wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:50 PM GMT

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

This is a 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:

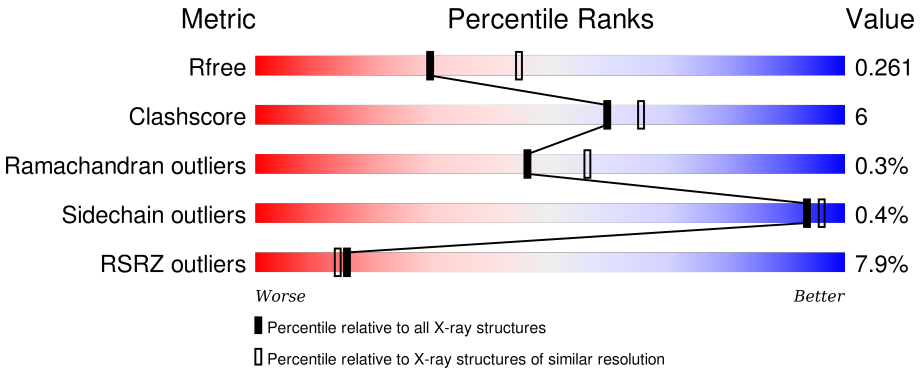
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.44 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	3% 80% 17% ·
1	a	344	2% 97% ·
2	B	510	5% 80% 19% ·
2	b	510	7% 98% ··
3	C	461	3% 77% 20% ·

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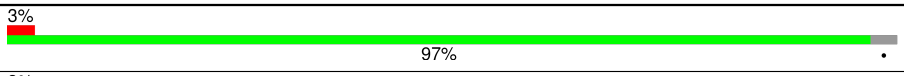
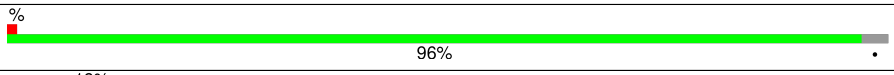
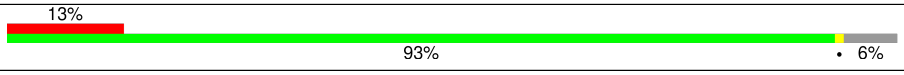
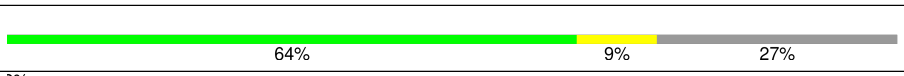
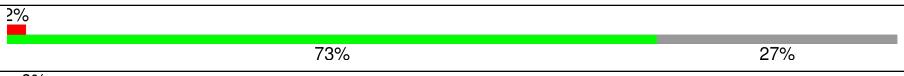
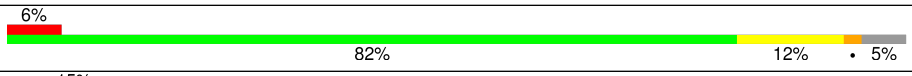
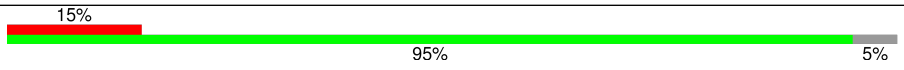
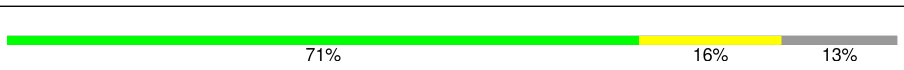
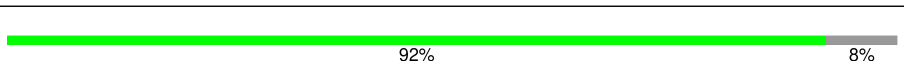
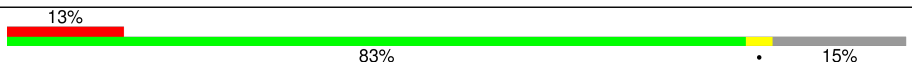
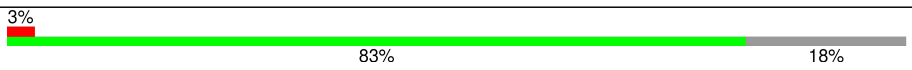
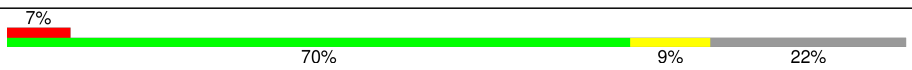
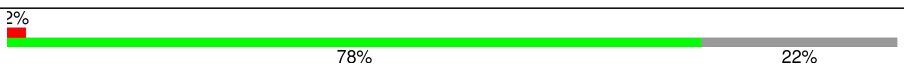
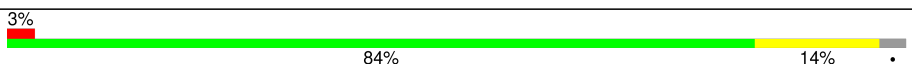
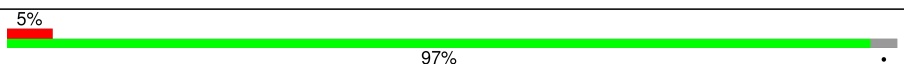
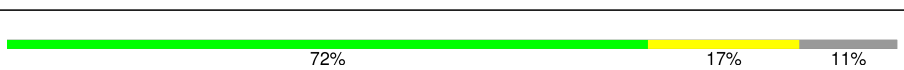
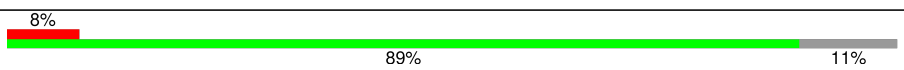
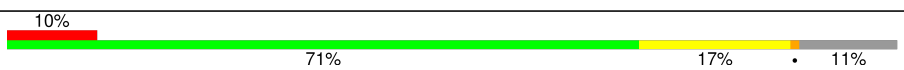
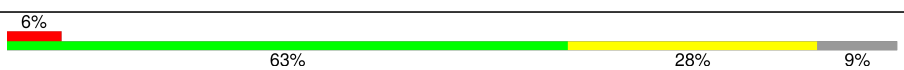
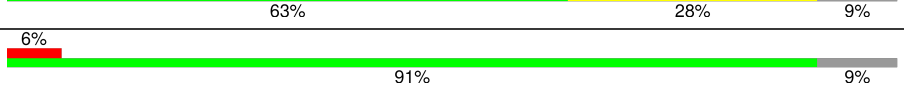
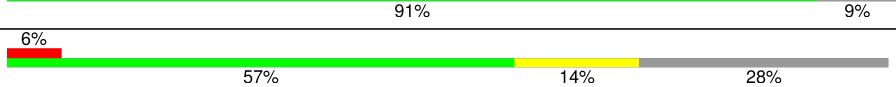
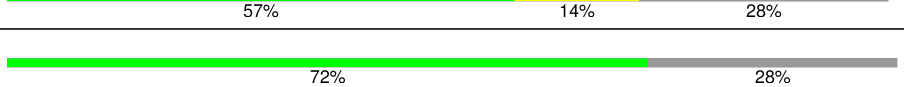
Mol	Chain	Length	Quality of chain
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	

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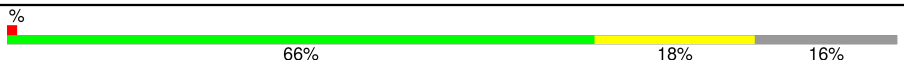
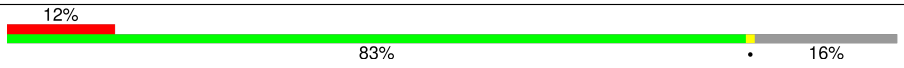
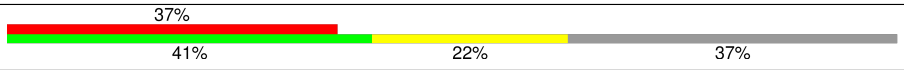
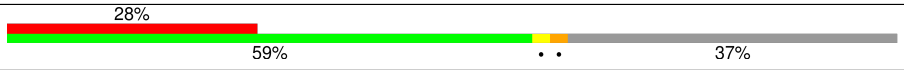
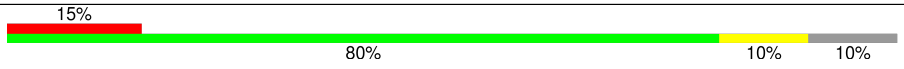
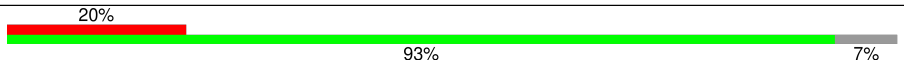
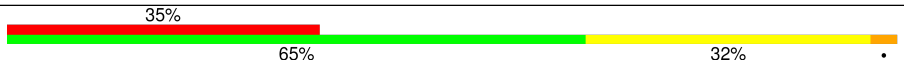
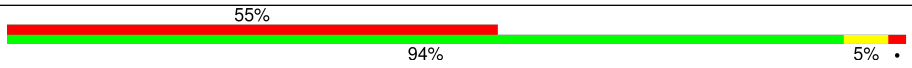
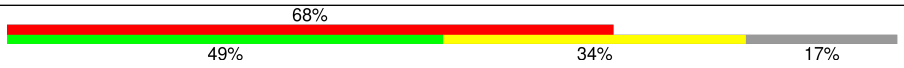
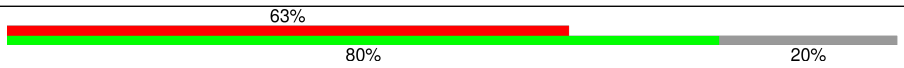
Mol	Chain	Length	Quality of chain
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	LMG	A	603	-	-	-	X
23	LMG	A	612	-	-	-	X
23	LMG	B	620	-	-	-	X
23	LMG	B	624	-	-	-	X
23	LMG	C	521	-	-	-	X
23	LMG	a	603	-	-	-	X
23	LMG	a	614	-	-	-	X
23	LMG	b	624	-	-	-	X
23	LMG	c	520	-	-	-	X
24	CL	a	604	-	-	-	X
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	608	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
26	BCR	D	406	-	-	-	X
26	BCR	b	617	-	-	-	X
26	BCR	d	404	-	-	-	X
26	BCR	t	102	-	-	-	X
27	PL9	A	610	-	-	-	X
27	PL9	D	407	-	-	-	X
27	PL9	a	612	-	-	-	X
27	PL9	d	405	-	-	-	X
28	SQD	L	101	-	-	-	X
28	SQD	L	103	-	-	-	X
29	LHG	a	616	-	-	-	X
29	LHG	d	407	-	-	-	X
30	SO4	V	202	-	-	-	X
32	UNL	B	621	-	-	-	X
32	UNL	B	622	-	-	-	X
32	UNL	B	623	-	-	-	X
32	UNL	D	410	-	-	-	X
32	UNL	J	101	-	-	-	X
32	UNL	T	102	-	-	-	X
32	UNL	T	103	-	-	-	X
32	UNL	X	101	-	-	-	X
32	UNL	b	621	-	-	-	X
32	UNL	b	622	-	-	-	X
32	UNL	d	409	-	-	-	X

2 Entry composition (i)

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

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

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

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

- Molecule 2 is a protein called CP47 protein.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total 269	C 184	N 44	O 40	S 1	0	0	0
6	f	33	Total 269	C 184	N 44	O 40	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	63	Total 498	C 333	N 80	O 83	S 2	0	0	0
7	h	63	Total 498	C 333	N 80	O 83	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	33	Total 266	C 183	N 39	O 43	S 1	0	0	0
8	i	35	Total 286	C 195	N 45	O 45	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	34	Total 249	C 170	N 38	O 40	S 1	0	0	0
9	j	33	Total 238	C 164	N 34	O 39	S 1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

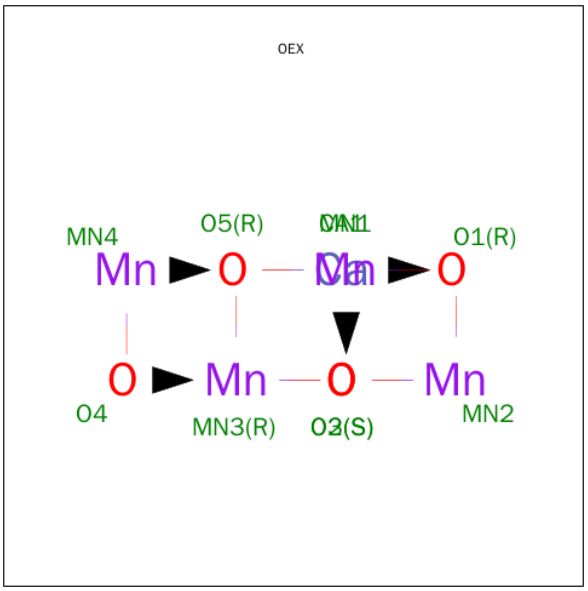
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

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

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

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

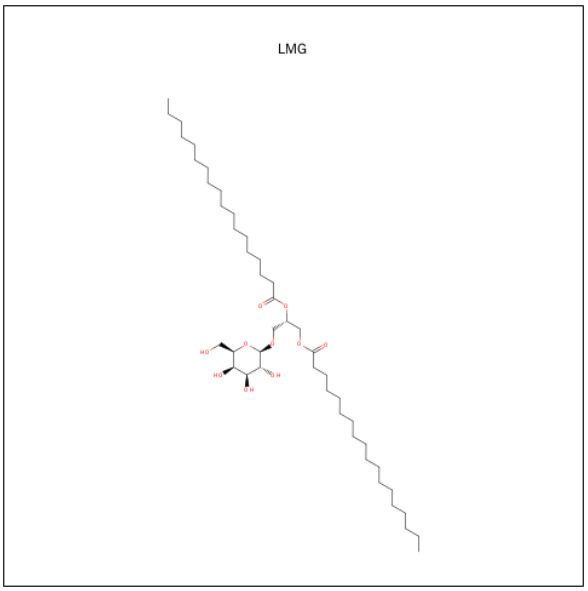


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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

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

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

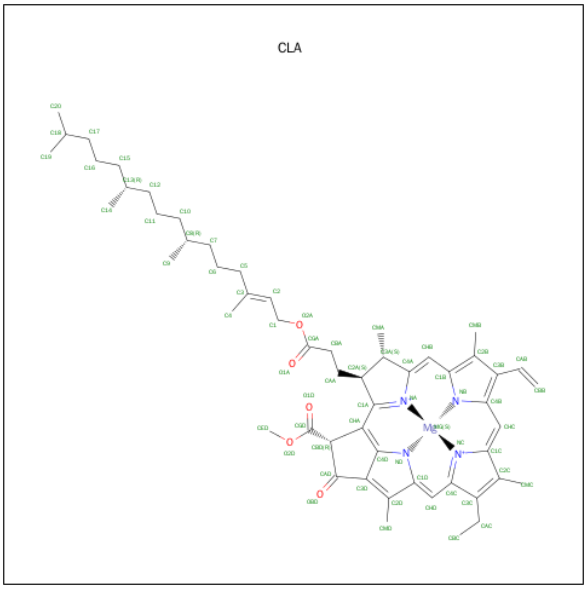


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 51 41 10	0	0
23	A	1	Total C O 51 41 10	0	0
23	B	1	Total C O 51 41 10	0	0
23	B	1	Total C O 51 41 10	0	0
23	C	1	Total C O 51 41 10	0	0
23	C	1	Total C O 51 41 10	0	0
23	D	1	Total C O 51 41 10	0	0
23	a	1	Total C O 51 41 10	0	0
23	a	1	Total C O 51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

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

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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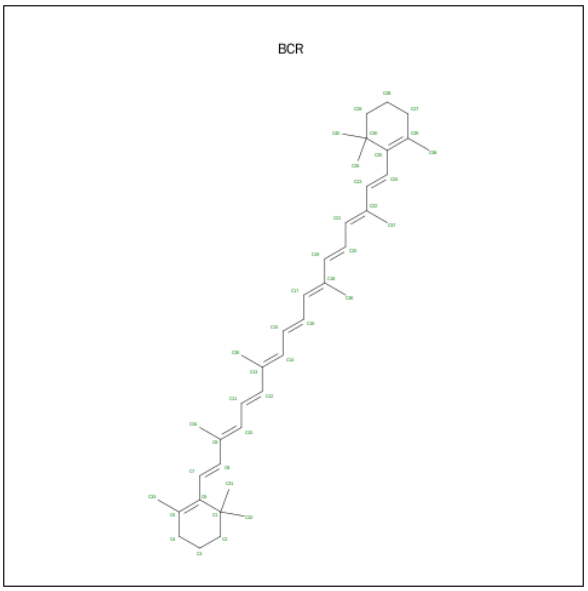
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	c	1	Total C Mg N O 65 55 1 4 5	0	0
25	c	1	Total C Mg N O 65 55 1 4 5	0	0
25	c	1	Total C Mg N O 65 55 1 4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

- 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	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

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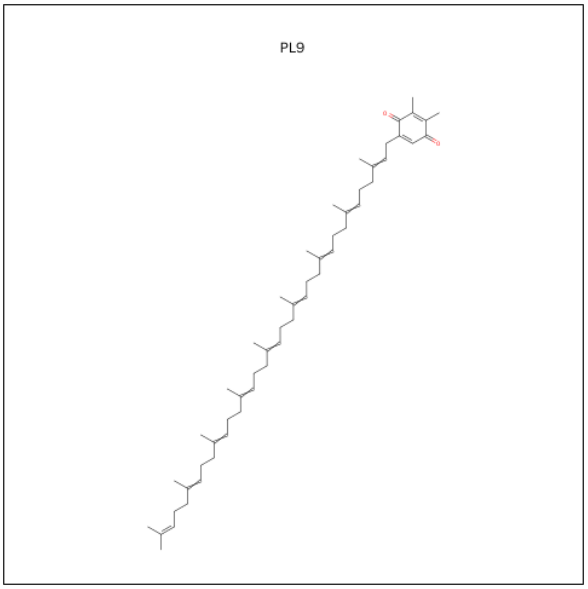
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

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



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

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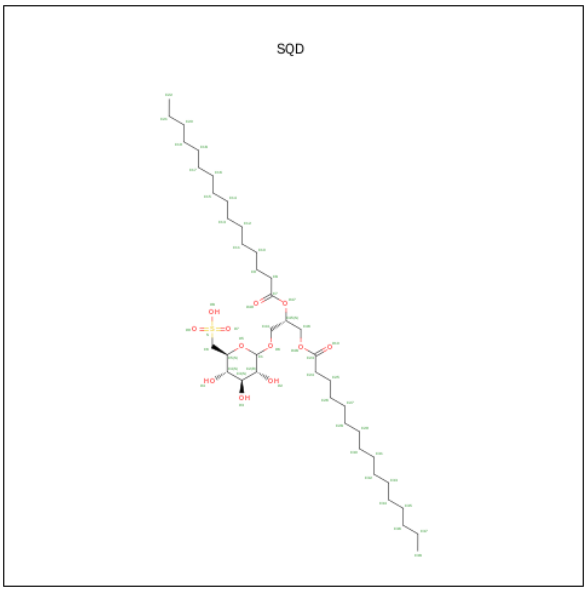
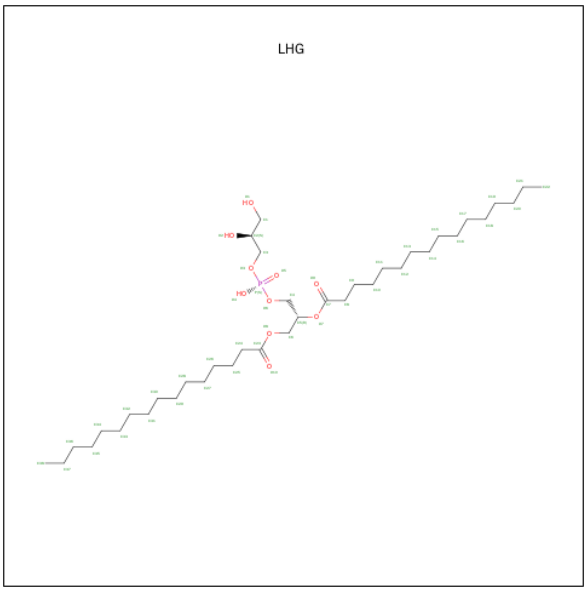
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

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



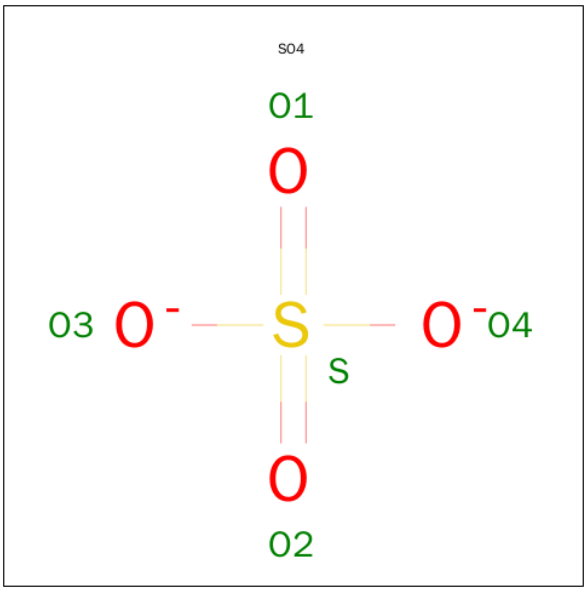
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 54 41 12 1	0	0
28	F	1	Total C O S 43 30 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	f	1	Total C O S 43 30 12 1	0	0

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



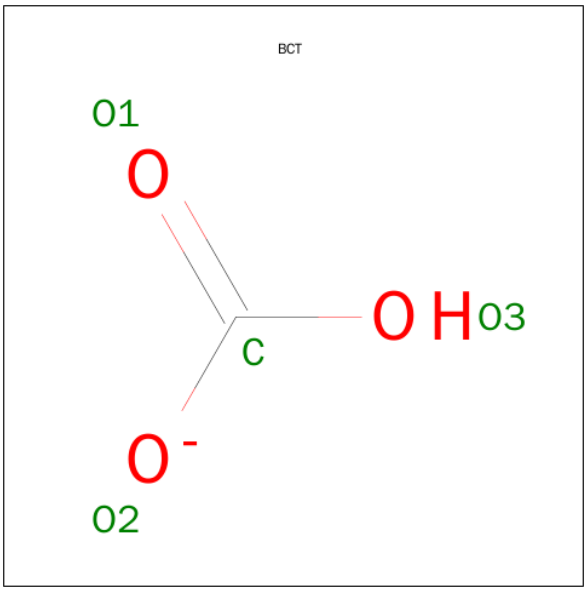
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	A	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	E	1	Total	C	O	P	0	0
			42	31	10	1		
29	L	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0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

- Molecule 30 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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

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

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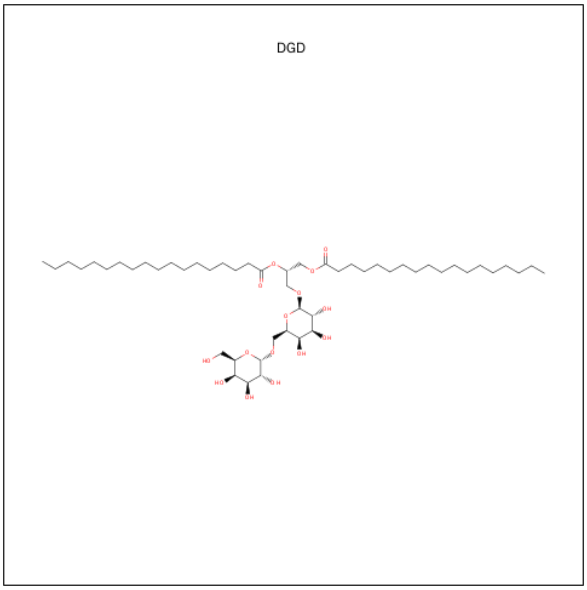
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	T	2	Total C 27 27	0	0
32	X	1	Total C 10 10	0	0
32	d	1	Total C 15 15	0	0
32	t	1	Total C 15 15	0	0
32	m	2	Total C 25 25	0	0
32	b	5	Total C 60 60	0	0
32	M	2	Total C 26 26	0	0

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



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

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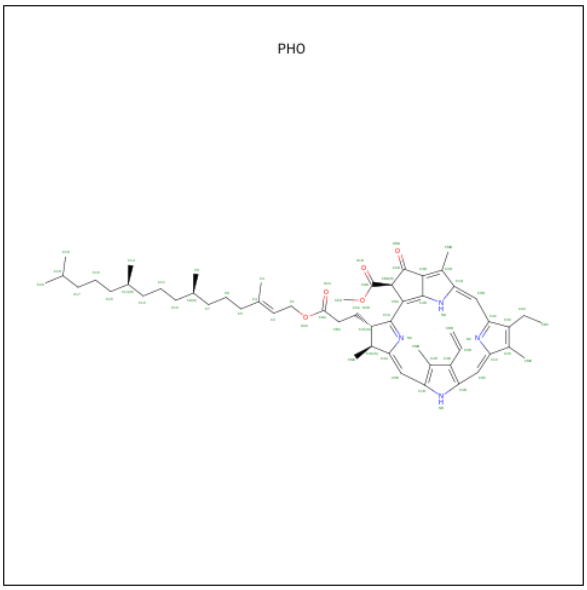
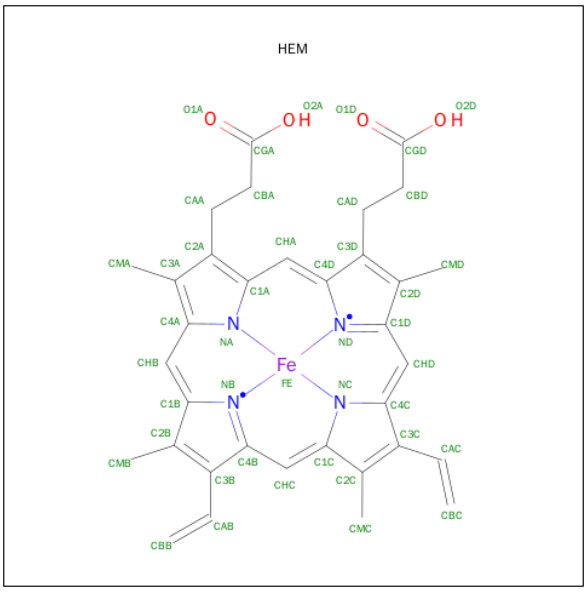
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	h	1	Total C O 62 47 15	0	0

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



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

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



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

- Molecule 36 is water.

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

Continued on next page...

Continued from previous page...

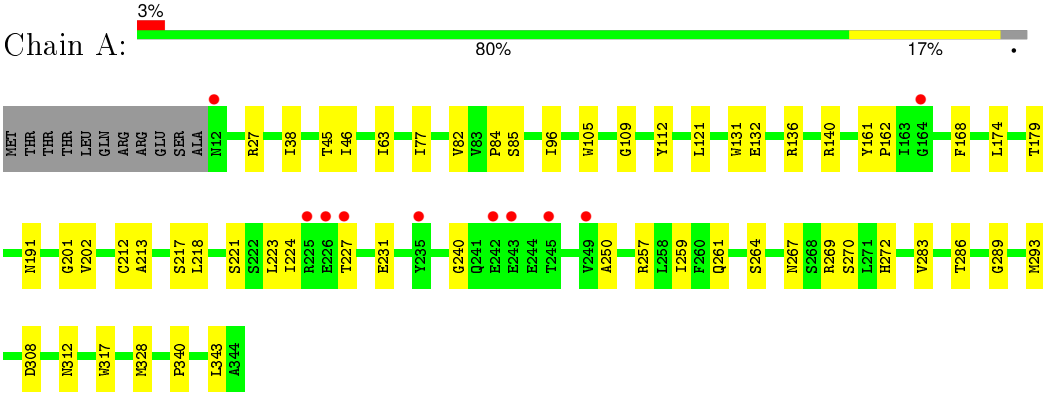
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	T	3	Total O 3 3	0	0
36	U	6	Total O 6 6	0	0
36	V	9	Total O 9 9	0	0
36	X	1	Total O 1 1	0	0
36	a	24	Total O 24 24	0	0
36	b	37	Total O 37 37	0	0
36	c	26	Total O 26 26	0	0
36	d	17	Total O 17 17	0	0
36	h	1	Total O 1 1	0	0
36	i	1	Total O 1 1	0	0
36	j	1	Total O 1 1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

3 Residue-property plots (i)

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

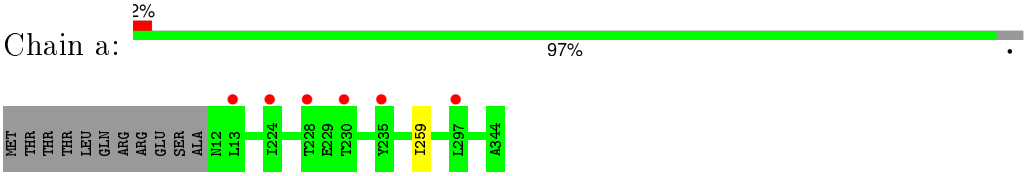
- Molecule 1: Photosystem Q(B) protein 1

Chain A:



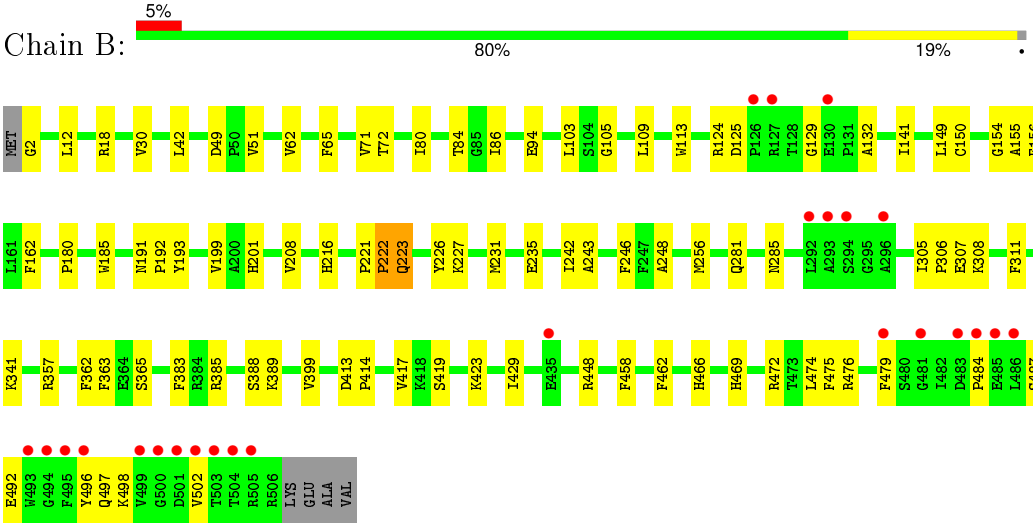
- Molecule 1: Photosystem Q(B) protein 1

Chain a:



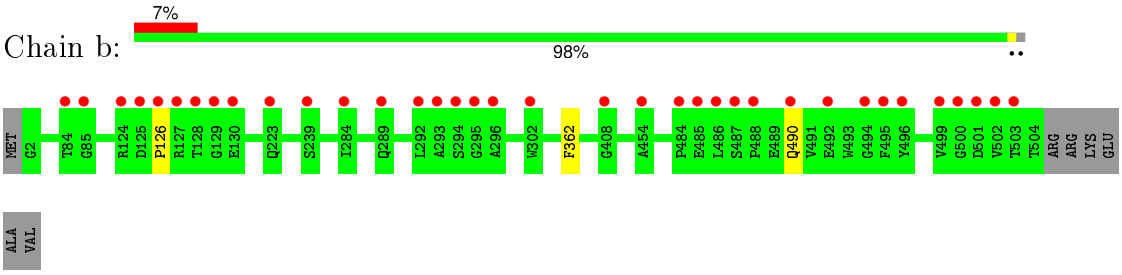
- Molecule 2: CP47 protein

Chain B:



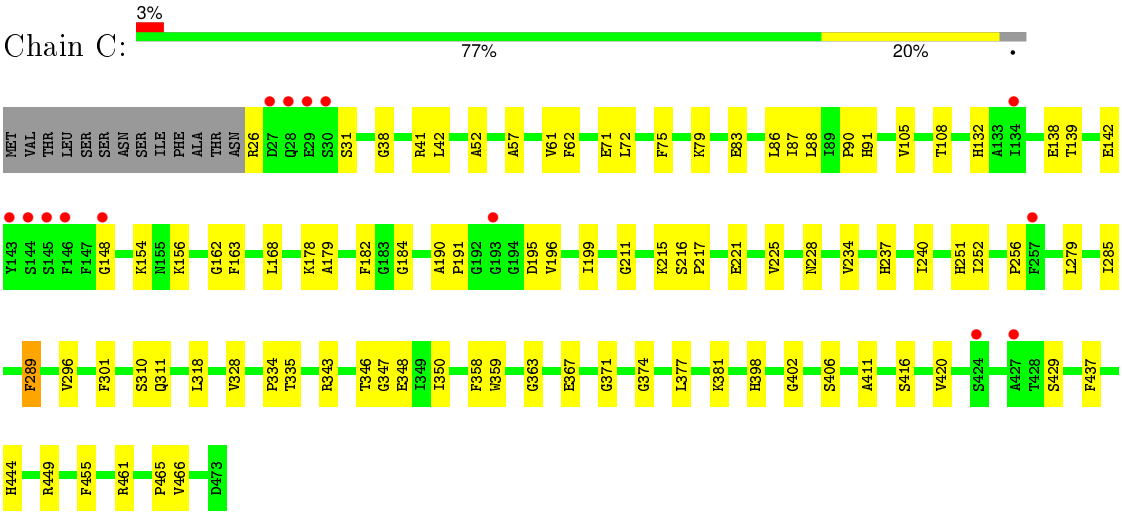
- Molecule 2: CP47 protein

Chain b:



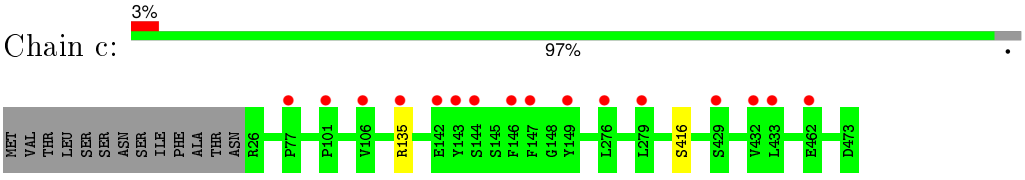
• Molecule 3: Photosystem II CP43 protein

Chain C:



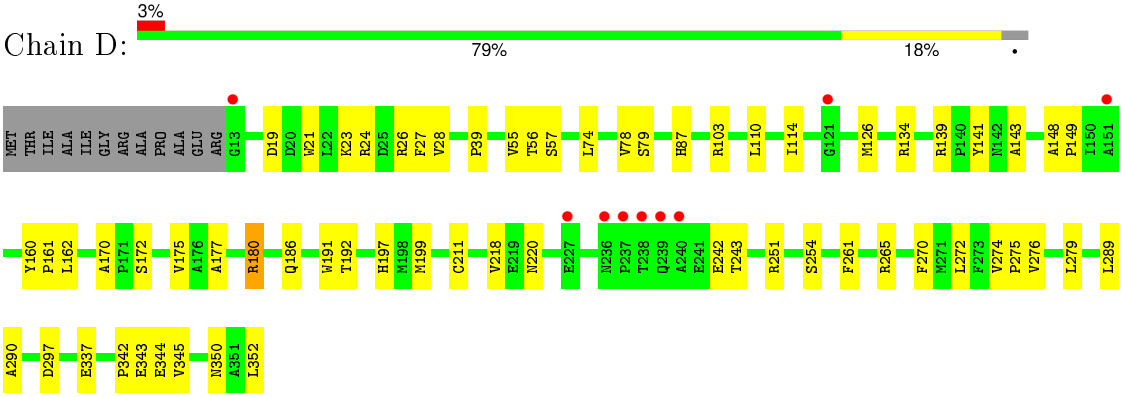
• Molecule 3: Photosystem II CP43 protein

Chain c:



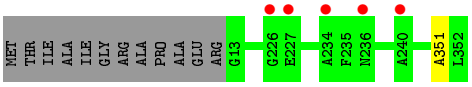
• Molecule 4: Photosystem II D2 protein

Chain D:

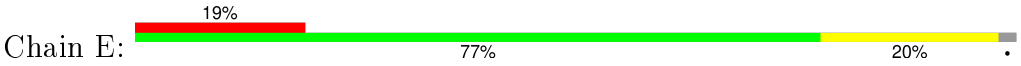


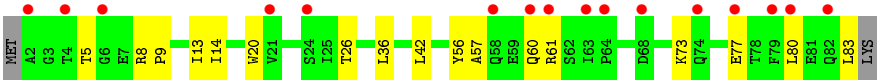
• Molecule 4: Photosystem II D2 protein

Chain d:

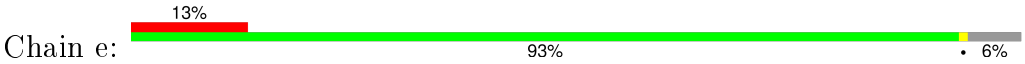


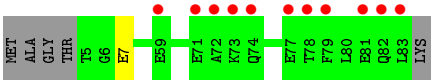
• Molecule 5: Cytochrome b559 subunit alpha





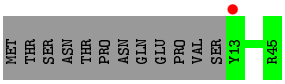
• Molecule 5: Cytochrome b559 subunit alpha



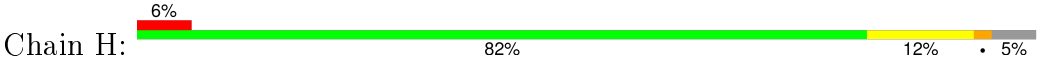


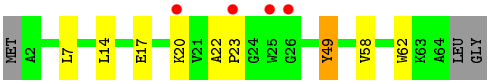
• Molecule 6: Cytochrome b559 subunit beta

• Molecule 6: Cytochrome b559 subunit beta

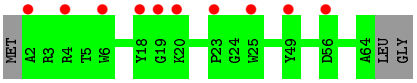


• Molecule 7: Photosystem II reaction center protein H

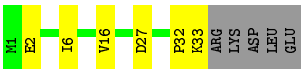




• Molecule 7: Photosystem II reaction center protein H

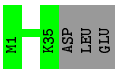


• Molecule 8: Photosystem II reaction center protein I



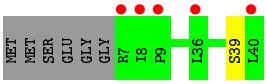
• Molecule 8: Photosystem II reaction center protein I

Chain i:



• Molecule 9: Photosystem II reaction center protein J

Chain J:

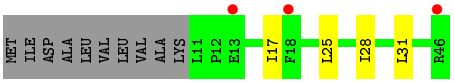


• Molecule 9: Photosystem II reaction center protein J

Chain j:

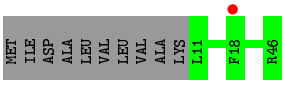
• Molecule 10: Photosystem II reaction center protein K

Chain K:



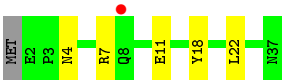
• Molecule 10: Photosystem II reaction center protein K

Chain k:



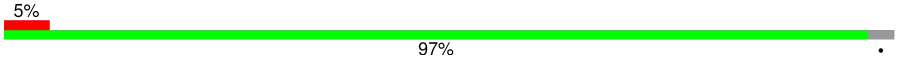
• Molecule 11: Photosystem II reaction center protein L

Chain L:



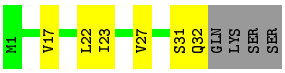
• Molecule 11: Photosystem II reaction center protein L

Chain l:



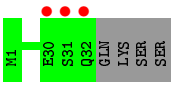
• Molecule 12: Photosystem II reaction center protein M

Chain M:



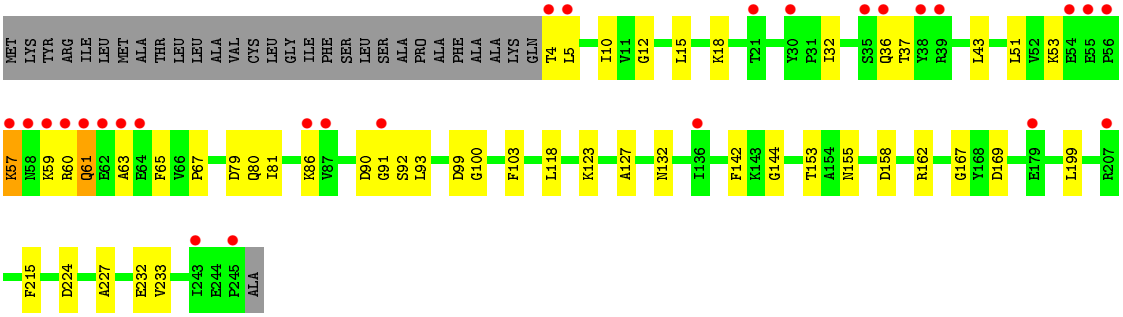
• Molecule 12: Photosystem II reaction center protein M

Chain m:



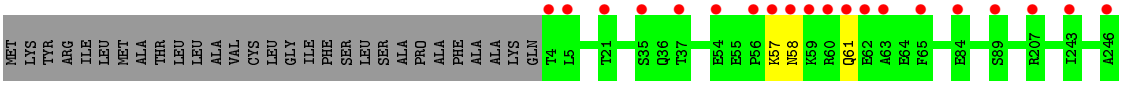
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



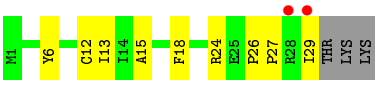
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



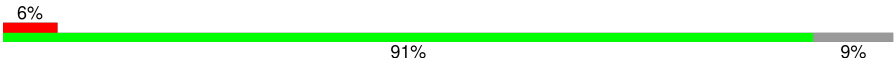
• Molecule 14: Photosystem II reaction center protein T

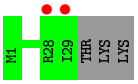
Chain T:



• Molecule 14: Photosystem II reaction center protein T

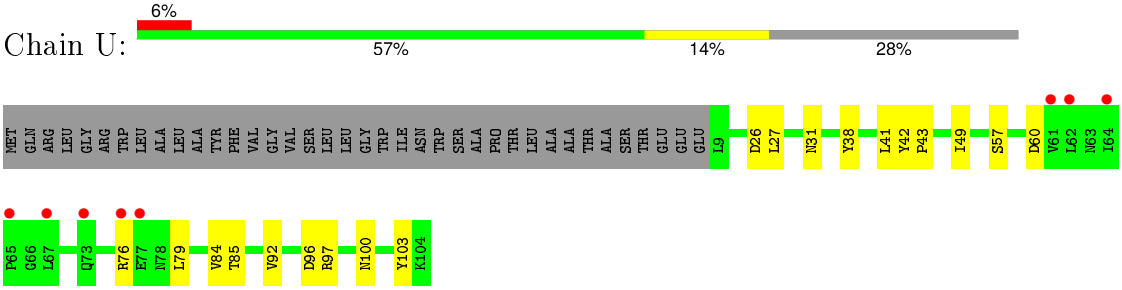
Chain t:





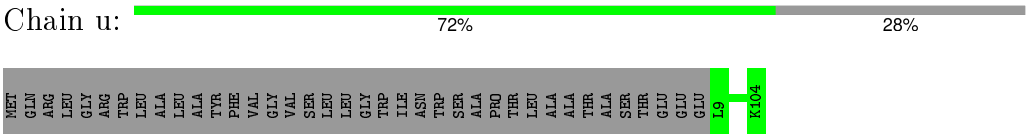
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



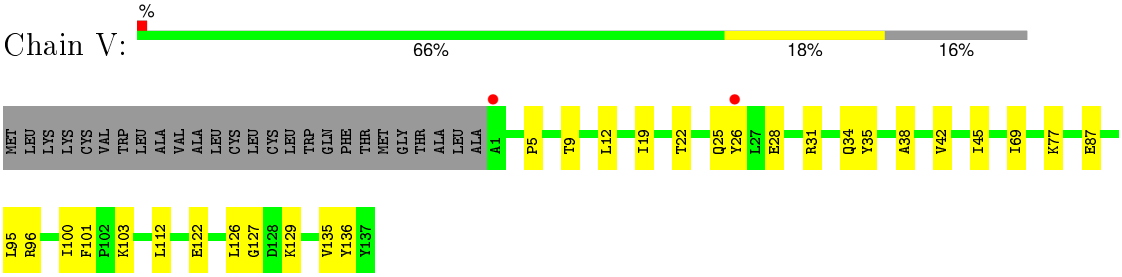
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



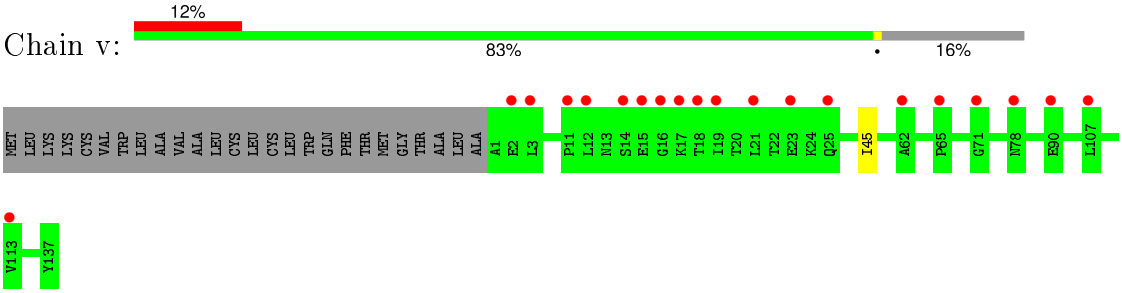
• Molecule 16: Cytochrome c-550

Chain V:



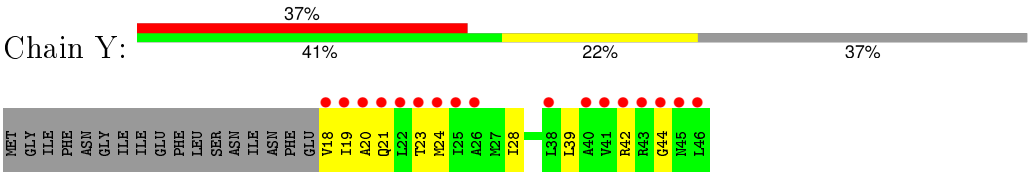
• Molecule 16: Cytochrome c-550

Chain v:



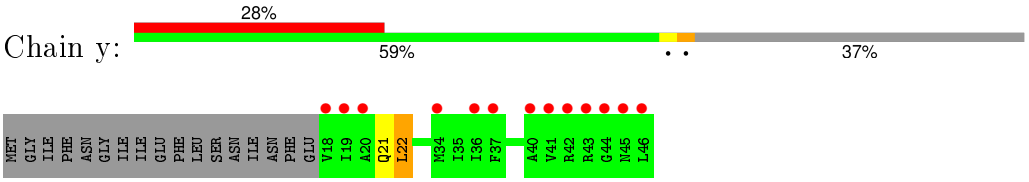
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



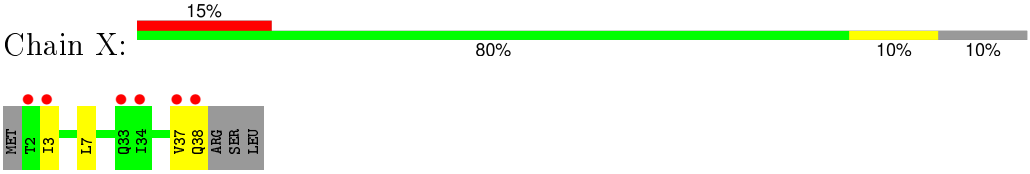
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



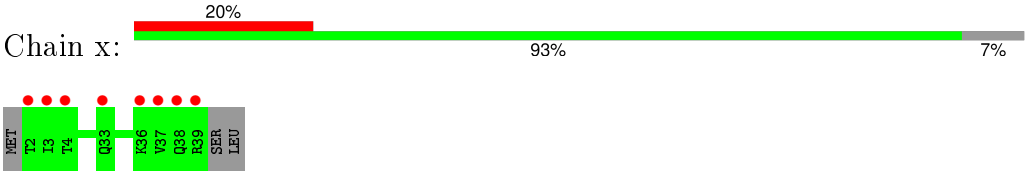
- Molecule 18: Photosystem II reaction center X protein

Chain X:



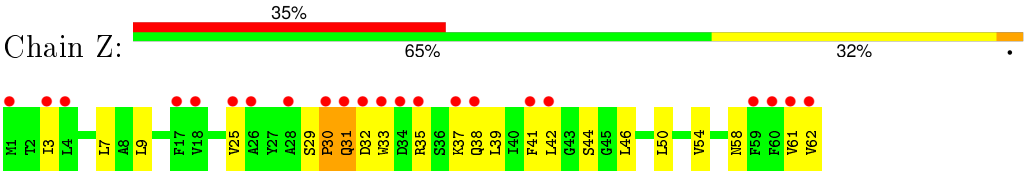
- Molecule 18: Photosystem II reaction center X protein

Chain x:



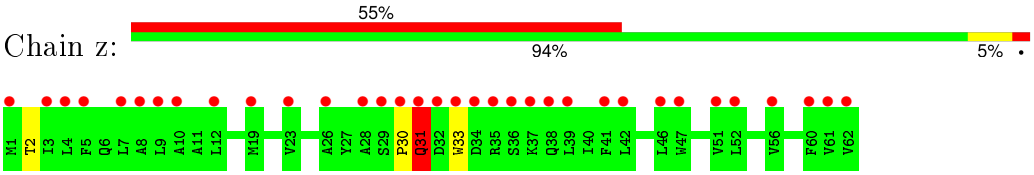
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:



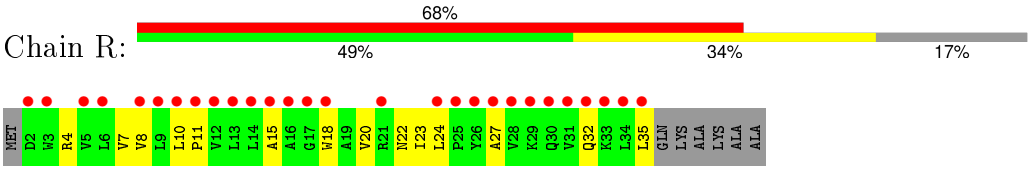
- Molecule 19: Photosystem II reaction center protein Z

Chain z:



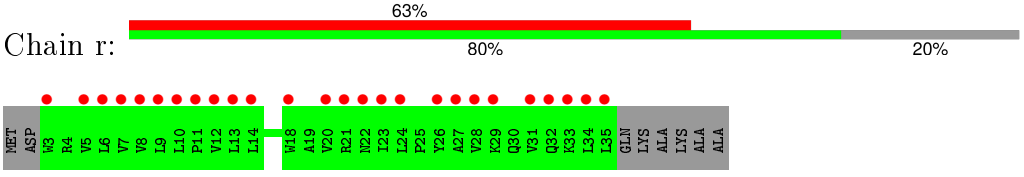
- Molecule 20: Photosystem II protein Y

Chain R:



- 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	116.45Å 218.89Å 302.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.44 49.12 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.12-2.44) 98.4 (49.12-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.216 , 0.256 0.223 , 0.261	Depositor DCC
R_{free} test set	14111 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	39.0	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 282213 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	50236	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

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

[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 (i)

5.1 Standard geometry (i)

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

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

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

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

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 498 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:18:VAL:HG23	17:Y:19:ILE:HD12	4.34	0.83
25:B:604:CLA:H93	25:B:605:CLA:HAB	1.66	0.77
3:C:79:LYS:HG3	16:V:103:LYS:HD3	4.60	0.75
25:C:503:CLA:H172	25:C:510:CLA:HBB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:607:CLA:HAB	25:D:404:CLA:H72	1.69	0.73

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	46	56
1	a	331/344 (96%)	324 (98%)	6 (2%)	1 (0%)	46	56
2	B	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
2	b	501/510 (98%)	482 (96%)	18 (4%)	1 (0%)	52	64
3	C	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	52	64
3	c	446/461 (97%)	435 (98%)	9 (2%)	2 (0%)	39	49
4	D	338/352 (96%)	326 (96%)	12 (4%)	0	100	100
4	d	338/352 (96%)	323 (96%)	14 (4%)	1 (0%)	46	56
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	31 (100%)	0	0	100	100
7	H	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	31/38 (82%)	31 (100%)	0	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/40 (80%)	32 (100%)	0	0	100	100
9	j	31/40 (78%)	31 (100%)	0	0	100	100
10	K	34/46 (74%)	31 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	34/46 (74%)	34 (100%)	0	0	100	100
11	L	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
11	l	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
12	M	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	228 (95%)	11 (5%)	1 (0%)	39	49
13	o	241/272 (89%)	225 (93%)	13 (5%)	3 (1%)	16	17
14	T	27/32 (84%)	27 (100%)	0	0	100	100
14	t	27/32 (84%)	26 (96%)	1 (4%)	0	100	100
15	U	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
15	u	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
16	v	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	26	32
17	Y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
17	y	27/46 (59%)	24 (89%)	2 (7%)	1 (4%)	4	1
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	10
19	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	5	2
20	R	32/41 (78%)	32 (100%)	0	0	100	100
20	r	31/41 (76%)	29 (94%)	2 (6%)	0	100	100
All	All	5199/5700 (91%)	5010 (96%)	173 (3%)	16 (0%)	46	56

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	30	PRO
13	o	57	LYS
3	c	416	SER
13	o	58	ASN

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	270/280 (96%)	269 (100%)	1 (0%)	93 96
1	a	270/280 (96%)	270 (100%)	0	100 100
2	B	403/407 (99%)	401 (100%)	2 (0%)	92 95
2	b	401/407 (98%)	399 (100%)	2 (0%)	92 95
3	C	350/362 (97%)	349 (100%)	1 (0%)	94 97
3	c	350/362 (97%)	350 (100%)	0	100 100
4	D	275/283 (97%)	274 (100%)	1 (0%)	93 96
4	d	275/283 (97%)	275 (100%)	0	100 100
5	E	71/73 (97%)	70 (99%)	1 (1%)	74 84
5	e	70/73 (96%)	69 (99%)	1 (1%)	74 84
6	F	27/39 (69%)	27 (100%)	0	100 100
6	f	27/39 (69%)	27 (100%)	0	100 100
7	H	53/55 (96%)	52 (98%)	1 (2%)	65 78
7	h	53/55 (96%)	53 (100%)	0	100 100
8	I	30/35 (86%)	30 (100%)	0	100 100
8	i	32/35 (91%)	32 (100%)	0	100 100
9	J	24/28 (86%)	24 (100%)	0	100 100
9	j	23/28 (82%)	23 (100%)	0	100 100
10	K	29/37 (78%)	29 (100%)	0	100 100
10	k	29/37 (78%)	29 (100%)	0	100 100
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	34/35 (97%)	34 (100%)	0	100 100
12	M	29/33 (88%)	29 (100%)	0	100 100
12	m	29/33 (88%)	29 (100%)	0	100 100
13	O	206/228 (90%)	205 (100%)	1 (0%)	92 95
13	o	206/228 (90%)	206 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	T	26/29 (90%)	26 (100%)	0	100 100
14	t	26/29 (90%)	26 (100%)	0	100 100
15	U	83/112 (74%)	83 (100%)	0	100 100
15	u	83/112 (74%)	83 (100%)	0	100 100
16	V	117/138 (85%)	117 (100%)	0	100 100
16	v	117/138 (85%)	117 (100%)	0	100 100
17	Y	22/37 (60%)	21 (96%)	1 (4%)	34 47
17	y	22/37 (60%)	21 (96%)	1 (4%)	34 47
18	X	30/34 (88%)	30 (100%)	0	100 100
18	x	31/34 (91%)	31 (100%)	0	100 100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65 78
19	z	52/52 (100%)	49 (94%)	3 (6%)	25 34
20	R	29/33 (88%)	29 (100%)	0	100 100
20	r	28/33 (85%)	28 (100%)	0	100 100
All	All	4318/4660 (93%)	4301 (100%)	17 (0%)	93 96

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	61	GLN
17	Y	23	THR
17	y	22	LEU
7	H	49	TYR
19	z	2	THR

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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 191 ligands modelled in this entry, 29 are unknown and 6 are monoatomic - leaving 156 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	OEX	A	601	1,3,36	0,15,15	0.00	-	0,32,32	0.00	-
23	LMG	A	603	-	51,51,55	0.90	2 (3%)	59,59,63	1.02	3 (5%)
25	CLA	A	606	-	55,73,73	1.09	2 (3%)	61,113,113	0.96	7 (11%)
25	CLA	A	607	-	55,73,73	1.14	3 (5%)	61,113,113	0.89	5 (8%)
25	CLA	A	608	-	55,73,73	1.15	3 (5%)	61,113,113	0.92	5 (8%)
26	BCR	A	609	-	41,41,41	0.65	0	56,56,56	1.87	11 (19%)
27	PL9	A	610	-	55,55,55	0.62	1 (1%)	68,69,69	1.87	20 (29%)
28	SQD	A	611	-	53,54,54	1.63	4 (7%)	61,65,65	1.33	6 (9%)
23	LMG	A	612	-	51,51,55	0.90	2 (3%)	59,59,63	1.02	3 (5%)
29	LHG	A	613	-	48,48,48	0.89	2 (4%)	49,54,54	1.01	3 (6%)
29	LHG	A	614	-	48,48,48	0.91	2 (4%)	49,54,54	1.03	2 (4%)
30	SO4	A	615	-	4,4,4	0.22	0	6,6,6	0.09	0
31	BCT	A	616	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	B	601	-	55,73,73	1.13	3 (5%)	61,113,113	0.92	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	602	-	55,73,73	1.14	3 (5%)	61,113,113	0.91	6 (9%)
25	CLA	B	603	-	55,73,73	1.08	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	B	604	-	55,73,73	1.14	3 (5%)	61,113,113	1.00	5 (8%)
25	CLA	B	605	-	55,73,73	1.12	3 (5%)	61,113,113	0.97	5 (8%)
25	CLA	B	606	-	55,73,73	1.13	3 (5%)	61,113,113	0.94	5 (8%)
25	CLA	B	607	36	55,73,73	1.12	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	B	608	-	55,73,73	1.12	3 (5%)	61,113,113	0.90	4 (6%)
25	CLA	B	609	-	55,73,73	1.17	3 (5%)	61,113,113	0.94	5 (8%)
25	CLA	B	610	-	55,73,73	1.14	3 (5%)	61,113,113	0.92	5 (8%)
25	CLA	B	611	-	55,73,73	1.14	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	B	612	-	55,73,73	1.12	2 (3%)	61,113,113	0.93	5 (8%)
25	CLA	B	613	-	55,73,73	1.11	3 (5%)	61,113,113	0.97	5 (8%)
25	CLA	B	614	-	55,73,73	1.11	3 (5%)	61,113,113	0.92	5 (8%)
25	CLA	B	615	-	55,73,73	1.15	3 (5%)	61,113,113	0.96	5 (8%)
25	CLA	B	616	-	55,73,73	1.12	3 (5%)	61,113,113	0.97	5 (8%)
26	BCR	B	617	-	41,41,41	0.66	0	56,56,56	2.00	17 (30%)
26	BCR	B	618	-	41,41,41	0.65	0	56,56,56	1.88	11 (19%)
26	BCR	B	619	-	41,41,41	0.70	0	56,56,56	1.95	14 (25%)
23	LMG	B	620	-	51,51,55	0.91	2 (3%)	59,59,63	0.98	3 (5%)
23	LMG	B	624	-	51,51,55	0.90	2 (3%)	59,59,63	0.99	3 (5%)
25	CLA	C	501	-	55,73,73	1.12	3 (5%)	61,113,113	0.97	5 (8%)
25	CLA	C	502	-	55,73,73	1.15	3 (5%)	61,113,113	0.92	5 (8%)
25	CLA	C	503	-	55,73,73	1.14	3 (5%)	61,113,113	0.97	5 (8%)
25	CLA	C	504	-	55,73,73	1.12	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	C	505	-	55,73,73	1.10	3 (5%)	61,113,113	0.89	4 (6%)
25	CLA	C	506	-	55,73,73	1.11	3 (5%)	61,113,113	0.94	5 (8%)
25	CLA	C	507	-	55,73,73	1.11	3 (5%)	61,113,113	0.96	5 (8%)
25	CLA	C	508	-	55,73,73	1.12	3 (5%)	61,113,113	0.94	5 (8%)
25	CLA	C	509	-	55,73,73	1.13	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	C	510	-	55,73,73	1.13	3 (5%)	61,113,113	0.94	5 (8%)
25	CLA	C	511	3	55,73,73	1.12	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	C	512	-	55,73,73	1.12	3 (5%)	61,113,113	0.97	5 (8%)
25	CLA	C	513	-	55,73,73	1.12	3 (5%)	61,113,113	0.93	5 (8%)
26	BCR	C	514	-	41,41,41	0.67	0	56,56,56	1.93	11 (19%)
26	BCR	C	515	-	41,41,41	0.68	0	56,56,56	1.85	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	DGD	C	516	-	63,63,67	0.84	2 (3%)	77,77,81	0.95	4 (5%)
33	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	0.98	4 (5%)
33	DGD	C	518	-	63,63,67	0.84	2 (3%)	77,77,81	0.90	3 (3%)
23	LMG	C	519	-	51,51,55	0.91	2 (3%)	59,59,63	0.98	3 (5%)
23	LMG	C	521	-	51,51,55	0.93	3 (5%)	59,59,63	1.16	4 (6%)
26	BCR	C	522	-	41,41,41	0.63	0	56,56,56	2.08	15 (26%)
34	PHO	D	401	-	67,69,69	0.64	1 (1%)	84,99,99	0.88	3 (3%)
34	PHO	D	402	-	67,69,69	0.63	1 (1%)	84,99,99	0.90	3 (3%)
25	CLA	D	403	36	55,73,73	1.12	3 (5%)	61,113,113	0.92	5 (8%)
25	CLA	D	404	-	55,73,73	1.10	3 (5%)	61,113,113	0.88	4 (6%)
25	CLA	D	405	-	55,73,73	1.13	3 (5%)	61,113,113	0.93	6 (9%)
26	BCR	D	406	-	41,41,41	0.65	0	56,56,56	2.26	15 (26%)
27	PL9	D	407	-	55,55,55	0.61	1 (1%)	68,69,69	1.82	20 (29%)
29	LHG	D	408	-	48,48,48	0.89	2 (4%)	49,54,54	1.04	3 (6%)
23	LMG	D	409	-	51,51,55	0.92	2 (3%)	59,59,63	1.00	3 (5%)
29	LHG	E	101	-	41,41,48	0.98	2 (4%)	42,47,54	1.11	3 (7%)
35	HEM	E	102	5,6	30,50,50	2.51	7 (23%)	24,82,82	2.45	11 (45%)
28	SQD	F	101	-	42,43,54	1.83	4 (9%)	50,54,65	1.40	7 (14%)
26	BCR	H	101	-	41,41,41	0.63	0	56,56,56	2.06	14 (25%)
33	DGD	H	102	-	63,63,67	0.86	2 (3%)	77,77,81	0.90	3 (3%)
26	BCR	K	101	-	41,41,41	0.69	0	56,56,56	1.82	15 (26%)
28	SQD	L	101	-	53,54,54	1.60	4 (7%)	61,65,65	4.26	7 (11%)
29	LHG	L	102	-	48,48,48	0.90	2 (4%)	49,54,54	1.11	3 (6%)
28	SQD	L	103	-	53,54,54	1.68	4 (7%)	61,65,65	1.14	4 (6%)
30	SO4	O	301	-	4,4,4	0.23	0	6,6,6	0.10	0
30	SO4	O	302	-	4,4,4	0.24	0	6,6,6	0.07	0
26	BCR	T	101	-	41,41,41	0.65	0	56,56,56	2.06	11 (19%)
30	SO4	U	201	-	4,4,4	0.22	0	6,6,6	0.09	0
35	HEM	V	201	16	30,50,50	2.79	10 (33%)	24,82,82	3.27	11 (45%)
30	SO4	V	202	-	4,4,4	0.24	0	6,6,6	0.09	0
21	OEX	a	601	1,3,36	0,15,15	0.00	-	0,32,32	0.00	-
23	LMG	a	603	-	51,51,55	0.91	2 (3%)	59,59,63	1.08	4 (6%)
25	CLA	a	606	-	55,73,73	1.07	2 (3%)	61,113,113	0.97	7 (11%)
25	CLA	a	607	36	55,73,73	1.11	3 (5%)	61,113,113	0.90	5 (8%)
25	CLA	a	608	-	55,73,73	1.15	3 (5%)	61,113,113	0.94	5 (8%)
34	PHO	a	609	-	67,69,69	0.63	2 (2%)	84,99,99	0.88	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	610	-	55,73,73	1.14	3 (5%)	61,113,113	0.91	5 (8%)
26	BCR	a	611	-	41,41,41	0.65	0	56,56,56	1.81	10 (17%)
27	PL9	a	612	-	55,55,55	0.63	1 (1%)	68,69,69	1.79	20 (29%)
28	SQD	a	613	-	53,54,54	1.65	4 (7%)	61,65,65	1.28	7 (11%)
23	LMG	a	614	-	51,51,55	0.88	2 (3%)	59,59,63	1.04	3 (5%)
29	LHG	a	615	-	48,48,48	0.90	2 (4%)	49,54,54	1.03	3 (6%)
29	LHG	a	616	-	41,41,48	0.97	2 (4%)	42,47,54	1.12	3 (7%)
30	SO4	a	617	-	4,4,4	0.22	0	6,6,6	0.08	0
31	BCT	a	618	22	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	b	601	-	55,73,73	1.13	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	b	602	-	55,73,73	1.13	3 (5%)	61,113,113	0.89	6 (9%)
25	CLA	b	603	-	55,73,73	1.12	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	b	604	-	55,73,73	1.13	3 (5%)	61,113,113	1.00	6 (9%)
25	CLA	b	605	-	55,73,73	1.14	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	b	606	-	55,73,73	1.12	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	b	607	36	55,73,73	1.09	2 (3%)	61,113,113	0.95	5 (8%)
25	CLA	b	608	-	55,73,73	1.13	3 (5%)	61,113,113	0.90	5 (8%)
25	CLA	b	609	-	55,73,73	1.15	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	b	610	36	55,73,73	1.15	3 (5%)	61,113,113	0.91	5 (8%)
25	CLA	b	611	-	55,73,73	1.15	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	b	612	-	55,73,73	1.12	2 (3%)	61,113,113	0.96	5 (8%)
25	CLA	b	613	-	55,73,73	1.12	2 (3%)	61,113,113	0.99	6 (9%)
25	CLA	b	614	-	55,73,73	1.13	3 (5%)	61,113,113	0.91	5 (8%)
25	CLA	b	615	-	55,73,73	1.16	3 (5%)	61,113,113	0.94	5 (8%)
25	CLA	b	616	-	55,73,73	1.12	3 (5%)	61,113,113	0.93	5 (8%)
26	BCR	b	617	-	41,41,41	0.64	0	56,56,56	2.07	15 (26%)
26	BCR	b	618	-	41,41,41	0.63	0	56,56,56	1.98	17 (30%)
26	BCR	b	619	-	41,41,41	0.69	0	56,56,56	1.95	13 (23%)
23	LMG	b	620	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	3 (5%)
23	LMG	b	624	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	3 (5%)
25	CLA	c	501	-	55,73,73	1.13	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	c	502	-	55,73,73	1.16	3 (5%)	61,113,113	0.92	5 (8%)
25	CLA	c	503	-	55,73,73	1.17	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	c	504	-	55,73,73	1.12	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	c	505	-	55,73,73	1.10	3 (5%)	61,113,113	0.89	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	c	506	-	55,73,73	1.11	3 (5%)	61,113,113	0.92	5 (8%)
25	CLA	c	507	-	55,73,73	1.14	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	c	508	-	55,73,73	1.12	3 (5%)	61,113,113	0.93	5 (8%)
25	CLA	c	509	-	55,73,73	1.12	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	c	510	-	55,73,73	1.12	3 (5%)	61,113,113	0.97	5 (8%)
25	CLA	c	511	3	55,73,73	1.16	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	c	512	-	55,73,73	1.15	3 (5%)	61,113,113	0.95	5 (8%)
25	CLA	c	513	-	55,73,73	1.15	3 (5%)	61,113,113	0.92	5 (8%)
26	BCR	c	514	-	41,41,41	0.67	0	56,56,56	1.84	12 (21%)
33	DGD	c	515	-	63,63,67	0.84	2 (3%)	77,77,81	0.95	4 (5%)
33	DGD	c	516	-	63,63,67	0.84	2 (3%)	77,77,81	0.96	3 (3%)
33	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	0.90	3 (3%)
23	LMG	c	518	-	51,51,55	0.90	2 (3%)	59,59,63	0.98	3 (5%)
23	LMG	c	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.05	4 (6%)
26	BCR	c	521	-	41,41,41	0.63	0	56,56,56	2.07	14 (25%)
25	CLA	d	401	-	55,73,73	1.09	3 (5%)	61,113,113	0.89	4 (6%)
34	PHO	d	402	-	67,69,69	0.63	0	84,99,99	0.90	3 (3%)
25	CLA	d	403	-	55,73,73	1.14	3 (5%)	61,113,113	0.94	5 (8%)
26	BCR	d	404	-	41,41,41	0.68	0	56,56,56	2.06	12 (21%)
27	PL9	d	405	-	55,55,55	0.61	1 (1%)	68,69,69	1.82	18 (26%)
29	LHG	d	406	-	48,48,48	0.91	2 (4%)	49,54,54	1.04	3 (6%)
29	LHG	d	407	-	48,48,48	0.90	2 (4%)	49,54,54	1.01	2 (4%)
23	LMG	d	408	-	51,51,55	0.91	2 (3%)	59,59,63	0.99	3 (5%)
30	SO4	d	410	-	4,4,4	0.23	0	6,6,6	0.07	0
35	HEM	e	101	5,6	30,50,50	2.53	8 (26%)	24,82,82	2.42	11 (45%)
28	SQD	f	101	-	42,43,54	1.86	4 (9%)	50,54,65	1.40	7 (14%)
26	BCR	h	101	-	41,41,41	0.64	0	56,56,56	1.98	13 (23%)
33	DGD	h	102	-	63,63,67	0.84	2 (3%)	77,77,81	0.91	2 (2%)
26	BCR	k	102	-	41,41,41	0.69	0	56,56,56	1.87	16 (28%)
29	LHG	l	101	-	48,48,48	0.91	2 (4%)	49,54,54	1.09	3 (6%)
30	SO4	o	301	-	4,4,4	0.23	0	6,6,6	0.09	0
26	BCR	t	102	-	41,41,41	0.63	0	56,56,56	2.07	15 (26%)
30	SO4	u	201	-	4,4,4	0.23	0	6,6,6	0.08	0
30	SO4	u	202	-	4,4,4	0.21	0	6,6,6	0.09	0
35	HEM	v	201	16	30,50,50	2.82	10 (33%)	24,82,82	3.33	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	z	101	-	41,41,41	0.67	0	56,56,56	1.86	11 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	OEX	A	601	1,3,36	-	0/0/68/68	0/0/6/6
23	LMG	A	603	-	-	0/46/66/70	0/1/1/1
25	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	608	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	A	609	-	-	0/29/63/63	0/2/2/2
27	PL9	A	610	-	-	0/53/73/73	0/1/1/1
28	SQD	A	611	-	-	0/49/69/69	0/1/1/1
23	LMG	A	612	-	-	0/46/66/70	0/1/1/1
29	LHG	A	613	-	-	0/53/53/53	0/0/0/0
29	LHG	A	614	-	-	0/53/53/53	0/0/0/0
30	SO4	A	615	-	-	0/0/0/0	0/0/0/0
31	BCT	A	616	22	-	0/0/0/0	0/0/0/0
25	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	607	36	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	617	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	LMG	B	620	-	-	0/46/66/70	0/1/1/1
23	LMG	B	624	-	-	0/46/66/70	0/1/1/1
25	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
33	DGD	C	516	-	-	0/51/91/95	0/2/2/2
33	DGD	C	517	-	-	0/51/91/95	0/2/2/2
33	DGD	C	518	-	-	0/51/91/95	0/2/2/2
23	LMG	C	519	-	-	0/46/66/70	0/1/1/1
23	LMG	C	521	-	-	1/46/66/70	0/1/1/1
26	BCR	C	522	-	-	0/29/63/63	0/2/2/2
34	PHO	D	401	-	-	0/53/103/103	0/1/6/6
34	PHO	D	402	-	-	0/53/103/103	0/1/6/6
25	CLA	D	403	36	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
27	PL9	D	407	-	-	0/53/73/73	0/1/1/1
29	LHG	D	408	-	-	0/53/53/53	0/0/0/0
23	LMG	D	409	-	-	0/46/66/70	0/1/1/1
29	LHG	E	101	-	-	0/46/46/53	0/0/0/0
35	HEM	E	102	5,6	-	0/10/54/54	0/0/8/8
28	SQD	F	101	-	-	0/38/58/69	0/1/1/1
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	SQD	L	101	-	-	0/49/69/69	0/1/1/1
29	LHG	L	102	-	-	0/53/53/53	0/0/0/0
28	SQD	L	103	-	-	0/49/69/69	0/1/1/1
30	SO4	O	301	-	-	0/0/0/0	0/0/0/0
30	SO4	O	302	-	-	0/0/0/0	0/0/0/0
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
30	SO4	U	201	-	-	0/0/0/0	0/0/0/0
35	HEM	V	201	16	-	0/10/54/54	0/0/8/8
30	SO4	V	202	-	-	0/0/0/0	0/0/0/0
21	OEX	a	601	1,3,36	-	0/0/68/68	0/0/6/6
23	LMG	a	603	-	-	0/46/66/70	0/1/1/1
25	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	607	36	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	608	-	3/3/20/25	0/37/135/135	0/0/9/9
34	PHO	a	609	-	-	0/53/103/103	0/1/6/6
25	CLA	a	610	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	a	611	-	-	0/29/63/63	0/2/2/2
27	PL9	a	612	-	-	0/53/73/73	0/1/1/1
28	SQD	a	613	-	-	0/49/69/69	0/1/1/1
23	LMG	a	614	-	-	0/46/66/70	0/1/1/1
29	LHG	a	615	-	-	0/53/53/53	0/0/0/0
29	LHG	a	616	-	-	0/46/46/53	0/0/0/0
30	SO4	a	617	-	-	0/0/0/0	0/0/0/0
31	BCT	a	618	22	-	0/0/0/0	0/0/0/0
25	CLA	b	601	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	607	36	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	610	36	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	617	-	-	0/29/63/63	0/2/2/2
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
23	LMG	b	620	-	-	0/46/66/70	0/1/1/1
23	LMG	b	624	-	-	0/46/66/70	0/1/1/1
25	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
33	DGD	c	515	-	-	0/51/91/95	0/2/2/2
33	DGD	c	516	-	-	0/51/91/95	0/2/2/2
33	DGD	c	517	-	-	0/51/91/95	0/2/2/2
23	LMG	c	518	-	-	0/46/66/70	0/1/1/1
23	LMG	c	520	-	-	0/46/66/70	0/1/1/1
26	BCR	c	521	-	-	0/29/63/63	0/2/2/2
25	CLA	d	401	-	3/3/20/25	0/37/135/135	0/0/9/9
34	PHO	d	402	-	-	0/53/103/103	0/1/6/6
25	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	d	404	-	-	0/29/63/63	0/2/2/2
27	PL9	d	405	-	-	0/53/73/73	0/1/1/1
29	LHG	d	406	-	-	0/53/53/53	0/0/0/0
29	LHG	d	407	-	-	0/53/53/53	0/0/0/0
23	LMG	d	408	-	-	0/46/66/70	0/1/1/1
30	SO4	d	410	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HEM	e	101	5,6	-	0/10/54/54	0/0/8/8
28	SQD	f	101	-	-	0/38/58/69	0/1/1/1
26	BCR	h	101	-	-	0/29/63/63	0/2/2/2
33	DGD	h	102	-	-	0/51/91/95	0/2/2/2
26	BCR	k	102	-	-	0/29/63/63	0/2/2/2
29	LHG	l	101	-	-	0/53/53/53	0/0/0/0
30	SO4	o	301	-	-	0/0/0/0	0/0/0/0
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
30	SO4	u	201	-	-	0/0/0/0	0/0/0/0
30	SO4	u	202	-	-	0/0/0/0	0/0/0/0
35	HEM	v	201	16	-	0/10/54/54	0/0/8/8
26	BCR	z	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 336 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	v	201	HEM	C3B-C4B	-8.69	1.44	1.51
35	e	101	HEM	C3B-C4B	-8.65	1.44	1.51
35	V	201	HEM	C3B-C4B	-8.51	1.44	1.51
35	E	102	HEM	C3B-C4B	-8.47	1.44	1.51
28	L	103	SQD	C6-S	-7.88	1.66	1.77

The worst 5 of 919 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L	101	SQD	O9-S-C6	-25.13	85.76	106.94
28	L	101	SQD	O8-S-O9	-12.47	82.59	111.61
28	L	101	SQD	O9-S-O7	-8.65	81.97	113.48
35	V	201	HEM	C3C-CAC-CBC	-8.64	111.20	124.46
35	v	201	HEM	C3C-CAC-CBC	-8.63	111.22	124.46

5 of 210 chirality outliers are listed below:

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

All (1) torsion outliers are listed below:

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

There are no ring outliers.

68 monomers are involved in 220 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	508	CLA	6	0
25	C	509	CLA	4	0
25	C	510	CLA	8	0
25	C	511	CLA	4	0
25	C	512	CLA	6	0
25	C	513	CLA	6	0
26	C	514	BCR	7	0
26	C	515	BCR	2	0
33	C	516	DGD	7	0
33	C	517	DGD	4	0
33	C	518	DGD	1	0
23	C	519	LMG	1	0
23	C	521	LMG	3	0
26	C	522	BCR	2	0
34	D	401	PHO	1	0
34	D	402	PHO	5	0
25	D	403	CLA	4	0
25	D	404	CLA	6	0
25	D	405	CLA	1	0
26	D	406	BCR	2	0
27	D	407	PL9	3	0
29	D	408	LHG	5	0
35	E	102	HEM	3	0
28	F	101	SQD	2	0
26	H	101	BCR	5	0
33	H	102	DGD	3	0
26	K	101	BCR	4	0
28	L	101	SQD	6	0
29	L	102	LHG	4	0
28	L	103	SQD	4	0
26	T	101	BCR	6	0

5.7 Other polymers

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	333/344 (96%)	0.17	10 (3%) 54 52	24, 32, 54, 72	0
1	a	333/344 (96%)	0.05	6 (1%) 71 70	24, 34, 62, 76	0
2	B	505/510 (99%)	0.10	27 (5%) 30 29	24, 35, 61, 84	0
2	b	503/510 (98%)	0.20	36 (7%) 18 16	26, 38, 67, 87	0
3	C	448/461 (97%)	0.15	14 (3%) 52 51	24, 40, 59, 77	0
3	c	448/461 (97%)	0.10	16 (3%) 46 45	29, 42, 60, 80	0
4	D	340/352 (96%)	0.05	9 (2%) 59 59	25, 34, 52, 70	0
4	d	340/352 (96%)	-0.08	5 (1%) 76 77	26, 37, 59, 74	0
5	E	82/84 (97%)	1.11	16 (19%) 1 1	39, 57, 71, 75	0
5	e	79/84 (94%)	0.63	11 (13%) 4 3	43, 58, 71, 81	0
6	F	33/45 (73%)	-0.10	0 100 100	42, 49, 63, 71	0
6	f	33/45 (73%)	-0.04	1 (3%) 54 52	46, 52, 73, 82	0
7	H	63/66 (95%)	0.17	4 (6%) 23 21	34, 41, 48, 60	0
7	h	63/66 (95%)	0.56	10 (15%) 3 1	39, 48, 59, 69	0
8	I	33/38 (86%)	-0.29	0 100 100	30, 36, 44, 55	0
8	i	35/38 (92%)	-0.19	0 100 100	31, 39, 56, 66	0
9	J	34/40 (85%)	0.19	5 (14%) 3 2	40, 53, 64, 78	0
9	j	33/40 (82%)	0.20	1 (3%) 54 52	43, 52, 61, 65	0
10	K	36/46 (78%)	0.49	3 (8%) 14 13	52, 61, 75, 77	0
10	k	36/46 (78%)	0.22	1 (2%) 56 56	48, 60, 76, 78	0
11	L	36/37 (97%)	-0.23	1 (2%) 56 56	26, 33, 53, 59	0
11	l	36/37 (97%)	-0.04	2 (5%) 28 26	28, 35, 50, 62	0
12	M	32/36 (88%)	-0.08	0 100 100	30, 36, 56, 58	0
12	m	32/36 (88%)	0.16	3 (9%) 11 9	30, 38, 57, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	242/272 (88%)	0.54	27 (11%) 7 5	30, 44, 70, 104	0
13	o	243/272 (89%)	0.35	20 (8%) 14 13	28, 45, 72, 108	0
14	T	29/32 (90%)	0.26	2 (6%) 20 18	26, 35, 56, 62	0
14	t	29/32 (90%)	0.22	2 (6%) 20 18	31, 36, 55, 67	0
15	U	96/134 (71%)	0.45	8 (8%) 14 13	34, 43, 64, 72	0
15	u	96/134 (71%)	0.06	0 100 100	35, 45, 58, 65	0
16	V	137/163 (84%)	0.17	2 (1%) 76 77	33, 44, 56, 64	0
16	v	137/163 (84%)	0.79	20 (14%) 3 2	37, 50, 67, 82	0
17	Y	29/46 (63%)	2.72	17 (58%) 0 0	63, 76, 95, 96	0
17	y	29/46 (63%)	1.73	13 (44%) 0 0	61, 71, 90, 91	0
18	X	37/41 (90%)	0.30	6 (16%) 3 1	42, 50, 65, 79	0
18	x	38/41 (92%)	0.66	8 (21%) 1 1	41, 52, 74, 84	0
19	Z	62/62 (100%)	1.88	22 (35%) 0 0	57, 73, 104, 111	0
19	z	62/62 (100%)	2.41	34 (54%) 0 0	62, 74, 100, 107	0
20	R	34/41 (82%)	3.39	28 (82%) 0 0	61, 74, 88, 92	0
20	r	33/41 (80%)	3.16	26 (78%) 0 0	64, 73, 86, 91	0
All	All	5279/5700 (92%)	0.30	416 (7%) 15 14	24, 41, 72, 111	0

The worst 5 of 416 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	56	PRO	9.4
13	O	61	GLN	9.2
13	O	63	ALA	8.8
19	Z	33	TRP	7.6
19	Z	30	PRO	7.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

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

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

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

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

6.5 Other polymers (i)

There are no such residues in this entry.