.13	15 (24%)
24	CLA	c	508	-	55,73,73	1.88	12 (21%)	61,113,113	2.10	21 (34%)
24	CLA	c	509	40	55,73,73	1.91	12 (21%)	61,113,113	2.25	18 (29%)
24	CLA	c	510	-	55,73,73	2.01	12 (21%)	61,113,113	2.16	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	511	-	55,73,73	2.01	12 (21%)	61,113,113	2.20	18 (29%)
24	CLA	c	512	-	55,73,73	1.94	12 (21%)	61,113,113	2.09	18 (29%)
24	CLA	c	513	3	55,73,73	1.90	11 (20%)	61,113,113	2.08	19 (31%)
24	CLA	c	514	-	55,73,73	1.93	12 (21%)	61,113,113	2.18	21 (34%)
24	CLA	c	515	-	55,73,73	1.94	12 (21%)	61,113,113	2.06	19 (31%)
26	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	9 (16%)
36	DGD	c	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.10	5 (6%)
36	DGD	c	518	-	63,63,67	0.87	2 (3%)	77,77,81	0.99	3 (3%)
36	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	3 (3%)
34	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	0.93	2 (3%)
34	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	4 (6%)
35	HTG	c	522	-	19,19,19	0.93	2 (10%)	22,24,24	1.85	2 (9%)
35	HTG	c	523	-	19,19,19	0.97	2 (10%)	22,24,24	1.69	2 (9%)
28	GOL	c	524	-	5,5,5	0.28	0	5,5,5	0.33	0
28	GOL	c	525	-	5,5,5	0.34	0	5,5,5	0.60	0
26	BCR	c	526	-	41,41,41	1.02	1 (2%)	56,56,56	1.52	11 (19%)
28	GOL	c	527	-	5,5,5	0.39	0	5,5,5	0.29	0
24	CLA	d	401	40	55,73,73	1.95	11 (20%)	61,113,113	2.18	20 (32%)
24	CLA	d	402	-	55,73,73	1.92	12 (21%)	61,113,113	2.26	22 (36%)
25	PHO	d	403	-	67,69,69	2.12	15 (22%)	84,99,99	1.96	20 (23%)
24	CLA	d	404	-	55,73,73	1.88	12 (21%)	61,113,113	2.04	20 (32%)
26	BCR	d	405	-	41,41,41	1.01	1 (2%)	56,56,56	1.82	13 (23%)
32	PL9	d	406	-	55,55,55	0.74	1 (1%)	68,69,69	1.63	19 (27%)
36	DGD	d	407	-	63,63,67	0.90	2 (3%)	77,77,81	1.07	6 (7%)
37	LHG	d	408	-	48,48,48	0.85	2 (4%)	49,54,54	1.02	5 (10%)
37	LHG	d	409	-	48,48,48	0.87	2 (4%)	49,54,54	1.11	4 (8%)
37	LHG	d	410	-	48,48,48	0.91	2 (4%)	49,54,54	0.99	3 (6%)
35	HTG	d	411	-	16,16,19	1.13	2 (12%)	19,21,24	1.97	1 (5%)
37	LHG	e	101	-	41,41,48	1.00	2 (4%)	42,47,54	1.07	2 (4%)
38	HEM	e	102	5,6	30,50,50	2.24	7 (23%)	24,82,82	2.59	10 (41%)
27	SQD	f	101	-	42,43,54	1.57	3 (7%)	50,54,65	1.56	7 (14%)
30	LMT	f	102	-	36,36,36	0.46	0	47,47,47	0.78	0
28	GOL	f	104	33	5,5,5	0.31	0	5,5,5	0.22	0
26	BCR	h	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.34	8 (14%)
36	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.01	7 (9%)
34	LMG	j	101	39	51,51,55	0.90	2 (3%)	59,59,63	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	k	103	-	41,41,41	1.01	1 (2%)	56,56,56	1.36	4 (7%)
27	SQD	l	101	-	53,54,54	1.27	3 (5%)	61,65,65	1.52	8 (13%)
37	LHG	l	102	-	48,48,48	0.92	2 (4%)	49,54,54	1.03	3 (6%)
30	LMT	m	102	-	36,36,36	0.48	0	47,47,47	1.04	3 (6%)
30	LMT	m	103	-	36,36,36	0.54	1 (2%)	47,47,47	1.08	4 (8%)
26	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.33	8 (14%)
28	GOL	t	102	-	5,5,5	0.31	0	5,5,5	0.34	0
28	GOL	v	201	-	5,5,5	0.32	0	5,5,5	0.34	0
38	HEM	v	202	16	30,50,50	2.16	7 (23%)	24,82,82	2.27	10 (41%)
28	GOL	v	203	-	5,5,5	0.22	0	5,5,5	0.47	0
28	GOL	v	204	-	5,5,5	0.30	0	5,5,5	0.35	0
28	GOL	v	205	-	5,5,5	0.32	0	5,5,5	0.39	0
26	BCR	y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.57	11 (19%)
34	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.20	5 (10%)

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
23	BCT	A	404	21	-	0/0/0/0	0/0/0/0
24	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	406	40	2/2/20/25	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	-	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
28	GOL	A	413	-	-	0/4/4/4	0/0/0/0
28	GOL	A	414	-	-	0/4/4/4	0/0/0/0
27	SQD	A	416	-	-	0/49/69/69	0/1/1/1
30	LMT	A	417	-	-	0/19/59/61	0/2/2/2
31	OEX	A	418	1,3,40	-	0/0/68/68	0/0/6/6
32	PL9	A	419	-	-	0/53/73/73	0/1/1/1
24	CLA	B	602	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
34	LMG	B	621	-	-	0/46/66/70	0/1/1/1
35	HTG	B	622	-	-	0/10/30/30	0/1/1/1
35	HTG	B	623	-	-	0/10/30/30	0/1/1/1
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
28	GOL	B	625	-	-	0/4/4/4	0/0/0/0
28	GOL	B	626	-	-	0/4/4/4	0/0/0/0
28	GOL	B	627	-	-	0/4/4/4	0/0/0/0
28	GOL	B	628	-	-	0/4/4/4	0/0/0/0
28	GOL	B	629	-	-	0/4/4/4	0/0/0/0
35	HTG	B	630	-	-	0/10/30/30	0/1/1/1
35	HTG	B	631	-	-	0/10/30/30	0/1/1/1
28	GOL	B	633	-	-	0/4/4/4	0/0/0/0
30	LMT	B	634	-	-	0/17/37/61	0/1/1/2
28	GOL	B	635	-	-	0/4/4/4	0/0/0/0
34	LMG	C	501	-	-	0/46/66/70	0/1/1/1
24	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	40	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	C	509	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	-	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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	514	-	2/2/20/25	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
34	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	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	524	-	-	0/4/4/4	0/0/0/0
28	GOL	C	525	-	-	0/4/4/4	0/0/0/0
24	CLA	D	401	40	3/3/20/25	0/37/135/135	0/0/9/9
30	LMT	D	402	-	-	0/21/61/61	0/2/2/2
24	CLA	D	403	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	405	-	-	0/29/63/63	0/2/2/2
32	PL9	D	406	-	-	0/53/73/73	0/1/1/1
36	DGD	D	407	-	-	1/51/91/95	0/2/2/2
37	LHG	D	408	-	-	0/53/53/53	0/0/0/0
37	LHG	D	409	-	-	0/53/53/53	0/0/0/0
37	LHG	D	410	-	-	0/53/53/53	0/0/0/0
35	HTG	D	411	-	-	0/7/27/30	0/1/1/1
37	LHG	E	101	-	-	0/46/46/53	0/0/0/0
30	LMT	E	102	-	-	0/21/61/61	0/2/2/2
38	HEM	E	103	5,6	-	0/10/54/54	0/0/8/8
27	SQD	F	101	-	-	0/38/58/69	0/1/1/1
28	GOL	F	103	33	-	0/4/4/4	0/0/0/0
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
30	LMT	I	102	-	-	0/21/61/61	0/2/2/2
34	LMG	J	101	39	-	0/46/66/70	0/1/1/1
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
37	LHG	L	101	-	-	0/53/53/53	0/0/0/0
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
28	GOL	O	302	-	-	0/4/4/4	0/0/0/0
35	HTG	O	303	-	-	0/10/30/30	0/1/1/1
28	GOL	T	101	-	-	0/4/4/4	0/0/0/0
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
28	GOL	T	103	-	-	0/4/4/4	0/0/0/0
28	GOL	V	201	-	-	0/4/4/4	0/0/0/0
38	HEM	V	203	16	-	0/10/54/54	0/0/8/8
35	HTG	V	204	-	-	0/10/30/30	0/1/1/1
28	GOL	V	205	-	-	0/4/4/4	0/0/0/0
28	GOL	V	206	-	-	0/4/4/4	0/0/0/0
28	GOL	V	207	-	-	0/4/4/4	0/0/0/0
28	GOL	V	208	-	-	0/4/4/4	0/0/0/0
26	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
34	LMG	Z	101	-	-	1/31/51/70	0/1/1/1
30	LMT	a	401	-	-	0/21/61/61	0/2/2/2
27	SQD	a	402	-	-	0/49/69/69	0/1/1/1
24	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	407	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	a	408	-	-	0/53/103/103	0/1/6/6
24	CLA	a	409	-	3/3/20/25	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
28	GOL	a	413	-	-	0/4/4/4	0/0/0/0
31	OEX	a	415	1,3,40	-	0/0/68/68	0/0/6/6
32	PL9	a	416	-	-	0/53/73/73	0/1/1/1
30	LMT	a	417	-	-	0/21/61/61	0/2/2/2
23	BCT	a	418	21	-	0/0/0/0	0/0/0/0
27	SQD	b	601	-	-	1/49/69/69	0/1/1/1
30	LMT	b	602	-	-	0/17/37/61	0/1/1/2
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
35	HTG	b	604	-	-	0/10/30/30	0/1/1/1
24	CLA	b	606	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	40	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	613	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	621	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	622	-	-	0/29/63/63	0/2/2/2
26	BCR	b	623	-	-	0/29/63/63	0/2/2/2
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
34	LMG	b	625	-	-	0/46/66/70	0/1/1/1
30	LMT	b	626	-	-	0/17/37/61	0/1/1/2
35	HTG	b	627	-	-	0/10/30/30	0/1/1/1
35	HTG	b	628	-	-	0/10/30/30	0/1/1/1
28	GOL	b	629	-	-	0/4/4/4	0/0/0/0
28	GOL	b	630	-	-	0/4/4/4	0/0/0/0
28	GOL	b	631	-	-	0/4/4/4	0/0/0/0
28	GOL	b	632	-	-	0/4/4/4	0/0/0/0
28	GOL	b	633	-	-	0/4/4/4	0/0/0/0
34	LMG	c	501	-	-	0/46/66/70	0/1/1/1
24	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	509	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	-	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	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	515	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
36	DGD	c	517	-	-	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	c	518	-	-	0/51/91/95	0/2/2/2
36	DGD	c	519	-	-	0/51/91/95	0/2/2/2
34	LMG	c	520	-	-	0/46/66/70	0/1/1/1
34	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	524	-	-	0/4/4/4	0/0/0/0
28	GOL	c	525	-	-	0/4/4/4	0/0/0/0
26	BCR	c	526	-	-	0/29/63/63	0/2/2/2
28	GOL	c	527	-	-	0/4/4/4	0/0/0/0
24	CLA	d	401	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	d	402	-	1/1/20/25	0/37/135/135	0/0/9/9
25	PHO	d	403	-	-	0/53/103/103	0/1/6/6
24	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	d	405	-	-	0/29/63/63	0/2/2/2
32	PL9	d	406	-	-	0/53/73/73	0/1/1/1
36	DGD	d	407	-	-	0/51/91/95	0/2/2/2
37	LHG	d	408	-	-	0/53/53/53	0/0/0/0
37	LHG	d	409	-	-	0/53/53/53	0/0/0/0
37	LHG	d	410	-	-	0/53/53/53	0/0/0/0
35	HTG	d	411	-	-	0/7/27/30	0/1/1/1
37	LHG	e	101	-	-	0/46/46/53	0/0/0/0
38	HEM	e	102	5,6	-	0/10/54/54	0/0/8/8
27	SQD	f	101	-	-	2/38/58/69	0/1/1/1
30	LMT	f	102	-	-	0/21/61/61	0/2/2/2
28	GOL	f	104	33	-	0/4/4/4	0/0/0/0
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	LMG	j	101	39	-	0/46/66/70	0/1/1/1
26	BCR	k	103	-	-	0/29/63/63	0/2/2/2
27	SQD	l	101	-	-	0/49/69/69	0/1/1/1
37	LHG	l	102	-	-	0/53/53/53	0/0/0/0
30	LMT	m	102	-	-	0/21/61/61	0/2/2/2
30	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	t	102	-	-	0/4/4/4	0/0/0/0
28	GOL	v	201	-	-	0/4/4/4	0/0/0/0
38	HEM	v	202	16	-	0/10/54/54	0/0/8/8
28	GOL	v	203	-	-	0/4/4/4	0/0/0/0
28	GOL	v	204	-	-	0/4/4/4	0/0/0/0
28	GOL	v	205	-	-	0/4/4/4	0/0/0/0
26	BCR	y	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	z	101	-	-	0/34/54/70	0/1/1/1

The worst 5 of 1069 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	416	SQD	C6-S	-7.63	1.66	1.77
27	a	402	SQD	C6-S	-7.59	1.66	1.77
27	A	411	SQD	C6-S	-7.59	1.66	1.77
27	f	101	SQD	C6-S	-7.57	1.66	1.77
27	a	411	SQD	C6-S	-7.13	1.67	1.77

The worst 5 of 1991 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	616	CLA	CHD-C4C-C3C	-6.38	115.08	124.94
24	B	610	CLA	CHD-C4C-C3C	-6.37	115.09	124.94
24	b	618	CLA	CHD-C4C-C3C	-6.34	115.14	124.94
24	b	612	CLA	CHD-C4C-C3C	-6.23	115.31	124.94
24	C	508	CLA	CHD-C4C-C3C	-6.20	115.36	124.94

5 of 180 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA
24	B	612	CLA	NC
24	D	403	CLA	ND

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	b	601	SQD	C45-O47-C7-C8
36	D	407	DGD	C2G-O2G-C1B-C2B
34	Z	101	LMG	C8-O7-C10-C11
27	f	101	SQD	C45-O47-C7-O49
27	f	101	SQD	C45-O47-C7-C8

There are no ring outliers.

86 monomers are involved in 236 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	405	CLA	4	0
24	A	406	CLA	6	0
25	A	408	PHO	2	0
24	A	409	CLA	3	0
26	A	410	BCR	3	0
27	A	411	SQD	6	0
28	A	412	GOL	2	0
28	A	413	GOL	2	0
27	A	416	SQD	2	0
32	A	419	PL9	4	0
24	B	602	CLA	1	0
24	B	604	CLA	3	0
24	B	605	CLA	1	0
24	B	606	CLA	6	0
24	B	607	CLA	2	0
24	B	608	CLA	2	0
24	B	609	CLA	2	0
24	B	610	CLA	7	0
24	B	611	CLA	4	0
24	B	612	CLA	1	0
24	B	613	CLA	5	0
24	B	614	CLA	5	0
24	B	615	CLA	4	0
24	B	616	CLA	1	0
24	B	617	CLA	10	0
26	B	618	BCR	2	0
26	B	619	BCR	1	0
26	B	620	BCR	3	0
34	B	621	LMG	2	0
35	B	623	HTG	1	0
28	B	628	GOL	1	0
28	B	633	GOL	1	0
30	B	634	LMT	1	0
28	B	635	GOL	2	0
34	C	501	LMG	5	0
24	C	502	CLA	4	0
24	C	503	CLA	7	0
24	C	504	CLA	4	0
24	C	505	CLA	4	0
24	C	506	CLA	1	0
24	C	507	CLA	7	0
24	C	508	CLA	6	0
24	C	509	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	510	CLA	4	0
24	C	511	CLA	6	0
24	C	512	CLA	4	0
24	C	513	CLA	6	0
24	C	514	CLA	9	0
26	C	515	BCR	3	0
26	C	516	BCR	4	0
36	C	517	DGD	4	0
36	C	518	DGD	3	0
36	C	519	DGD	3	0
34	C	520	LMG	4	0
34	C	521	LMG	2	0
35	C	522	HTG	1	0
35	C	523	HTG	2	0
28	C	524	GOL	1	0
28	C	525	GOL	2	0
24	D	401	CLA	6	0
30	D	402	LMT	1	0
24	D	403	CLA	1	0
24	D	404	CLA	4	0
26	D	405	BCR	4	0
36	D	407	DGD	6	0
37	D	408	LHG	2	0
37	D	410	LHG	10	0
35	D	411	HTG	3	0
37	E	101	LHG	6	0
27	F	101	SQD	5	0
26	H	101	BCR	6	0
36	H	102	DGD	2	0
30	I	102	LMT	2	0
34	J	101	LMG	3	0
26	K	101	BCR	2	0
37	L	101	LHG	1	0
30	M	101	LMT	1	0
30	M	102	LMT	2	0
28	T	101	GOL	1	0
26	T	102	BCR	5	0
35	V	204	HTG	1	0
28	V	205	GOL	2	0
28	V	207	GOL	1	0
28	V	208	GOL	1	0
26	Y	101	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	Z	101	LMG	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	0.72	47 (14%) 4 6	16, 23, 42, 79	0
1	a	334/344 (97%)	0.88	68 (20%) 1 1	17, 25, 48, 82	0
2	B	504/505 (99%)	0.31	44 (8%) 13 20	18, 27, 52, 90	0
2	b	504/505 (99%)	0.51	53 (10%) 8 13	19, 29, 60, 108	0
3	C	451/455 (99%)	0.28	28 (6%) 24 34	20, 32, 49, 89	0
3	c	455/455 (100%)	0.48	40 (8%) 12 20	23, 35, 50, 87	0
4	D	342/342 (100%)	0.93	67 (19%) 1 2	15, 24, 40, 114	0
4	d	341/342 (99%)	0.64	41 (12%) 6 10	18, 26, 42, 90	0
5	E	81/84 (96%)	1.27	19 (23%) 1 1	27, 40, 68, 97	0
5	e	81/84 (96%)	1.14	16 (19%) 1 2	32, 45, 77, 97	0
6	F	34/44 (77%)	0.39	6 (17%) 2 3	26, 35, 56, 64	0
6	f	32/44 (72%)	0.46	4 (12%) 5 9	31, 37, 84, 99	0
7	H	65/65 (100%)	0.39	3 (4%) 36 47	24, 34, 52, 97	0
7	h	65/65 (100%)	0.61	6 (9%) 11 18	28, 37, 58, 113	0
8	I	37/38 (97%)	0.86	5 (13%) 4 7	30, 34, 91, 101	0
8	i	37/38 (97%)	0.78	5 (13%) 4 7	29, 34, 79, 102	0
9	J	38/39 (97%)	0.79	8 (21%) 1 1	26, 38, 85, 109	0
9	j	38/39 (97%)	0.29	4 (10%) 8 13	30, 41, 84, 85	0
10	K	37/37 (100%)	0.20	0 100 100	31, 38, 55, 64	0
10	k	37/37 (100%)	0.91	8 (21%) 1 1	33, 42, 56, 66	0
11	L	37/37 (100%)	1.23	11 (29%) 1 0	16, 20, 66, 91	0
11	l	37/37 (100%)	1.10	7 (18%) 2 2	17, 21, 61, 91	0
12	M	33/36 (91%)	0.95	7 (21%) 1 1	18, 23, 44, 100	0
12	m	33/36 (91%)	0.82	6 (18%) 2 2	19, 23, 44, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.42	23 (9%) 10 17	16, 34, 65, 113	0
13	o	243/244 (99%)	0.93	53 (21%) 1 1	18, 35, 75, 122	0
14	T	29/31 (93%)	1.03	4 (13%) 4 7	17, 23, 48, 85	0
14	t	29/31 (93%)	0.59	2 (6%) 20 30	17, 23, 49, 85	0
15	U	97/104 (93%)	0.30	6 (6%) 24 34	22, 33, 53, 85	0
15	u	97/104 (93%)	-0.07	0 100 100	25, 34, 51, 85	0
16	V	137/137 (100%)	0.01	0 100 100	23, 33, 54, 70	0
16	v	137/137 (100%)	0.53	14 (10%) 9 14	26, 38, 57, 72	0
17	Y	29/30 (96%)	2.12	9 (31%) 1 0	38, 50, 91, 107	0
17	y	29/30 (96%)	2.00	9 (31%) 1 0	41, 54, 91, 107	0
18	X	39/40 (97%)	0.82	8 (20%) 1 1	32, 42, 80, 92	0
18	x	39/40 (97%)	1.65	11 (28%) 1 0	35, 45, 93, 96	0
19	Z	62/62 (100%)	1.35	19 (30%) 1 0	40, 52, 87, 98	0
19	z	62/62 (100%)	3.06	37 (59%) 0 0	44, 53, 87, 98	0
20	R	34/34 (100%)	9.53	34 (100%) 0 0	69, 93, 111, 118	0
All	All	5293/5382 (98%)	0.70	732 (13%) 4 7	15, 31, 63, 122	0

The worst 5 of 732 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	18.7
20	R	6	LEU	14.4
20	R	14	LEU	13.7
20	R	31	VAL	13.3
20	R	20	VAL	12.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.96	0.14	-	23,34,56,61	0
14	FME	T	1	10/11	0.96	0.14	-	21,27,45,56	0
12	FME	m	1	10/11	0.93	0.15	-	25,31,61,62	0
9	FME	j	1	10/11	0.76	0.34	-	53,71,94,136	0
14	FME	t	1	10/11	0.95	0.11	-	13,22,33,65	0
8	FME	i	1	10/11	0.97	0.15	-	23,34,37,42	0
8	FME	I	1	10/11	0.97	0.11	-	22,34,37,40	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	UNL	k	102	10/-	0.58	0.61	26.13	54,83,94,102	0
28	GOL	b	633	6/6	0.95	0.29	15.05	32,54,63,71	0
29	UNL	j	103	10/-	0.61	0.32	12.31	44,61,67,73	0
29	UNL	k	101	32/-	0.70	0.38	10.71	42,75,105,108	0
30	LMT	B	634	25/35	0.78	0.27	9.82	32,63,105,111	0
28	GOL	c	525	6/6	0.90	0.24	9.13	43,46,61,62	0
28	GOL	t	102	6/6	0.77	0.34	8.12	29,60,65,69	0
27	SQD	a	402	54/54	0.76	0.23	7.65	34,61,79,100	0
30	LMT	f	102	35/35	0.60	0.36	7.63	56,83,109,113	0
28	GOL	C	524	6/6	0.88	0.21	7.38	39,45,57,60	0
36	DGD	d	407	62/66	0.59	0.44	7.05	41,88,117,122	0
28	GOL	V	205	6/6	0.79	0.40	6.97	37,54,59,72	0
28	GOL	b	632	6/6	0.81	0.29	6.03	40,46,68,69	0
32	PL9	a	416	55/55	0.75	0.27	5.87	50,76,94,95	0
30	LMT	E	102	35/35	0.61	0.34	5.82	43,81,105,107	0
28	GOL	v	203	6/6	0.75	0.29	5.78	50,69,71,78	0
35	HTG	V	204	19/19	0.88	0.26	5.70	40,65,99,175	0
29	UNL	X	101	10/-	0.85	0.15	5.37	29,37,41,42	0
35	HTG	b	627	19/19	0.89	0.23	5.36	27,44,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	LMT	M	101	35/35	0.66	0.28	5.35	35,60,79,85	0
29	UNL	J	103	10/-	0.71	0.43	5.30	38,53,73,75	0
29	UNL	I	101	40/-	0.76	0.29	5.11	27,63,114,119	0
30	LMT	b	602	25/35	0.79	0.30	5.10	22,63,102,106	0
28	GOL	F	103	6/6	0.91	0.18	4.95	52,59,65,68	0
28	GOL	c	527	6/6	0.89	0.21	4.95	36,57,61,63	0
28	GOL	B	629	6/6	0.94	0.24	4.90	24,40,61,78	0
32	PL9	A	419	55/55	0.68	0.29	4.81	38,66,87,92	0
28	GOL	B	628	6/6	0.88	0.23	4.66	35,46,67,70	0
28	GOL	B	627	6/6	0.85	0.22	4.59	31,35,43,44	0
30	LMT	m	103	35/35	0.65	0.27	4.55	30,60,86,90	0
28	GOL	a	413	6/6	0.79	0.23	4.18	38,67,69,71	0
26	BCR	B	619	40/40	0.90	0.16	3.93	17,25,44,46	0
30	LMT	a	417	35/35	0.76	0.42	3.77	52,76,90,94	0
30	LMT	a	401	35/35	0.82	0.19	3.67	28,61,79,86	0
29	UNL	i	101	40/-	0.73	0.24	3.62	36,64,96,108	0
29	UNL	D	413	40/-	0.81	0.20	3.54	33,55,105,108	0
24	CLA	b	606	65/65	0.92	0.18	3.51	30,46,82,98	0
34	LMG	J	101	51/55	0.92	0.22	3.49	20,37,78,86	0
34	LMG	Z	101	37/55	0.62	0.32	3.46	32,81,104,105	0
28	GOL	A	414	6/6	0.78	0.19	3.45	40,60,69,70	0
28	GOL	V	208	6/6	0.86	0.27	3.35	41,56,62,63	0
34	LMG	j	101	51/55	0.90	0.19	3.33	26,39,70,82	0
28	GOL	A	413	6/6	0.86	0.19	3.31	35,38,41,42	0
35	HTG	C	523	19/19	0.75	0.29	3.28	46,75,97,109	0
26	BCR	d	405	40/40	0.87	0.16	3.27	29,35,63,64	0
34	LMG	z	101	39/55	0.72	0.39	3.25	47,74,94,101	0
35	HTG	c	523	19/19	0.83	0.31	3.08	60,84,93,98	0
28	GOL	f	104	6/6	0.92	0.22	3.07	45,51,59,61	0
28	GOL	a	412	6/6	0.91	0.16	2.97	22,37,41,45	0
35	HTG	D	411	16/19	0.69	0.25	2.86	38,100,111,113	0
23	BCT	a	418	4/4	0.95	0.17	2.84	30,33,42,44	0
27	SQD	l	101	54/54	0.68	0.25	2.77	31,67,98,101	0
34	LMG	C	501	51/55	0.84	0.19	2.62	37,54,74,82	0
28	GOL	B	625	6/6	0.92	0.14	2.61	28,43,48,55	0
27	SQD	A	416	54/54	0.80	0.18	2.59	28,52,75,76	0
30	LMT	A	417	33/35	0.85	0.19	2.55	27,65,78,85	0
29	UNL	d	413	36/-	0.80	0.19	2.52	35,58,94,99	0
29	UNL	C	526	34/-	0.65	0.34	2.51	46,71,82,84	0
24	CLA	B	617	65/65	0.95	0.17	2.51	19,28,88,91	0
26	BCR	b	623	40/40	0.91	0.21	2.48	15,27,40,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	LMG	b	625	51/55	0.87	0.28	2.42	24,39,59,71	0
24	CLA	B	602	65/65	0.92	0.16	2.40	24,39,82,104	0
35	HTG	B	631	19/19	0.76	0.21	2.39	25,84,104,120	0
28	GOL	V	207	6/6	0.95	0.21	2.32	35,38,41,44	0
39	MG	j	102	1/1	0.98	0.16	2.30	34,34,34,34	0
28	GOL	B	626	6/6	0.89	0.21	2.24	32,37,40,59	0
29	UNL	d	412	17/-	0.84	0.16	2.23	31,48,79,85	0
30	LMT	I	102	35/35	0.75	0.34	2.09	59,81,95,100	0
28	GOL	V	206	6/6	0.87	0.21	2.09	21,38,44,48	0
36	DGD	D	407	62/66	0.51	0.49	2.09	44,89,114,119	0
27	SQD	b	601	54/54	0.72	0.23	1.96	36,58,91,95	0
35	HTG	B	630	19/19	0.86	0.18	1.84	30,54,78,81	0
37	LHG	L	101	49/49	0.93	0.23	1.81	15,29,47,58	0
34	LMG	c	501	51/55	0.80	0.21	1.72	39,60,77,85	0
37	LHG	d	408	49/49	0.90	0.23	1.67	26,34,46,50	0
29	UNL	x	101	10/-	0.76	0.17	1.63	35,44,57,58	0
27	SQD	a	411	54/54	0.90	0.23	1.62	32,56,75,78	0
29	UNL	D	412	17/-	0.91	0.16	1.59	24,45,74,78	0
37	LHG	D	408	49/49	0.90	0.25	1.50	16,31,43,54	0
34	LMG	B	621	51/55	0.83	0.25	1.46	20,35,52,64	0
28	GOL	b	629	6/6	0.93	0.13	1.42	32,40,48,57	0
32	PL9	d	406	55/55	0.90	0.21	1.41	16,23,35,47	0
28	GOL	T	101	6/6	0.89	0.18	1.38	35,60,64,65	0
28	GOL	v	204	6/6	0.84	0.20	1.36	47,64,70,92	0
37	LHG	l	102	49/49	0.90	0.19	1.33	19,30,48,57	0
37	LHG	E	101	42/49	0.69	0.25	1.33	38,73,93,103	0
24	CLA	c	515	65/65	0.86	0.27	1.33	37,51,79,88	0
35	HTG	B	623	19/19	0.84	0.16	1.33	29,42,64,71	0
26	BCR	B	618	40/40	0.93	0.16	1.31	15,23,33,41	0
28	GOL	B	633	6/6	0.92	0.10	1.31	27,36,40,41	0
25	PHO	A	408	64/64	0.95	0.26	1.30	16,22,30,32	0
32	PL9	D	406	55/55	0.91	0.24	1.28	14,23,36,43	0
24	CLA	A	409	65/65	0.95	0.12	1.28	18,27,83,92	0
30	LMT	b	626	25/35	0.69	0.30	1.23	33,67,110,115	0
27	SQD	f	101	43/54	0.82	0.30	1.23	55,82,109,117	0
25	PHO	d	403	64/64	0.94	0.21	1.21	20,25,34,38	0
24	CLA	B	611	65/65	0.95	0.12	1.21	19,26,36,39	0
34	LMG	C	521	51/55	0.79	0.23	1.21	31,74,90,96	0
28	GOL	b	630	6/6	0.92	0.16	1.15	37,48,50,52	0
27	SQD	A	411	54/54	0.90	0.21	1.14	26,51,71,78	0
34	LMG	C	520	51/55	0.77	0.28	1.13	26,61,82,87	0
24	CLA	c	510	65/65	0.93	0.16	1.13	24,31,70,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	CLA	A	405	65/65	0.94	0.26	1.12	15,18,26,50	0
24	CLA	b	612	65/65	0.93	0.21	1.12	14,23,30,36	0
24	CLA	D	403	65/65	0.96	0.28	1.10	14,19,36,42	0
24	CLA	A	406	65/65	0.95	0.26	1.09	15,19,84,88	0
36	DGD	C	519	62/66	0.93	0.23	1.08	20,30,58,63	0
35	HTG	d	411	16/19	0.67	0.27	1.05	54,73,84,87	0
24	CLA	C	509	65/65	0.91	0.16	1.01	21,29,78,80	0
24	CLA	d	402	65/65	0.96	0.24	1.00	18,22,38,46	0
26	BCR	D	405	40/40	0.91	0.14	1.00	22,31,61,77	0
37	LHG	D	409	49/49	0.94	0.18	1.00	17,27,48,60	0
26	BCR	b	622	40/40	0.91	0.17	0.98	16,26,33,36	0
24	CLA	a	407	65/65	0.94	0.26	0.98	19,25,72,79	0
37	LHG	d	409	49/49	0.93	0.14	0.97	17,26,39,55	0
36	DGD	h	102	62/66	0.87	0.17	0.97	23,35,52,69	0
26	BCR	Y	101	40/40	0.90	0.12	0.96	28,35,49,50	0
34	LMG	c	521	51/55	0.76	0.28	0.92	35,79,91,98	0
36	DGD	C	518	62/66	0.92	0.23	0.90	22,32,76,92	0
35	HTG	b	628	19/19	0.60	0.31	0.90	48,90,106,124	0
35	HTG	B	622	19/19	0.92	0.11	0.90	26,30,44,56	0
24	CLA	D	401	65/65	0.96	0.24	0.89	13,18,30,32	0
24	CLA	c	512	65/65	0.93	0.17	0.84	26,32,44,59	0
24	CLA	b	609	65/65	0.95	0.15	0.84	16,25,56,66	0
24	CLA	C	514	65/65	0.91	0.16	0.83	32,42,69,72	0
36	DGD	c	519	62/66	0.92	0.20	0.83	26,34,65,72	0
37	LHG	D	410	49/49	0.94	0.18	0.81	20,33,91,95	0
24	CLA	b	618	65/65	0.94	0.18	0.81	15,23,48,56	0
24	CLA	B	615	65/65	0.92	0.14	0.78	15,24,67,78	0
35	HTG	b	603	19/19	0.89	0.14	0.77	34,44,64,67	0
38	HEM	e	102	43/43	0.94	0.18	0.77	38,48,65,84	0
24	CLA	c	505	65/65	0.89	0.13	0.75	29,35,46,60	0
28	GOL	v	201	6/6	0.93	0.13	0.75	31,40,49,50	0
34	LMG	c	520	51/55	0.85	0.22	0.74	33,63,86,88	0
36	DGD	c	517	62/66	0.93	0.17	0.74	23,32,68,76	0
36	DGD	H	102	62/66	0.86	0.19	0.72	20,29,42,58	0
24	CLA	a	409	65/65	0.94	0.13	0.70	20,27,83,88	0
26	BCR	K	101	40/40	0.93	0.12	0.68	27,33,42,47	0
24	CLA	C	505	65/65	0.92	0.21	0.66	22,29,59,77	0
37	LHG	d	410	49/49	0.94	0.18	0.65	23,35,85,104	0
37	LHG	e	101	42/49	0.74	0.23	0.64	49,87,117,128	0
26	BCR	t	101	40/40	0.92	0.12	0.63	15,24,45,49	0
24	CLA	B	610	65/65	0.91	0.12	0.60	19,26,36,40	0
30	LMT	m	102	35/35	0.70	0.23	0.60	16,51,73,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	CLA	d	401	65/65	0.96	0.21	0.60	16,19,26,42	0
27	SQD	F	101	43/54	0.88	0.30	0.56	39,70,96,105	0
24	CLA	b	619	65/65	0.93	0.14	0.55	15,25,72,77	0
26	BCR	T	102	40/40	0.91	0.16	0.55	14,28,36,42	0
24	CLA	d	404	65/65	0.94	0.12	0.52	27,34,74,81	0
25	PHO	A	407	64/64	0.94	0.18	0.50	15,18,23,28	0
28	GOL	A	412	6/6	0.92	0.10	0.48	29,31,34,37	0
36	DGD	C	517	62/66	0.94	0.14	0.48	22,33,75,83	0
24	CLA	a	406	65/65	0.96	0.24	0.47	17,20,35,51	0
24	CLA	B	612	65/65	0.91	0.17	0.47	15,21,37,41	0
21	FE2	a	403	1/1	0.99	0.11	0.46	30,30,30,30	0
26	BCR	k	103	40/40	0.86	0.17	0.46	32,40,48,52	0
30	LMT	M	102	35/35	0.78	0.20	0.44	22,50,66,76	0
26	BCR	C	515	40/40	0.92	0.12	0.43	31,42,49,53	0
24	CLA	b	616	65/65	0.93	0.13	0.41	18,26,38,52	0
24	CLA	B	607	65/65	0.93	0.11	0.41	18,26,51,75	0
25	PHO	a	408	64/64	0.95	0.18	0.40	16,21,29,37	0
24	CLA	b	611	65/65	0.94	0.10	0.40	19,31,58,74	0
24	CLA	b	614	65/65	0.89	0.12	0.37	24,31,41,50	0
24	CLA	C	507	65/65	0.92	0.16	0.36	28,42,81,88	0
24	CLA	B	604	65/65	0.91	0.12	0.35	18,25,32,40	0
30	LMT	D	402	35/35	0.68	0.25	0.34	32,75,96,97	0
24	CLA	b	610	65/65	0.95	0.11	0.33	18,24,37,42	0
28	GOL	V	201	6/6	0.92	0.11	0.31	27,29,40,41	0
24	CLA	B	614	65/65	0.94	0.17	0.30	14,22,45,52	0
28	GOL	v	205	6/6	0.93	0.17	0.28	25,39,52,58	0
36	DGD	c	518	62/66	0.90	0.19	0.28	24,35,79,94	0
24	CLA	b	621	65/65	0.92	0.15	0.27	21,35,82,84	0
26	BCR	c	516	40/40	0.91	0.12	0.26	29,36,47,57	0
24	CLA	b	608	65/65	0.94	0.11	0.24	22,29,38,42	0
24	CLA	B	608	65/65	0.92	0.18	0.24	13,20,31,35	0
24	CLA	B	616	65/65	0.95	0.11	0.22	19,28,48,60	0
24	CLA	c	514	65/65	0.90	0.18	0.22	34,43,67,76	0
24	CLA	c	507	65/65	0.91	0.12	0.22	22,31,52,62	0
26	BCR	H	101	40/40	0.88	0.13	0.19	21,32,48,52	0
24	CLA	C	504	65/65	0.92	0.12	0.17	24,33,42,48	0
24	CLA	b	617	65/65	0.94	0.11	0.17	18,26,36,50	0
24	CLA	C	510	65/65	0.95	0.11	0.16	25,32,51,57	0
24	CLA	c	506	65/65	0.90	0.17	0.15	26,33,51,61	0
24	CLA	C	511	65/65	0.93	0.15	0.15	23,29,41,62	0
24	CLA	c	503	65/65	0.93	0.11	0.13	29,34,45,54	0
24	CLA	b	607	65/65	0.92	0.12	0.10	23,30,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	GOL	b	631	6/6	0.91	0.11	0.09	39,46,48,60	0
24	CLA	B	605	65/65	0.94	0.14	0.08	15,22,51,63	0
26	BCR	y	101	40/40	0.92	0.12	0.06	31,40,53,60	0
26	BCR	b	624	40/40	0.92	0.10	0.05	20,32,46,52	0
21	FE2	A	401	1/1	0.99	0.10	0.01	27,27,27,27	0
26	BCR	B	620	40/40	0.95	0.10	0.01	22,29,42,47	0
24	CLA	b	620	65/65	0.91	0.11	-0.00	22,31,51,74	0
24	CLA	C	502	65/65	0.93	0.11	-0.03	25,32,47,58	0
24	CLA	c	513	65/65	0.91	0.12	-0.04	30,39,50,54	0
24	CLA	B	609	65/65	0.95	0.14	-0.04	17,22,32,36	0
24	CLA	b	615	65/65	0.94	0.11	-0.04	21,28,39,46	0
24	CLA	B	613	65/65	0.95	0.11	-0.05	15,23,32,35	0
24	CLA	B	606	65/65	0.95	0.09	-0.06	16,22,34,38	0
24	CLA	c	504	65/65	0.94	0.14	-0.06	26,32,45,55	0
24	CLA	C	513	65/65	0.93	0.12	-0.08	29,42,67,74	0
38	HEM	v	202	43/43	0.97	0.10	-0.10	29,33,40,48	0
24	CLA	C	512	65/65	0.93	0.11	-0.10	26,32,41,48	0
24	CLA	B	603	65/65	0.91	0.12	-0.12	18,25,32,38	0
24	CLA	b	613	65/65	0.94	0.11	-0.12	22,29,38,42	0
26	BCR	c	526	40/40	0.90	0.16	-0.13	39,48,59,63	0
24	CLA	C	506	65/65	0.95	0.10	-0.14	21,29,45,53	0
26	BCR	A	410	40/40	0.95	0.10	-0.16	16,26,33,35	0
24	CLA	D	404	65/65	0.95	0.12	-0.17	21,28,73,84	0
28	GOL	c	524	6/6	0.98	0.15	-0.17	25,28,30,34	0
23	BCT	A	404	4/4	0.96	0.10	-0.20	27,30,39,40	0
26	BCR	h	101	40/40	0.87	0.12	-0.23	27,35,46,49	0
35	HTG	O	303	19/19	0.94	0.09	-0.28	24,32,47,48	0
28	GOL	C	525	6/6	0.95	0.13	-0.31	20,24,26,27	0
26	BCR	a	410	40/40	0.94	0.09	-0.34	16,24,31,33	0
24	CLA	c	509	65/65	0.92	0.12	-0.36	27,34,49,58	0
24	CLA	C	508	65/65	0.93	0.11	-0.36	25,35,48,57	0
38	HEM	E	103	43/43	0.96	0.17	-0.45	27,38,50,56	0
24	CLA	c	508	65/65	0.93	0.12	-0.47	30,41,65,70	0
26	BCR	C	516	40/40	0.94	0.09	-0.56	25,34,43,46	0
24	CLA	c	511	65/65	0.96	0.10	-0.57	29,36,49,55	0
24	CLA	C	503	65/65	0.94	0.12	-0.59	22,28,40,51	0
22	CL	a	405	1/1	0.99	0.12	-0.92	26,26,26,26	0
38	HEM	V	203	43/43	0.97	0.08	-1.09	23,26,31,36	0
31	OEX	A	418	10/10	0.99	0.09	-1.53	16,23,28,32	0
31	OEX	a	415	10/10	0.99	0.11	-1.57	20,24,35,37	0
22	CL	a	404	1/1	1.00	0.10	-2.07	20,20,20,20	0
22	CL	A	403	1/1	0.98	0.07	-2.18	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CL	A	402	1/1	0.99	0.10	-2.49	19,19,19,19	0
33	CA	O	301	1/1	0.97	0.05	-2.99	56,56,56,56	0
33	CA	o	301	1/1	0.94	0.07	-3.37	62,62,62,62	0
33	CA	c	502	1/1	0.96	0.04	-3.41	44,44,44,44	0
39	MG	J	102	1/1	0.97	0.04	-3.51	28,28,28,28	0
29	UNL	M	103	10/-	0.85	0.18	-	34,42,59,64	0
33	CA	b	605	1/1	0.67	0.14	-	95,95,95,95	0
22	CL	V	202	1/1	0.95	0.05	-	63,63,63,63	0
22	CL	u	201	1/1	0.95	0.05	-	63,63,63,63	0
29	UNL	B	632	33/-	0.74	0.24	-	32,70,105,113	0
29	UNL	A	415	28/-	0.62	0.31	-	55,65,84,90	0
29	UNL	b	634	33/-	0.65	0.26	-	42,71,112,116	0
28	GOL	T	103	6/6	0.69	0.31	-	63,76,80,81	0
35	HTG	C	522	19/19	0.91	0.18	-	53,65,89,95	0
35	HTG	B	624	19/19	0.71	0.35	-	38,95,102,121	0
28	GOL	O	302	6/6	0.68	0.18	-	52,61,64,70	0
33	CA	f	103	1/1	0.89	0.12	-	72,72,72,72	0
35	HTG	c	522	19/19	0.86	0.17	-	63,69,80,85	0
35	HTG	b	604	19/19	0.62	0.19	-	50,80,106,112	0
33	CA	B	601	1/1	0.77	0.09	-	79,79,79,79	0
33	CA	F	102	1/1	0.88	0.14	-	72,72,72,72	0
29	UNL	m	101	10/-	0.86	0.25	-	37,51,60,62	0
29	UNL	a	414	30/-	0.63	0.28	-	45,65,86,89	0
28	GOL	B	635	6/6	0.22	0.43	-	82,91,97,98	0

6.5 Other polymers (i)

There are no such residues in this entry.