wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:48 PM GMT

PDB ID	:	4TNJ
Title	:	RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 A resolution
Authors	:	Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on	:	2014-06-04
Resolution	:	4.50 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 (i)) were used in the production of this report:

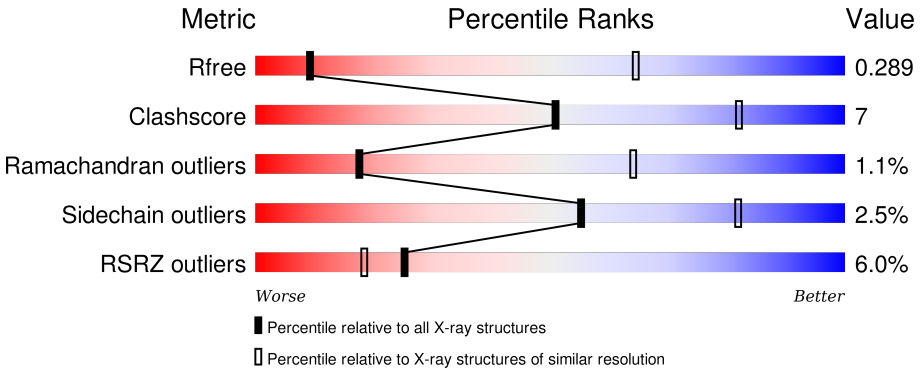
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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 4.50 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	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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	9% 70% 26%
1	a	344	9% 95%
2	B	510	7% 77% 19%
2	b	510	5% 94%

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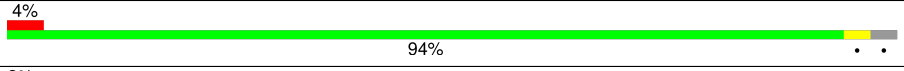
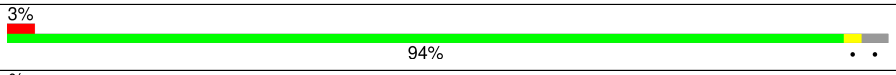
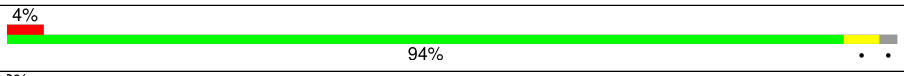
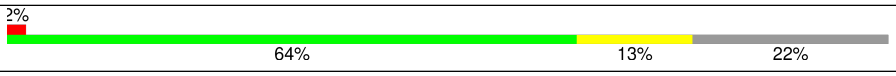
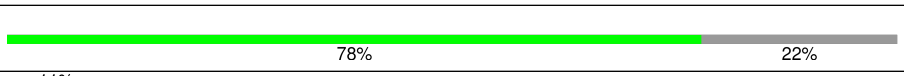
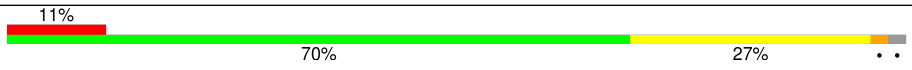
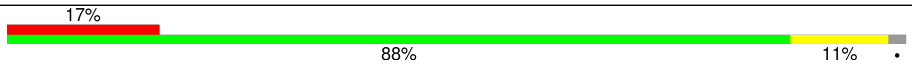
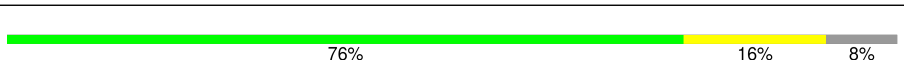
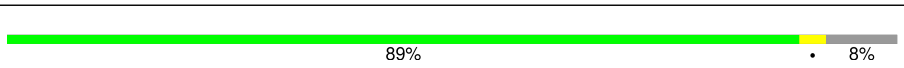
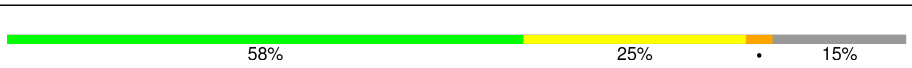
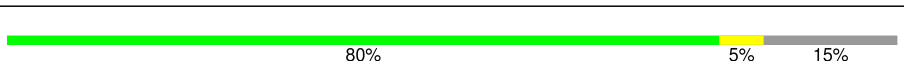
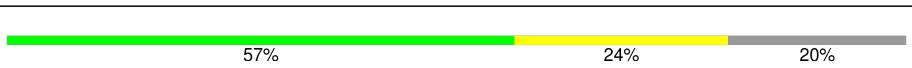
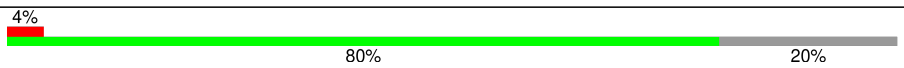
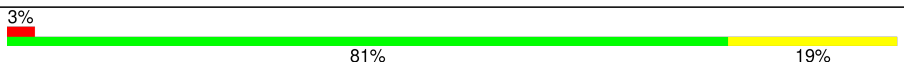
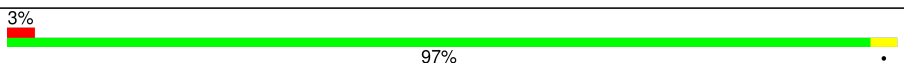
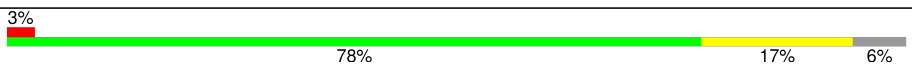
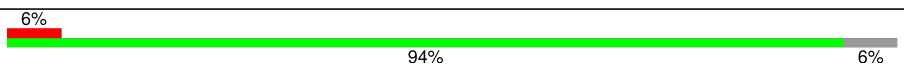
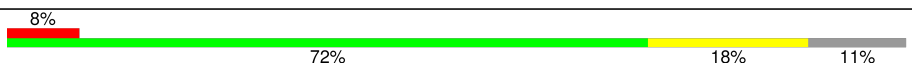
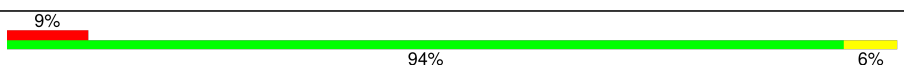
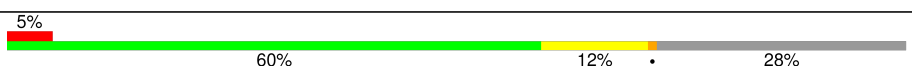
Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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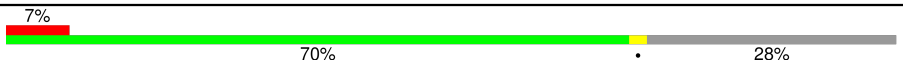
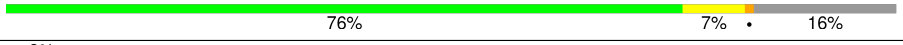
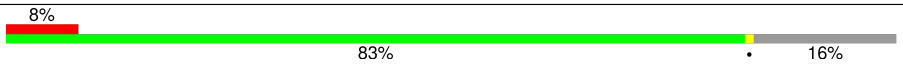
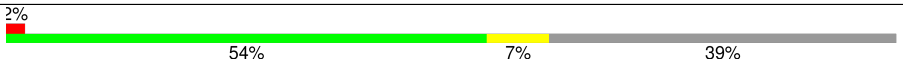
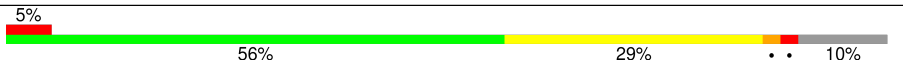
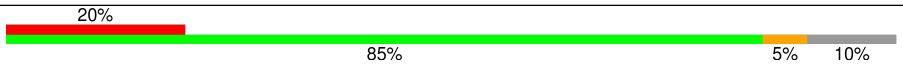
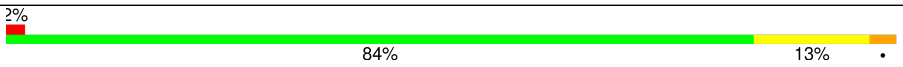
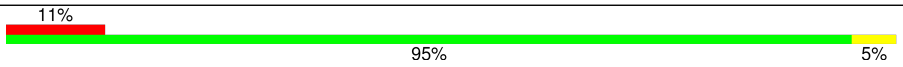
Mol	Chain	Length	Quality of chain
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	X
22	CLA	A	403	X	-	-	X
22	CLA	A	404	X	-	-	X
22	CLA	A	405	X	-	-	X
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	X
22	CLA	B	604	X	-	-	X
22	CLA	B	605	X	-	-	X
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	X
22	CLA	B	608	X	-	-	X
22	CLA	B	609	X	-	-	X
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X
22	CLA	B	614	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	615	X	-	-	X
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	X
22	CLA	C	504	X	-	-	X
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	X
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	520	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	D	406	X	-	-	X
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	X
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	X
22	CLA	b	618	X	-	-	X
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	X
22	CLA	c	506	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	X
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	X
22	CLA	d	405	X	-	-	X
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	j	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	618	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	513	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	521	-	-	-	X
24	BCR	D	411	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	J	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	622	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	513	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	521	-	-	-	X
24	BCR	f	102	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	D	409	-	-	-	X
25	DGD	a	411	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	408	-	-	-	X
26	LHG	C	519	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	a	413	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	m	101	-	-	-	X
28	CL	A	411	-	-	-	X
29	OEX	A	412	-	-	-	X
29	OEX	a	414	-	-	-	X
30	SQD	A	414	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	D	403	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	d	402	-	-	-	X
30	SQD	f	103	-	-	-	X
31	LMT	B	623	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	102	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	M	103	-	-	-	X
31	LMT	b	603	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	409	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	D	401	-	-	-	X
32	PHO	d	401	-	-	-	X
33	BCT	d	403	-	-	-	X
34	HEM	F	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	v	201	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 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	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	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 666	C 434	N 108	O 124	0	0	0
5	e	82	Total 666	C 434	N 108	O 124	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total 282	C 192	N 46	O 43	S 1	0	0	0
6	f	35	Total 282	C 192	N 46	O 43	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 507	C 338	N 81	O 86	S 2	0	0	0
7	h	65	Total 507	C 338	N 81	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	35	Total 286	C 195	N 45	O 45	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	34	Total 249	C 170	N 38	O 40	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	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 293	C 204	N 43	O 46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 304	C 202	N 48	O 53	S 1	0	0	0
11	l	37	Total 304	C 202	N 48	O 53	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 267	C 178	N 40	O 48	S 1	0	0	0
12	m	34	Total 267	C 178	N 40	O 48	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	243	Total 1845	C 1154	N 308	O 379	S 4	0	0	0
13	o	243	Total 1845	C 1154	N 308	O 379	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	32	Total 275	C 192	N 40	O 41	S 2	0	0	0
14	t	32	Total 275	C 192	N 40	O 41	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	97	Total 774	C 491	N 129	O 154	0	0	0
15	u	97	Total 774	C 491	N 129	O 154	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
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	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	37	Total	C	N	O	0	0	0
			270	182	41	47			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	G	28	Total	C	N	O	0	0	0
			140	84	28	28			

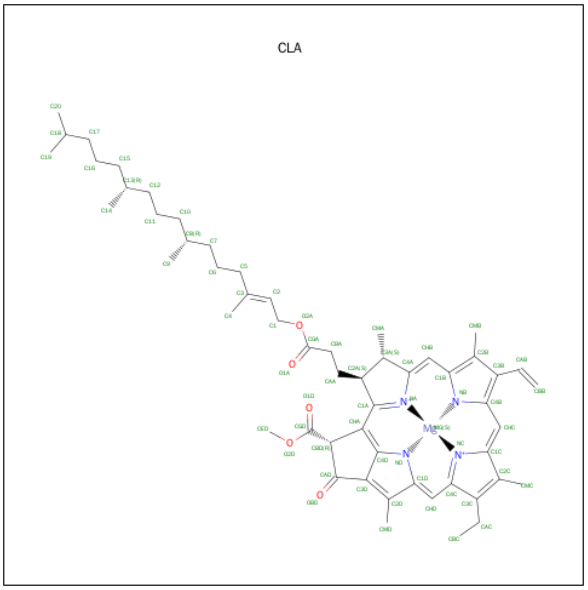
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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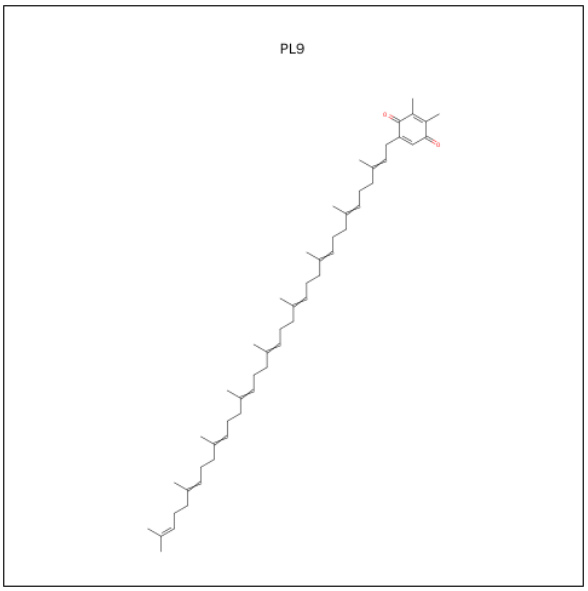
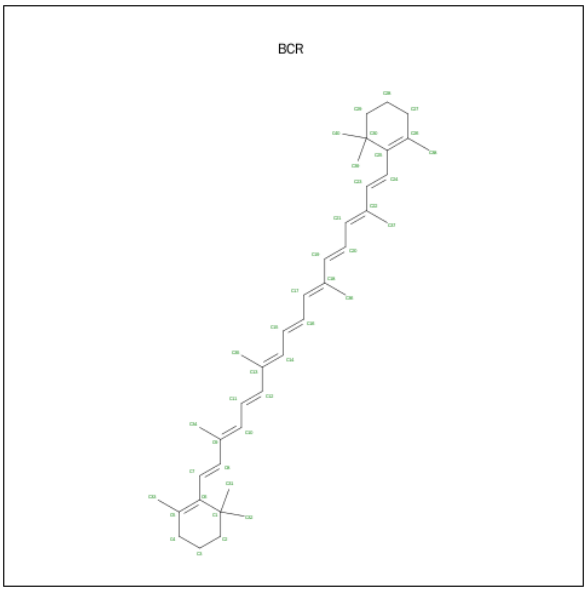
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N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

- Molecule 23 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
23	A	1	Total C O 45 43 2	0	0
23	D	1	Total C O 55 53 2	0	0
23	J	1	Total C O 35 33 2	0	0
23	a	1	Total C O 45 43 2	0	0
23	d	1	Total C O 55 53 2	0	0
23	j	1	Total C O 35 33 2	0	0

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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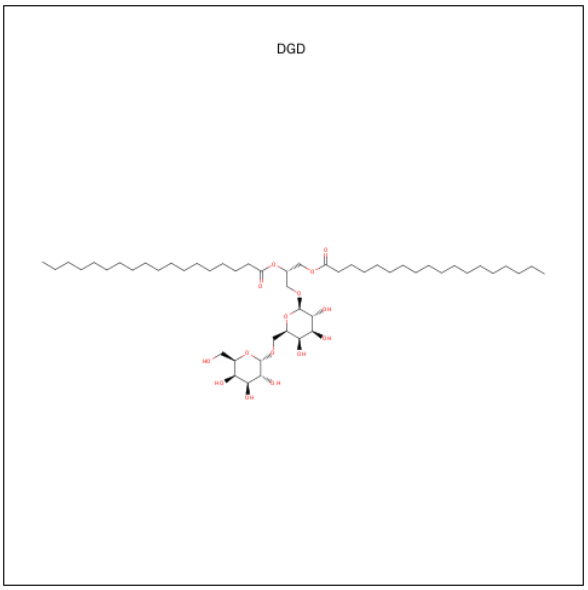
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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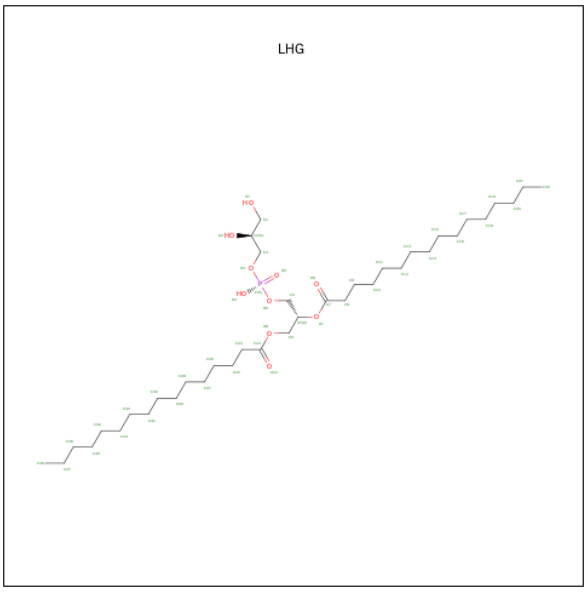
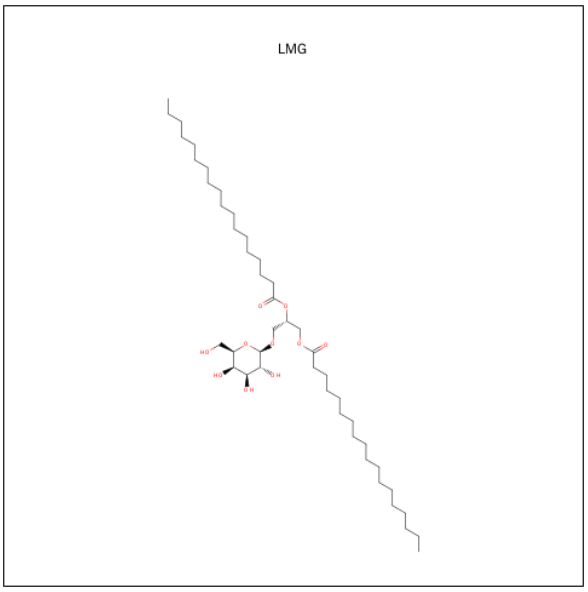
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 58 43 15	0	0
25	B	1	Total C O 52 37 15	0	0
25	C	1	Total C O 53 38 15	0	0
25	C	1	Total C O 62 47 15	0	0
25	C	1	Total C O 66 51 15	0	0
25	D	1	Total C O 63 48 15	0	0
25	a	1	Total C O 56 41 15	0	0
25	b	1	Total C O 52 37 15	0	0
25	b	1	Total C O 58 43 15	0	0
25	c	1	Total C O 53 38 15	0	0
25	c	1	Total C O 62 47 15	0	0
25	c	1	Total C O 66 51 15	0	0
25	d	1	Total C O 63 48 15	0	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

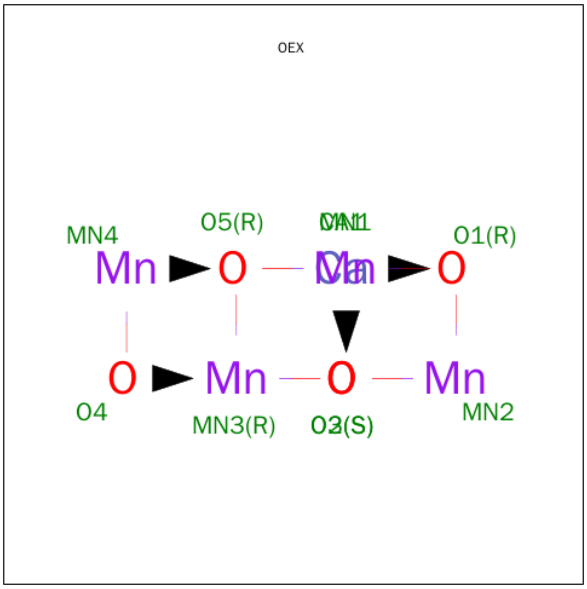


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 51 41 10	0	0
27	A	1	Total C O 42 32 10	0	0
27	B	1	Total C O 49 39 10	0	0
27	B	1	Total C O 49 39 10	0	0
27	C	1	Total C O 45 35 10	0	0
27	C	1	Total C O 48 38 10	0	0
27	D	1	Total C O 48 38 10	0	0
27	D	1	Total C O 46 36 10	0	0
27	E	1	Total C O 44 34 10	0	0
27	I	1	Total C O 43 33 10	0	0
27	M	1	Total C O 42 32 10	0	0
27	a	1	Total C O 42 32 10	0	0
27	a	1	Total C O 51 41 10	0	0
27	b	1	Total C O 49 39 10	0	0
27	b	1	Total C O 49 39 10	0	0
27	c	1	Total C O 45 35 10	0	0
27	c	1	Total C O 48 38 10	0	0
27	d	1	Total C O 48 38 10	0	0
27	d	1	Total C O 46 36 10	0	0
27	e	1	Total C O 44 34 10	0	0
27	i	1	Total C O 43 33 10	0	0
27	m	1	Total C O 42 32 10	0	0

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

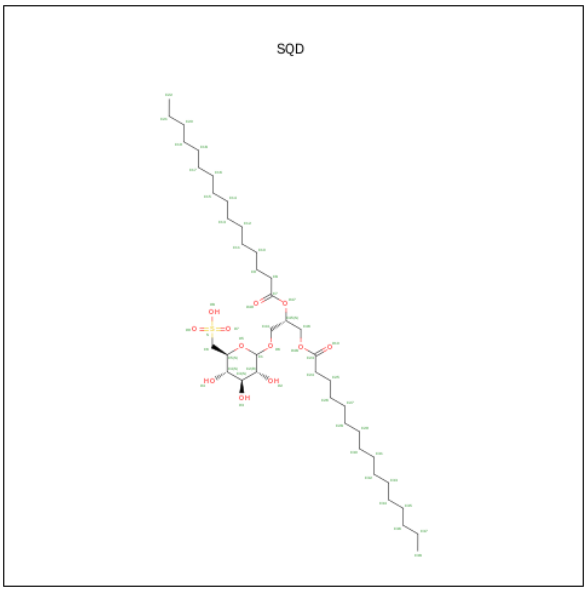
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Cl 1 1	0	0
28	a	1	Total Cl 1 1	0	0

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



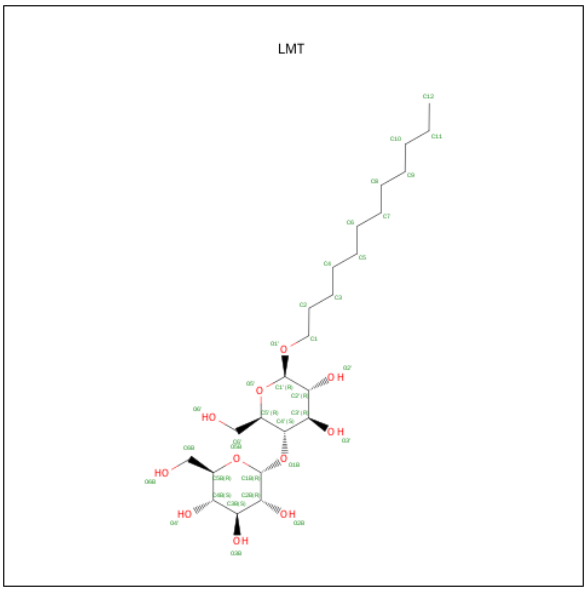
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0	0
29	a	1	Total Ca Mn O 10 1 4 5	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



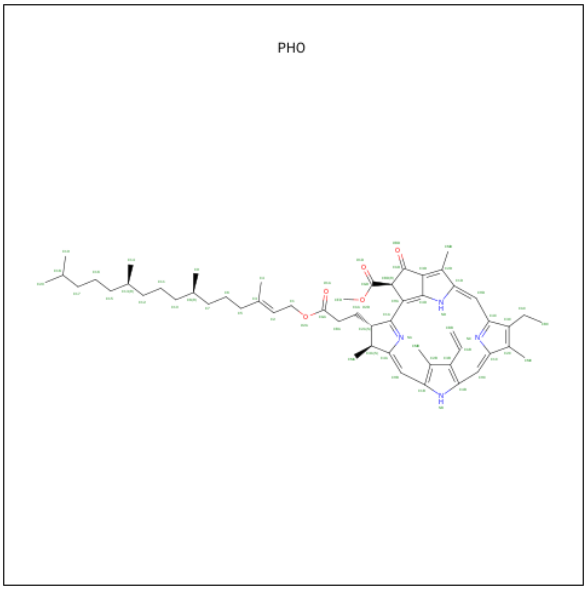
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



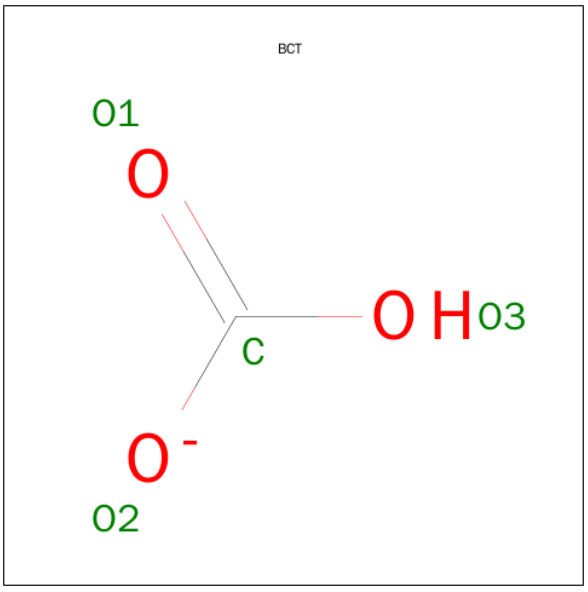
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	D	1	Total C O 31 20 11	0	0
31	I	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	d	1	Total C O 31 20 11	0	0
31	i	1	Total C O 35 24 11	0	0

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



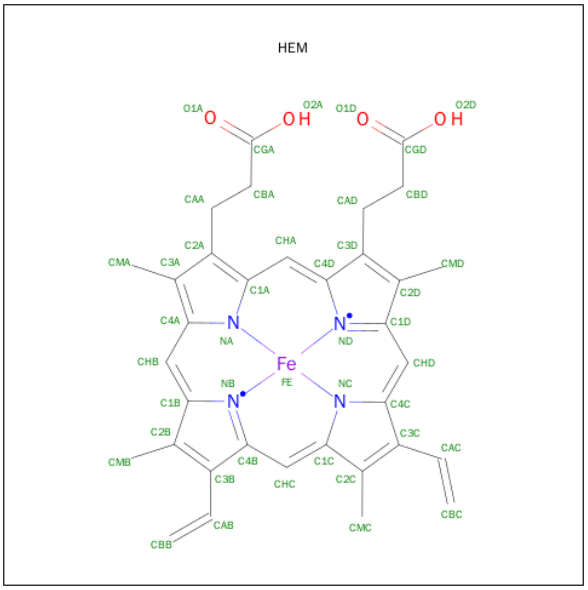
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 4 1 3	0	0
33	d	1	Total C O 4 1 3	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	F	1	Total C Fe N O 43 34 1 4 4	0	0
34	V	1	Total C Fe N O 43 34 1 4 4	0	0
34	f	1	Total C Fe N O 43 34 1 4 4	0	0
34	v	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	o	1	Total Ca 1 1	0	0
35	O	1	Total Ca 1 1	0	0
35	K	1	Total Ca 1 1	0	0

Continued on next page...

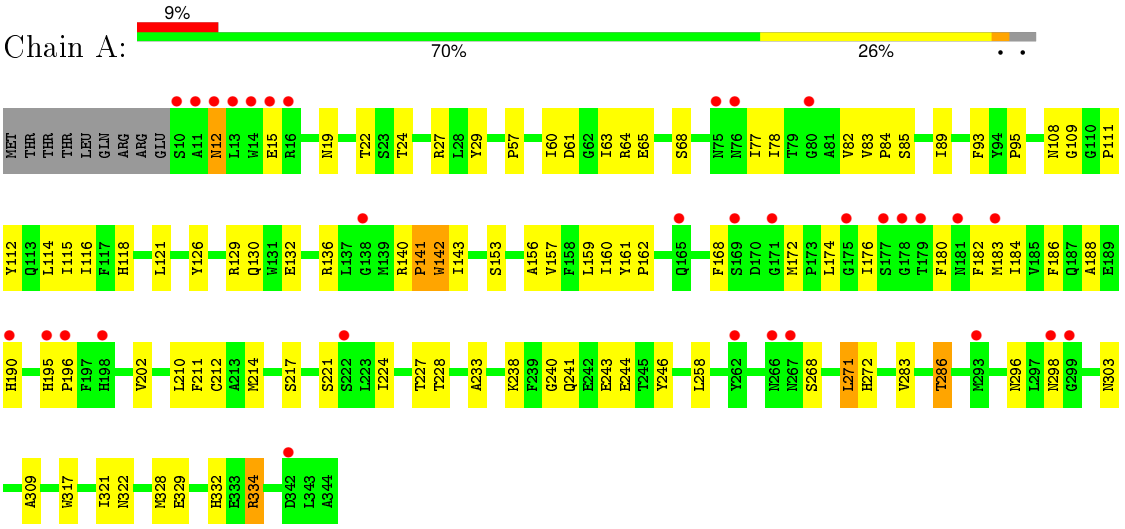
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
35	k	1	1	1	0	0

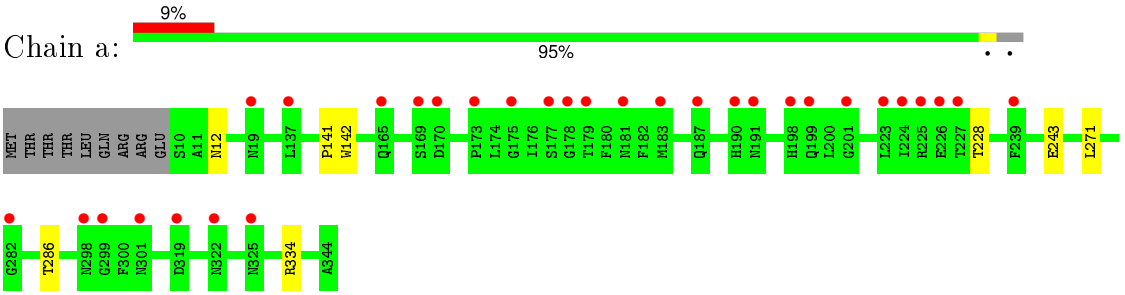
3 Residue-property plots (i)

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

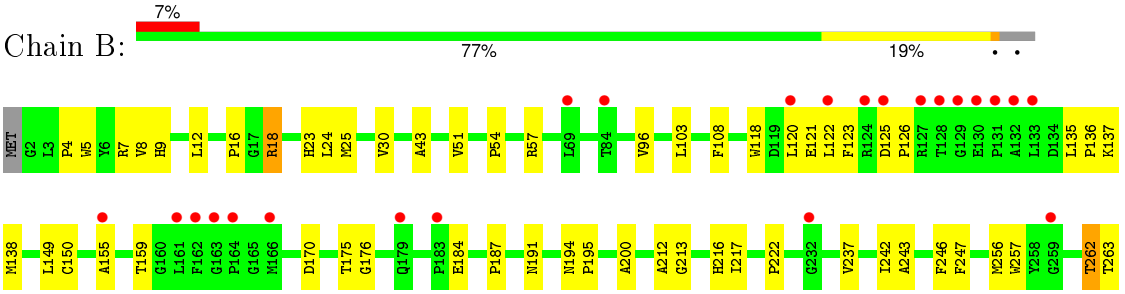
- Molecule 1: Photosystem Q(B) protein 1

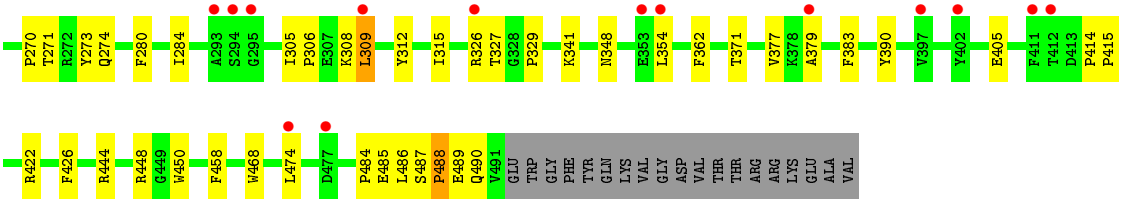


- Molecule 1: Photosystem Q(B) protein 1

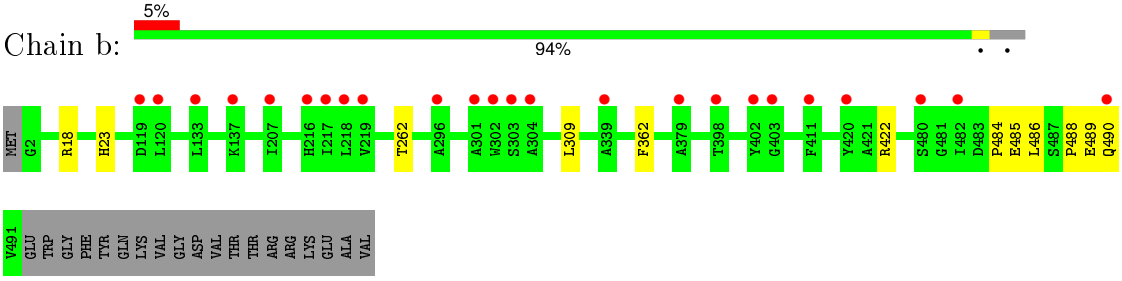


- Molecule 2: Photosystem II core light harvesting protein

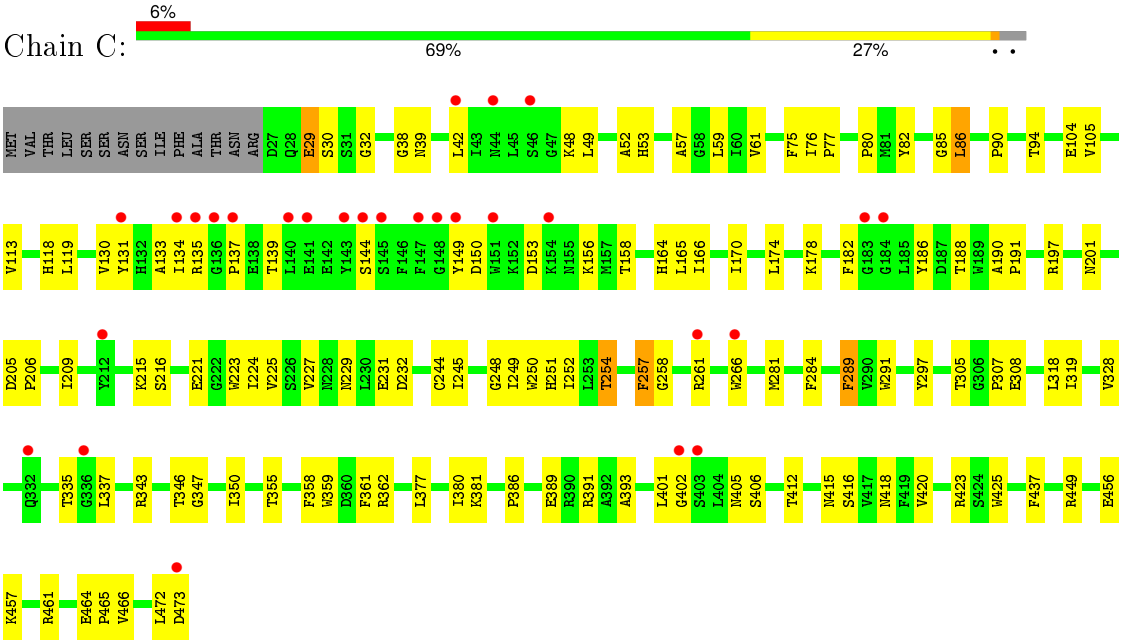




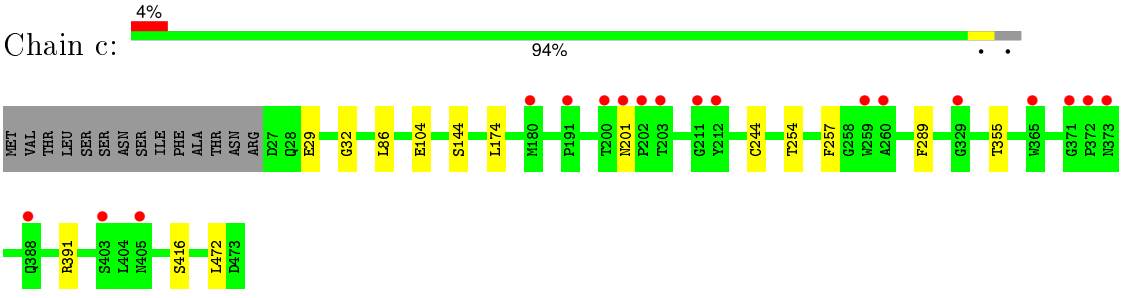
• Molecule 2: Photosystem II core light harvesting protein



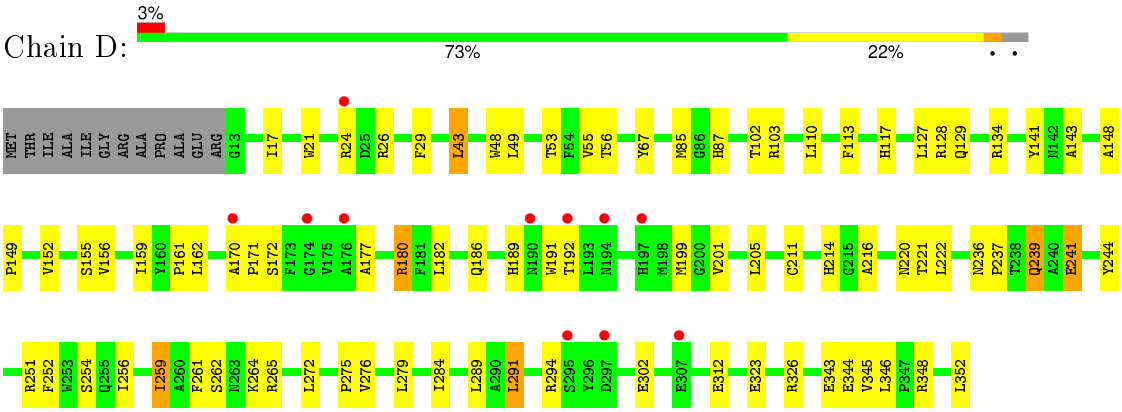
• Molecule 3: Photosystem II CP43 protein



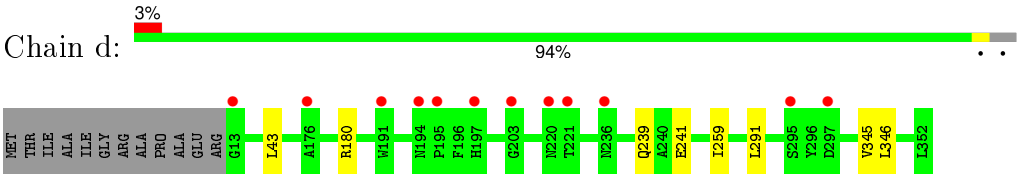
• Molecule 3: Photosystem II CP43 protein



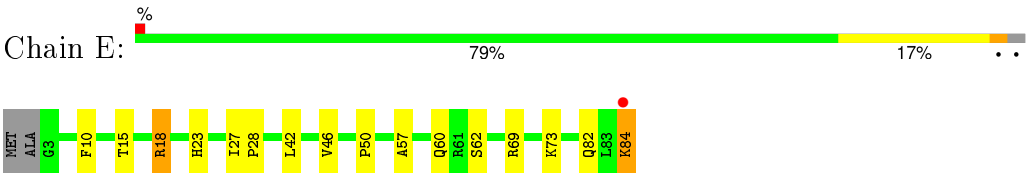
• Molecule 4: Photosystem II D2 protein



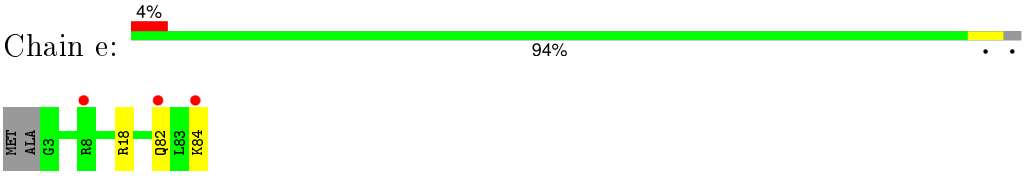
- Molecule 4: Photosystem II D2 protein



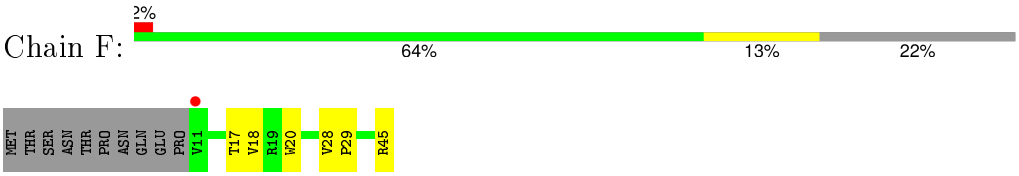
- Molecule 5: Cytochrome b559 subunit alpha



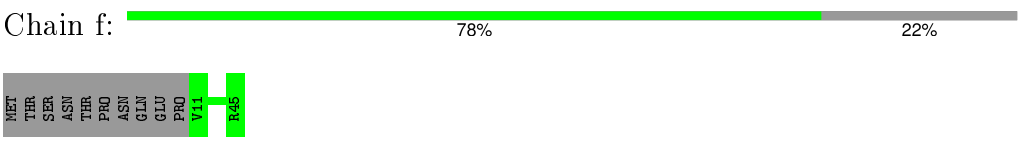
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

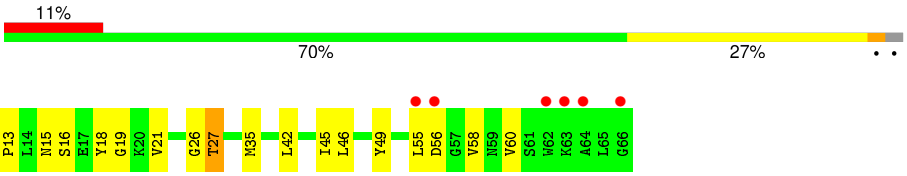


- Molecule 6: Cytochrome b559 subunit beta



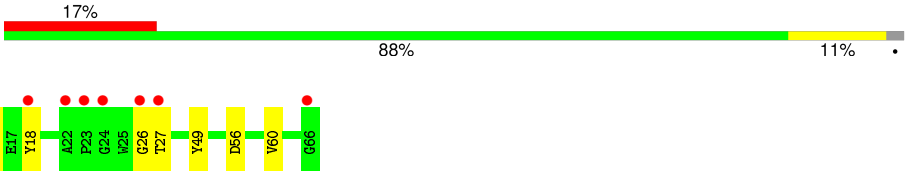
- Molecule 7: Photosystem II reaction center protein H

Chain H:



• Molecule 7: Photosystem II reaction center protein H

Chain h:

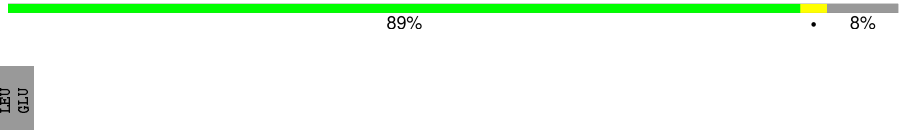


• Molecule 8: Photosystem II reaction center protein I

Chain I:

• Molecule 8: Photosystem II reaction center protein I

Chain i:



• Molecule 9: Photosystem II reaction center protein J

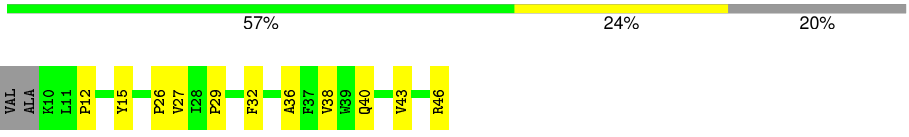
Chain J:

• Molecule 9: Photosystem II reaction center protein J

Chain j:

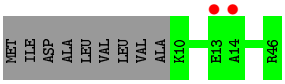
• Molecule 10: Photosystem II reaction center protein K

Chain K:



• Molecule 10: Photosystem II reaction center protein K

Chain k:

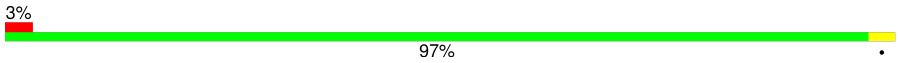


• Molecule 11: Photosystem II reaction center protein L

Chain L:

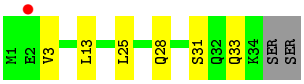
• Molecule 11: Photosystem II reaction center protein L

Chain l:



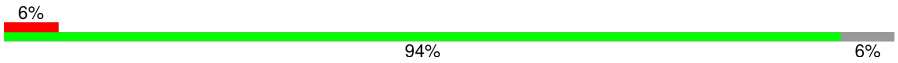
• Molecule 12: Photosystem II reaction center protein M

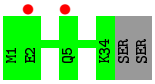
Chain M:



• Molecule 12: Photosystem II reaction center protein M

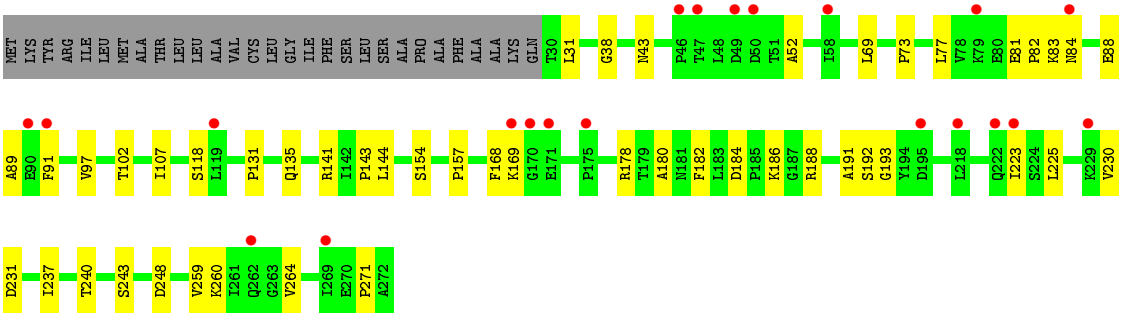
Chain m:





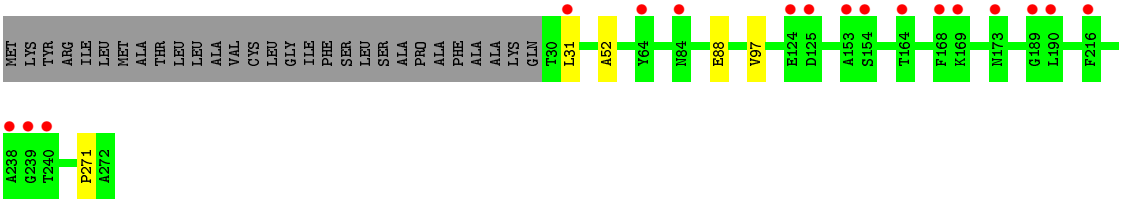
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

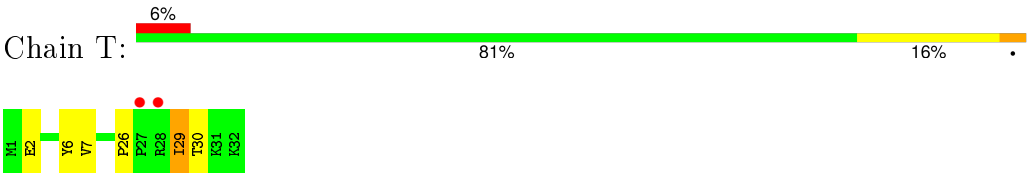


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

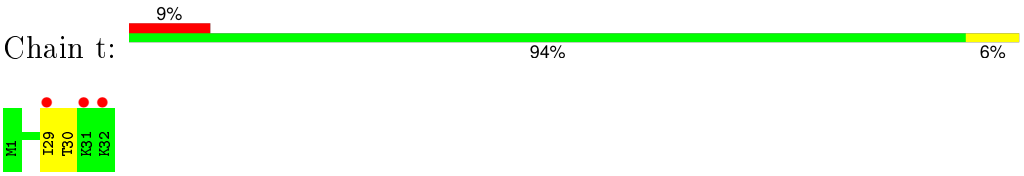
Chain o:



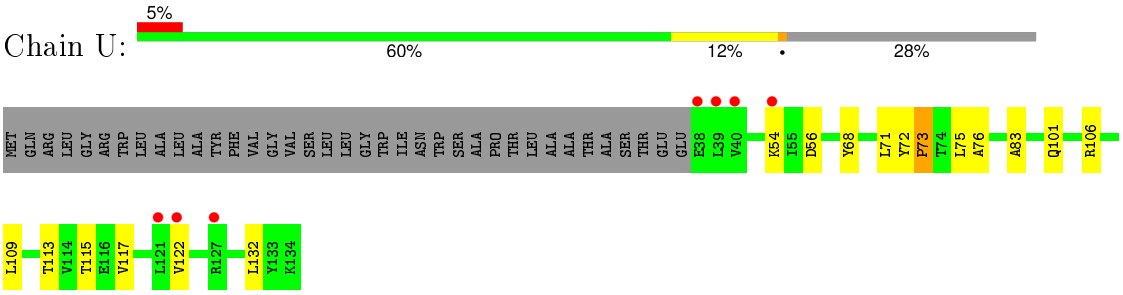
- Molecule 14: Photosystem II reaction center protein T



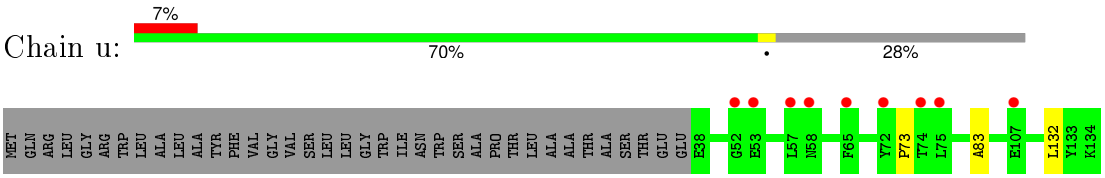
- Molecule 14: Photosystem II reaction center protein T



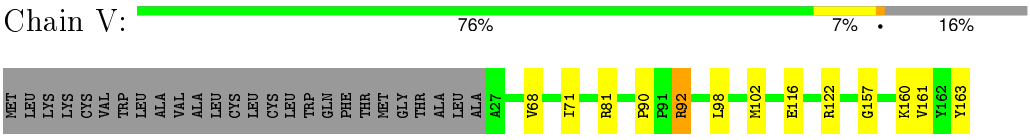
- Molecule 15: Photosystem II 12 kDa extrinsic protein



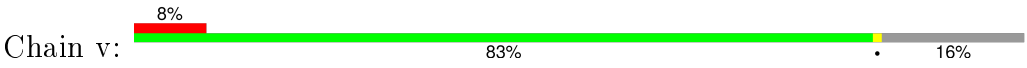
- Molecule 15: Photosystem II 12 kDa extrinsic protein

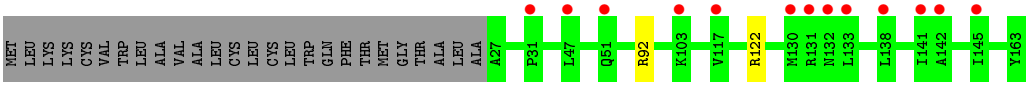


- Molecule 16: Cytochrome c-550



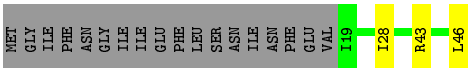
- Molecule 16: Cytochrome c-550





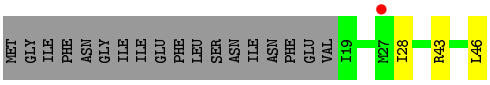
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



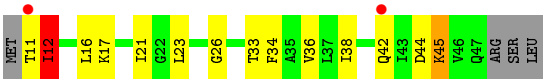
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



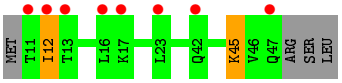
• Molecule 18: Photosystem II reaction center X protein

Chain X:



• Molecule 18: Photosystem II reaction center X protein

Chain x:



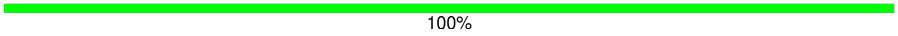
• Molecule 19: Photosystem II reaction center protein Y

Chain Y:

There are no outlier residues recorded for this chain.

• Molecule 19: Photosystem II reaction center protein Y

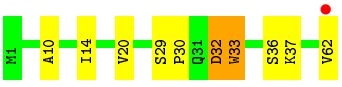
Chain G:



There are no outlier residues recorded for this chain.

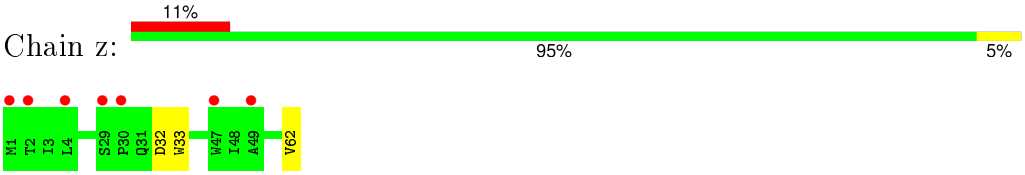
• Molecule 20: Photosystem II reaction center protein Z

Chain Z:



• Molecule 20: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 4.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.276 , 0.284 0.296 , 0.289	Depositor DCC
R_{free} test set	2668 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	153.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 115.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Outliers	0 of 54442 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å^2)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, BCT, HEM, LMG, 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	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.23	0/3556	0.41	0/4842
3	c	0.23	0/3556	0.41	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.43	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.46	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.25	0/293	0.43	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.25	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.44	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.26	0/273	0.44	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.25	0/490	0.44	0/669
All	All	0.23	0/41950	0.42	0/57100

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 (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	2628	0	2524	79	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	87	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	71	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	18	0
7	h	507	0	521	0	0
8	I	286	0	308	4	0
8	i	286	0	308	0	0
9	J	249	0	262	8	0
9	j	249	0	262	0	0
10	K	293	0	305	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	6	0
11	l	304	0	316	0	0
12	M	267	0	289	6	0
12	m	267	0	289	0	0
13	O	1845	0	1801	29	0
13	o	1845	0	1801	0	0
14	T	275	0	288	5	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	13	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	44	0
22	B	975	0	1080	92	0
22	C	845	0	936	49	0
22	D	130	0	144	14	0
22	H	65	0	72	11	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	3	0
23	D	55	0	80	8	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	11	0
24	C	120	0	168	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	40	0	56	3	0
24	H	40	0	56	1	0
24	J	40	0	56	2	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	2	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	98	0	136	6	0
27	C	93	0	126	7	0
27	D	94	0	128	7	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	1	0
27	a	93	0	126	0	0
27	b	98	0	136	0	0
27	c	93	0	126	0	0
27	d	94	0	128	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	m	42	0	54	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	47	0	61	3	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	1	0
31	M	70	0	92	0	0
31	b	140	0	184	0	0
31	d	31	0	35	0	0
31	i	35	0	46	0	0
32	D	128	0	148	16	0
32	a	64	0	74	0	0
32	d	64	0	74	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	586	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 7.

The worst 5 of 586 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)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.56	0.87
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.60	0.82
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.61	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.50	0.80
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.77

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	16 62
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	16 62
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	24 70
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	30 74
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	21 67
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	21 67
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	46 83
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	46 83
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15 60
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	15 60
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100 100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100 100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3 32
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3 32
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100 100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100 100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 44
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 44
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	16	62
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	16	62
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	42
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	42
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9	52
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9	52
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4	38
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	38
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2	28
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2	28
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	56
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	56
All	All	5138/5618 (92%)	4673 (91%)	410 (8%)	55 (1%)	17	64

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	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	271/280 (97%)	267 (98%)	4 (2%)	72	89
1	a	271/280 (97%)	267 (98%)	4 (2%)	72	89
2	B	390/407 (96%)	381 (98%)	9 (2%)	58	83
2	b	390/407 (96%)	381 (98%)	9 (2%)	58	83
3	C	347/362 (96%)	336 (97%)	11 (3%)	46	77
3	c	347/362 (96%)	336 (97%)	11 (3%)	46	77
4	D	275/283 (97%)	268 (98%)	7 (2%)	55	82
4	d	275/283 (97%)	268 (98%)	7 (2%)	55	82
5	E	72/73 (99%)	70 (97%)	2 (3%)	51	79
5	e	72/73 (99%)	70 (97%)	2 (3%)	51	79
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	17	56
7	h	53/55 (96%)	49 (92%)	4 (8%)	17	56
8	I	32/35 (91%)	31 (97%)	1 (3%)	47	78
8	i	32/35 (91%)	31 (97%)	1 (3%)	47	78
9	J	24/28 (86%)	23 (96%)	1 (4%)	36	72
9	j	24/28 (86%)	23 (96%)	1 (4%)	36	72
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	50	79
11	l	35/35 (100%)	34 (97%)	1 (3%)	50	79
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	82	91
13	o	202/228 (89%)	200 (99%)	2 (1%)	82	91
14	T	29/29 (100%)	28 (97%)	1 (3%)	44	77
14	t	29/29 (100%)	28 (97%)	1 (3%)	44	77
15	U	84/112 (75%)	83 (99%)	1 (1%)	78	90
15	u	84/112 (75%)	83 (99%)	1 (1%)	78	90
16	V	116/138 (84%)	114 (98%)	2 (2%)	68	88
16	v	116/138 (84%)	114 (98%)	2 (2%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	g	20/37 (54%)	18 (90%)	2 (10%)	9 41
17	y	20/37 (54%)	18 (90%)	2 (10%)	9 41
18	X	30/34 (88%)	28 (93%)	2 (7%)	20 59
18	x	30/34 (88%)	28 (93%)	2 (7%)	20 59
20	Z	52/52 (100%)	50 (96%)	2 (4%)	40 74
20	z	52/52 (100%)	50 (96%)	2 (4%)	40 74
All	All	4244/4594 (92%)	4140 (98%)	104 (2%)	55 82

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	y	46	LEU
2	b	262	THR
16	v	92	ARG
18	X	12	ILE
1	a	228	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	118	HIS
4	D	117	HIS
4	d	117	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	$\#\|Z\| > 2$
22	CLA	A	402	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	6 (9%)
22	CLA	A	403	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	6 (9%)
22	CLA	A	404	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	A	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	7 (11%)
23	PL9	A	406	-	45,45,55	1.07	3 (6%)	56,57,69	1.58	12 (21%)
24	BCR	A	407	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	5 (8%)
25	DGD	A	408	-	57,57,67	0.91	0	71,71,81	1.42	7 (9%)
26	LHG	A	409	-	38,38,48	0.67	0	39,44,54	1.18	3 (7%)
27	LMG	A	410	-	51,51,55	0.73	1 (1%)	59,59,63	1.37	6 (10%)
29	OEX	A	412	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	A	413	-	50,51,54	0.96	3 (6%)	58,62,65	1.96	8 (13%)
30	SQD	A	414	-	53,54,54	0.95	4 (7%)	61,65,65	1.70	9 (14%)
27	LMG	A	415	-	42,42,55	0.82	0	50,50,63	1.26	4 (8%)
22	CLA	B	601	-	55,73,73	0.96	4 (7%)	61,113,113	1.21	9 (14%)
22	CLA	B	602	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	9 (14%)
22	CLA	B	603	-	55,73,73	0.95	3 (5%)	61,113,113	1.25	8 (13%)
22	CLA	B	604	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	B	605	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	B	606	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	B	607	-	55,73,73	0.95	4 (7%)	61,113,113	1.21	7 (11%)
22	CLA	B	608	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	8 (13%)
22	CLA	B	609	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	B	610	-	55,73,73	1.01	4 (7%)	61,113,113	1.28	8 (13%)
22	CLA	B	611	-	55,73,73	0.94	4 (7%)	61,113,113	1.19	8 (13%)
22	CLA	B	612	-	55,73,73	0.93	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	B	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
22	CLA	B	614	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	9 (14%)
22	CLA	B	615	-	55,73,73	0.94	4 (7%)	61,113,113	1.18	7 (11%)
24	BCR	B	616	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	7 (12%)
24	BCR	B	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	6 (10%)
24	BCR	B	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.34	11 (19%)
24	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
25	DGD	B	620	-	59,59,67	0.88	1 (1%)	73,73,81	1.35	6 (8%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.33	6 (10%)
31	LMT	B	622	-	36,36,36	1.09	5 (13%)	47,47,47	0.99	2 (4%)
31	LMT	B	623	-	36,36,36	1.07	4 (11%)	47,47,47	1.04	3 (6%)
27	LMG	B	624	-	49,49,55	0.75	0	57,57,63	1.33	6 (10%)
25	DGD	B	625	-	53,53,67	1.05	3 (5%)	67,67,81	1.36	7 (10%)
30	SQD	B	626	-	46,47,54	1.01	4 (8%)	54,58,65	1.99	9 (16%)
31	LMT	B	627	-	36,36,36	1.09	5 (13%)	47,47,47	0.98	2 (4%)
31	LMT	B	628	-	36,36,36	1.10	5 (13%)	47,47,47	1.06	1 (2%)
22	CLA	C	501	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	7 (11%)
22	CLA	C	502	-	55,73,73	0.95	4 (7%)	61,113,113	1.23	8 (13%)
22	CLA	C	503	-	55,73,73	0.93	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	C	504	-	55,73,73	0.96	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	C	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	8 (13%)
22	CLA	C	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	9 (14%)
22	CLA	C	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.25	7 (11%)
22	CLA	C	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.16	6 (9%)
22	CLA	C	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	C	510	3	55,73,73	0.94	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	C	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	C	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	7 (11%)
24	BCR	C	513	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	9 (16%)
24	BCR	C	514	-	41,41,41	1.07	3 (7%)	56,56,56	1.30	9 (16%)
25	DGD	C	515	-	54,54,67	0.96	2 (3%)	68,68,81	1.29	8 (11%)
25	DGD	C	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.45	14 (18%)
25	DGD	C	517	-	67,67,67	0.87	2 (2%)	81,81,81	1.43	10 (12%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.29	5 (9%)
26	LHG	C	519	-	36,36,48	0.69	0	37,42,54	1.26	4 (10%)
22	CLA	C	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	C	521	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	8 (14%)
27	LMG	C	522	-	48,48,55	0.76	0	56,56,63	1.32	6 (10%)
32	PHO	D	401	-	67,69,69	1.21	8 (11%)	84,99,99	1.00	4 (4%)
32	PHO	D	402	-	67,69,69	1.23	10 (14%)	84,99,99	1.00	4 (4%)
30	SQD	D	403	-	42,43,54	1.03	3 (7%)	50,54,65	1.96	9 (18%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	405	-	55,73,73	0.95	4 (7%)	61,113,113	1.18	7 (11%)
22	CLA	D	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	D	407	-	55,55,55	1.13	3 (5%)	68,69,69	1.58	15 (22%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.39	5 (8%)
25	DGD	D	409	-	64,64,67	0.89	0	78,78,81	1.34	10 (12%)
31	LMT	D	410	-	32,32,36	1.15	5 (15%)	43,43,47	1.04	2 (4%)
24	BCR	D	411	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	5 (8%)
27	LMG	D	412	-	46,46,55	0.78	2 (4%)	54,54,63	1.31	5 (9%)
27	LMG	E	101	-	44,44,55	0.74	0	52,52,63	1.31	5 (9%)
34	HEM	F	101	5,6	30,50,50	2.10	11 (36%)	24,82,82	2.30	9 (37%)
30	SQD	F	102	-	44,45,54	1.03	3 (6%)	52,56,65	1.74	9 (17%)
22	CLA	H	101	-	55,73,73	0.95	4 (7%)	61,113,113	1.19	7 (11%)
24	BCR	H	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.28	5 (9%)
31	LMT	I	102	-	36,36,36	1.08	5 (13%)	47,47,47	1.06	2 (4%)
23	PL9	J	101	-	35,35,55	1.16	1 (2%)	44,45,69	1.55	6 (13%)
24	BCR	J	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.59	12 (21%)
27	LMG	M	101	-	42,42,55	0.85	1 (2%)	50,50,63	1.25	4 (8%)
31	LMT	M	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.03	3 (6%)
31	LMT	M	103	-	36,36,36	1.10	5 (13%)	47,47,47	1.01	3 (6%)
34	HEM	V	201	16	30,50,50	2.22	10 (33%)	24,82,82	2.24	6 (25%)
30	SQD	a	401	-	53,54,54	0.95	4 (7%)	61,65,65	1.69	8 (13%)
27	LMG	a	402	-	42,42,55	0.83	0	50,50,63	1.26	5 (10%)
22	CLA	a	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	6 (9%)
22	CLA	a	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	a	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
32	PHO	a	407	-	67,69,69	1.23	8 (11%)	84,99,99	1.00	4 (4%)
22	CLA	a	408	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	a	409	-	45,45,55	1.12	3 (6%)	56,57,69	1.59	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	a	410	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	7 (12%)
25	DGD	a	411	-	57,57,67	0.92	1 (1%)	71,71,81	1.41	7 (9%)
26	LHG	a	412	-	38,38,48	0.67	1 (2%)	39,44,54	1.19	3 (7%)
27	LMG	a	413	-	51,51,55	0.74	1 (1%)	59,59,63	1.35	7 (11%)
29	OEX	a	414	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	a	415	-	50,51,54	0.95	3 (6%)	58,62,65	1.98	9 (15%)
25	DGD	b	601	-	53,53,67	1.05	4 (7%)	67,67,81	1.36	7 (10%)
30	SQD	b	602	-	46,47,54	1.01	4 (8%)	54,58,65	2.03	9 (16%)
31	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	0.97	1 (2%)
31	LMT	b	604	-	36,36,36	1.10	5 (13%)	47,47,47	1.05	1 (2%)
22	CLA	b	605	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	b	606	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	8 (13%)
22	CLA	b	607	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	608	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	b	609	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	6 (9%)
22	CLA	b	610	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	b	611	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	b	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	b	613	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	b	614	-	55,73,73	1.02	4 (7%)	61,113,113	1.28	7 (11%)
22	CLA	b	615	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	8 (13%)
22	CLA	b	616	-	55,73,73	0.93	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	617	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	8 (13%)
22	CLA	b	618	-	55,73,73	0.94	4 (7%)	61,113,113	1.19	8 (13%)
22	CLA	b	619	-	55,73,73	0.95	4 (7%)	61,113,113	1.16	6 (9%)
24	BCR	b	620	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
24	BCR	b	621	-	41,41,41	1.05	2 (4%)	56,56,56	1.31	7 (12%)
24	BCR	b	622	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	10 (17%)
24	BCR	b	623	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	9 (16%)
25	DGD	b	624	-	59,59,67	0.89	1 (1%)	73,73,81	1.34	6 (8%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
31	LMT	b	626	-	36,36,36	1.09	5 (13%)	47,47,47	0.99	2 (4%)
31	LMT	b	627	-	36,36,36	1.06	3 (8%)	47,47,47	1.03	3 (6%)
27	LMG	b	628	-	49,49,55	0.76	0	57,57,63	1.32	5 (8%)
22	CLA	c	501	-	55,73,73	0.96	3 (5%)	61,113,113	1.17	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	502	-	55,73,73	0.96	4 (7%)	61,113,113	1.23	8 (13%)
22	CLA	c	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	c	504	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	8 (13%)
22	CLA	c	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	8 (13%)
22	CLA	c	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.28	7 (11%)
22	CLA	c	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	c	509	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	c	510	3	55,73,73	0.94	3 (5%)	61,113,113	1.22	6 (9%)
22	CLA	c	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	9 (14%)
22	CLA	c	512	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
24	BCR	c	513	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	10 (17%)
24	BCR	c	514	-	41,41,41	1.07	3 (7%)	56,56,56	1.30	8 (14%)
25	DGD	c	515	-	54,54,67	0.94	1 (1%)	68,68,81	1.30	7 (10%)
25	DGD	c	516	-	63,63,67	0.90	1 (1%)	77,77,81	1.46	13 (16%)
25	DGD	c	517	-	67,67,67	0.87	2 (2%)	81,81,81	1.42	11 (13%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.28	5 (9%)
26	LHG	c	519	-	36,36,48	0.72	0	37,42,54	1.26	3 (8%)
22	CLA	c	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	8 (13%)
24	BCR	c	521	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	8 (14%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.32	5 (8%)
32	PHO	d	401	-	67,69,69	1.21	10 (14%)	84,99,99	1.01	4 (4%)
30	SQD	d	402	-	42,43,54	1.03	3 (7%)	50,54,65	1.95	9 (18%)
33	BCT	d	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	404	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	7 (11%)
22	CLA	d	405	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	d	406	-	55,55,55	1.13	2 (3%)	68,69,69	1.60	15 (22%)
27	LMG	d	407	-	48,48,55	0.76	0	56,56,63	1.38	4 (7%)
25	DGD	d	408	-	64,64,67	0.90	2 (3%)	78,78,81	1.35	10 (12%)
31	LMT	d	409	-	32,32,36	1.14	5 (15%)	43,43,47	1.01	2 (4%)
27	LMG	d	410	-	46,46,55	0.79	1 (2%)	54,54,63	1.32	6 (11%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.30	5 (9%)
34	HEM	f	101	5,6	30,50,50	2.12	12 (40%)	24,82,82	2.31	9 (37%)
24	BCR	f	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	6 (10%)
30	SQD	f	103	-	44,45,54	1.03	4 (9%)	52,56,65	1.73	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	g	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	6 (10%)
22	CLA	h	101	-	55,73,73	0.95	4 (7%)	61,113,113	1.18	7 (11%)
27	LMG	i	101	-	43,43,55	0.81	0	51,51,63	1.28	5 (9%)
31	LMT	i	102	-	36,36,36	1.07	4 (11%)	47,47,47	1.06	2 (4%)
23	PL9	j	101	-	35,35,55	1.13	1 (2%)	44,45,69	1.54	7 (15%)
24	BCR	j	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.58	12 (21%)
27	LMG	m	101	-	42,42,55	0.85	1 (2%)	50,50,63	1.25	4 (8%)
34	HEM	v	201	16	30,50,50	2.22	11 (36%)	24,82,82	2.24	6 (25%)
24	BCR	x	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	5 (8%)
24	BCR	y	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	6 (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
22	CLA	A	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	BCR	A	407	-	-	0/29/63/63	0/2/2/2
25	DGD	A	408	-	-	0/45/85/95	0/2/2/2
26	LHG	A	409	-	-	0/43/43/53	0/0/0/0
27	LMG	A	410	-	-	0/46/66/70	0/1/1/1
29	OEX	A	412	1,3	-	0/0/68/68	0/0/6/6
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
30	SQD	A	414	-	-	0/49/69/69	0/1/1/1
27	LMG	A	415	-	-	0/37/57/70	0/1/1/1
22	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	B	616	-	-	0/29/63/63	0/2/2/2
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	DGD	B	620	-	-	0/47/87/95	0/2/2/2
27	LMG	B	621	-	-	0/44/64/70	0/1/1/1
31	LMT	B	622	-	-	0/21/61/61	0/2/2/2
31	LMT	B	623	-	-	0/21/61/61	0/2/2/2
27	LMG	B	624	-	-	0/44/64/70	0/1/1/1
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
30	SQD	B	626	-	-	0/42/62/69	0/1/1/1
31	LMT	B	627	-	-	0/21/61/61	0/2/2/2
31	LMT	B	628	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	C	513	-	-	0/29/63/63	0/2/2/2
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	DGD	C	515	-	-	0/42/82/95	0/2/2/2
25	DGD	C	516	-	-	1/51/91/95	0/2/2/2
25	DGD	C	517	-	-	0/55/95/95	0/2/2/2
27	LMG	C	518	-	-	0/40/60/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	C	519	-	-	0/41/41/53	0/0/0/0
22	CLA	C	520	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	C	521	-	-	0/29/63/63	0/2/2/2
27	LMG	C	522	-	-	0/43/63/70	0/1/1/1
32	PHO	D	401	-	-	0/53/103/103	0/1/6/6
32	PHO	D	402	-	-	0/53/103/103	0/1/6/6
30	SQD	D	403	-	-	1/38/58/69	0/1/1/1
33	BCT	D	404	21	-	0/0/0/0	0/0/0/0
22	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	D	406	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PL9	D	407	-	-	0/53/73/73	0/1/1/1
27	LMG	D	408	-	-	0/43/63/70	0/1/1/1
25	DGD	D	409	-	-	0/52/92/95	0/2/2/2
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
24	BCR	D	411	-	-	0/29/63/63	0/2/2/2
27	LMG	D	412	-	-	0/41/61/70	0/1/1/1
27	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
30	SQD	F	102	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	H	102	-	-	0/29/63/63	0/2/2/2
27	LMG	I	101	-	-	0/38/58/70	0/1/1/1
31	LMT	I	102	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	0/29/49/73	0/1/1/1
24	BCR	J	102	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	-	0/37/57/70	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/10/54/54	0/0/8/8
30	SQD	a	401	-	-	0/49/69/69	0/1/1/1
27	LMG	a	402	-	-	0/37/57/70	0/1/1/1
22	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
32	PHO	a	407	-	-	0/53/103/103	0/1/6/6
22	CLA	a	408	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	a	409	-	-	0/41/61/73	0/1/1/1
24	BCR	a	410	-	-	0/29/63/63	0/2/2/2
25	DGD	a	411	-	-	0/45/85/95	0/2/2/2
26	LHG	a	412	-	-	0/43/43/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	a	413	-	-	0/46/66/70	0/1/1/1
29	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
30	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2
30	SQD	b	602	-	-	0/42/62/69	0/1/1/1
31	LMT	b	603	-	-	0/21/61/61	0/2/2/2
31	LMT	b	604	-	-	0/21/61/61	0/2/2/2
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
24	BCR	b	621	-	-	0/29/63/63	0/2/2/2
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
24	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	DGD	b	624	-	-	0/47/87/95	0/2/2/2
27	LMG	b	625	-	-	0/44/64/70	0/1/1/1
31	LMT	b	626	-	-	0/21/61/61	0/2/2/2
31	LMT	b	627	-	-	0/21/61/61	0/2/2/2
27	LMG	b	628	-	-	0/44/64/70	0/1/1/1
22	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	513	-	-	0/29/63/63	0/2/2/2
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	DGD	c	515	-	-	0/42/82/95	0/2/2/2
25	DGD	c	516	-	-	1/51/91/95	0/2/2/2
25	DGD	c	517	-	-	0/55/95/95	0/2/2/2
27	LMG	c	518	-	-	0/40/60/70	0/1/1/1
26	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	c	521	-	-	0/29/63/63	0/2/2/2
27	LMG	c	522	-	-	0/43/63/70	0/1/1/1
32	PHO	d	401	-	-	0/53/103/103	0/1/6/6
30	SQD	d	402	-	-	1/38/58/69	0/1/1/1
33	BCT	d	403	21	-	0/0/0/0	0/0/0/0
22	CLA	d	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	d	406	-	-	0/53/73/73	0/1/1/1
27	LMG	d	407	-	-	0/43/63/70	0/1/1/1
25	DGD	d	408	-	-	0/52/92/95	0/2/2/2
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
27	LMG	d	410	-	-	0/41/61/70	0/1/1/1
27	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
24	BCR	f	102	-	-	0/29/63/63	0/2/2/2
30	SQD	f	103	-	-	0/40/60/69	0/1/1/1
24	BCR	g	101	-	-	0/29/63/63	0/2/2/2
22	CLA	h	101	-	3/3/20/25	0/37/135/135	0/0/9/9
27	LMG	i	101	-	-	0/38/58/70	0/1/1/1
31	LMT	i	102	-	-	0/21/61/61	0/2/2/2
23	PL9	j	101	-	-	0/29/49/73	0/1/1/1
24	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/10/54/54	0/0/8/8
24	BCR	x	101	-	-	0/29/63/63	0/2/2/2
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 501 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-7.33	1.45	1.51
34	v	201	HEM	C3B-C4B	-7.19	1.45	1.51
34	f	101	HEM	C3B-C4B	-6.16	1.46	1.51
34	F	101	HEM	C3B-C4B	-6.08	1.46	1.51
34	f	101	HEM	C3D-C4D	-5.27	1.44	1.51

The worst 5 of 1175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	j	101	PL9	C7-C3-C2	-6.05	118.40	123.42
23	J	101	PL9	C7-C3-C2	-6.00	118.44	123.42
23	d	406	PL9	C7-C3-C2	-5.80	118.61	123.42
23	D	407	PL9	C7-C3-C2	-5.68	118.71	123.42
23	A	406	PL9	C7-C3-C2	-5.66	118.73	123.42

5 of 209 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	C	516	DGD	C2G-O2G-C1B-C2B
25	c	516	DGD	C2G-O2G-C1B-C2B
30	d	402	SQD	C45-O47-C7-C8
30	D	403	SQD	C45-O47-C7-C8

There are no ring outliers.

80 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	11	0
22	A	403	CLA	12	0
22	A	404	CLA	16	0
22	A	405	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	406	PL9	3	0
24	A	407	BCR	2	0
25	A	408	DGD	1	0
26	A	409	LHG	3	0
27	A	410	LMG	2	0
30	A	413	SQD	3	0
30	A	414	SQD	3	0
27	A	415	LMG	1	0
22	B	601	CLA	1	0
22	B	602	CLA	11	0
22	B	603	CLA	3	0
22	B	604	CLA	10	0
22	B	605	CLA	6	0
22	B	606	CLA	16	0
22	B	607	CLA	10	0
22	B	608	CLA	14	0
22	B	609	CLA	3	0
22	B	610	CLA	6	0
22	B	611	CLA	10	0
22	B	612	CLA	10	0
22	B	613	CLA	4	0
22	B	614	CLA	2	0
22	B	615	CLA	6	0
24	B	616	BCR	6	0
24	B	617	BCR	1	0
24	B	618	BCR	3	0
24	B	619	BCR	2	0
25	B	620	DGD	2	0
27	B	621	LMG	3	0
31	B	622	LMT	2	0
27	B	624	LMG	3	0
25	B	625	DGD	2	0
30	B	626	SQD	3	0
31	B	627	LMT	2	0
31	B	628	LMT	2	0
22	C	501	CLA	6	0
22	C	503	CLA	5	0
22	C	504	CLA	4	0
22	C	505	CLA	2	0
22	C	506	CLA	6	0
22	C	507	CLA	4	0
22	C	508	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	509	CLA	6	0
22	C	510	CLA	10	0
22	C	511	CLA	1	0
22	C	512	CLA	3	0
24	C	513	BCR	8	0
24	C	514	BCR	7	0
25	C	515	DGD	3	0
25	C	516	DGD	4	0
25	C	517	DGD	5	0
27	C	518	LMG	4	0
26	C	519	LHG	2	0
22	C	520	CLA	5	0
24	C	521	BCR	5	0
27	C	522	LMG	3	0
32	D	401	PHO	11	0
32	D	402	PHO	5	0
30	D	403	SQD	3	0
22	D	405	CLA	11	0
22	D	406	CLA	3	0
23	D	407	PL9	8	0
27	D	408	LMG	6	0
25	D	409	DGD	2	0
24	D	411	BCR	3	0
27	D	412	LMG	1	0
27	E	101	LMG	1	0
34	F	101	HEM	4	0
30	F	102	SQD	2	0
22	H	101	CLA	11	0
24	H	102	BCR	1	0
27	I	101	LMG	1	0
31	I	102	LMT	1	0
24	J	102	BCR	2	0
27	M	101	LMG	1	0
34	V	201	HEM	3	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	335/344 (97%)	0.49	32 (9%) 10 8	172, 174, 175, 176	0
1	a	335/344 (97%)	0.52	31 (9%) 11 9	172, 174, 175, 176	0
2	B	490/510 (96%)	0.28	37 (7%) 17 13	172, 174, 175, 176	0
2	b	490/510 (96%)	0.34	24 (4%) 33 26	172, 174, 175, 176	0
3	C	447/461 (96%)	0.31	28 (6%) 23 17	172, 174, 175, 176	0
3	c	447/461 (96%)	0.19	18 (4%) 42 33	173, 174, 175, 176	0
4	D	340/352 (96%)	0.23	11 (3%) 51 40	171, 174, 175, 176	0
4	d	340/352 (96%)	0.22	12 (3%) 48 38	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.02	1 (1%) 81 73	172, 174, 175, 175	0
5	e	82/84 (97%)	0.07	3 (3%) 45 36	173, 174, 175, 177	0
6	F	35/45 (77%)	-0.10	1 (2%) 55 44	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.43	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.49	7 (10%) 8 7	173, 174, 175, 176	0
7	h	65/66 (98%)	0.79	11 (16%) 2 4	173, 174, 175, 176	0
8	I	35/38 (92%)	0.30	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	-0.07	0 100 100	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.06	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	-0.40	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.28	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	0.21	2 (5%) 29 23	174, 174, 175, 176	0
11	L	37/37 (100%)	0.40	1 (2%) 58 48	172, 174, 175, 175	0
11	l	37/37 (100%)	0.21	1 (2%) 58 48	173, 174, 175, 176	0
12	M	34/36 (94%)	0.27	1 (2%) 55 44	172, 174, 174, 176	0
12	m	34/36 (94%)	0.15	2 (5%) 26 19	173, 173, 174, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.54	21 (8%) 13 11	172, 174, 175, 176	0
13	o	243/272 (89%)	0.54	17 (6%) 19 15	172, 174, 175, 176	0
14	T	32/32 (100%)	0.31	2 (6%) 23 17	173, 174, 176, 176	0
14	t	32/32 (100%)	0.40	3 (9%) 11 9	173, 174, 175, 176	0
15	U	97/134 (72%)	0.54	7 (7%) 18 14	172, 174, 174, 175	0
15	u	97/134 (72%)	0.70	9 (9%) 11 9	173, 174, 175, 175	0
16	V	137/163 (84%)	0.10	0 100 100	172, 174, 175, 175	0
16	v	137/163 (84%)	0.56	13 (9%) 10 9	173, 174, 175, 176	0
17	g	28/46 (60%)	0.39	1 (3%) 46 37	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.01	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	0.39	2 (5%) 29 23	173, 174, 175, 176	0
18	x	37/41 (90%)	0.94	8 (21%) 1 2	173, 175, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.31	1 (1%) 74 65	173, 174, 175, 176	0
20	z	62/62 (100%)	0.98	7 (11%) 7 7	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.34	314 (6%) 25 18	171, 174, 175, 177	0

The worst 5 of 314 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.8
1	a	224	ILE	5.7
15	U	38	GLU	5.1
5	e	84	LYS	5.1
3	C	135	ARG	4.8

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
31	LMT	i	102	35/35	0.52	1.30	9.06	173,175,176,177	0
24	BCR	B	619	40/40	0.80	0.83	7.14	172,173,174,175	0
25	DGD	D	409	63/66	0.70	0.81	6.82	172,174,176,178	0
24	BCR	y	101	40/40	0.78	0.99	6.67	173,173,174,175	0
31	LMT	D	410	31/35	0.63	0.93	6.54	174,175,176,176	0
24	BCR	b	623	40/40	0.80	0.76	6.35	171,173,174,174	0
27	LMG	c	518	45/55	0.72	1.00	6.01	172,174,176,176	0
25	DGD	d	408	63/66	0.66	0.77	5.36	172,175,177,178	0
24	BCR	c	521	40/40	0.81	1.26	5.31	172,174,175,175	0
27	LMG	C	518	45/55	0.61	1.09	5.29	171,174,175,175	0
33	BCT	d	403	4/4	0.91	0.92	5.20	174,174,175,176	0
31	LMT	I	102	35/35	0.41	0.92	4.70	173,175,176,178	0
31	LMT	b	627	35/35	0.54	1.22	4.57	173,175,177,177	0
22	CLA	a	408	65/65	0.74	0.81	4.42	173,174,175,175	0
24	BCR	a	410	40/40	0.73	0.67	4.33	172,173,174,175	0
24	BCR	C	513	40/40	0.87	0.77	4.10	172,173,174,174	0
22	CLA	A	405	65/65	0.83	0.62	3.75	172,174,175,176	0
22	CLA	b	605	65/65	0.60	1.14	3.53	172,175,176,176	0
22	CLA	D	406	65/65	0.88	0.63	3.26	172,174,175,176	0
24	BCR	f	102	40/40	0.64	0.47	3.20	171,173,175,175	0
23	PL9	J	101	35/55	0.44	0.53	3.05	172,175,176,176	0
23	PL9	j	101	35/55	0.50	0.37	3.04	173,175,175,176	0
24	BCR	J	102	40/40	0.50	0.44	3.02	172,174,176,177	0
24	BCR	g	101	40/40	0.63	0.78	2.98	173,174,175,175	0
24	BCR	c	513	40/40	0.83	0.87	2.93	172,173,175,175	0
30	SQD	a	401	54/54	0.84	0.58	2.92	172,174,176,178	0
30	SQD	d	402	43/54	0.74	0.84	2.91	172,174,176,178	0
31	LMT	B	623	35/35	0.78	0.50	2.84	173,174,177,177	0
27	LMG	M	101	42/55	0.73	0.53	2.74	173,174,176,176	0
27	LMG	A	415	42/55	0.62	0.53	2.64	171,174,176,177	0
25	DGD	B	625	52/66	0.76	0.57	2.59	172,175,177,177	0
24	BCR	H	102	40/40	0.68	0.94	2.58	173,174,175,176	0
25	DGD	b	601	52/66	0.72	0.47	2.48	172,174,176,177	0
24	BCR	B	617	40/40	0.75	0.44	2.48	172,173,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	B	601	65/65	0.62	0.85	2.43	172,175,176,177	0
24	BCR	B	618	40/40	0.83	0.32	2.41	171,172,174,174	0
24	BCR	C	514	40/40	0.78	0.83	2.36	172,173,175,175	0
30	SQD	f	103	45/54	0.84	0.52	2.31	172,174,176,178	0
22	CLA	c	512	65/65	0.77	0.69	2.30	172,174,176,176	0
22	CLA	b	607	65/65	0.82	0.43	2.22	172,173,175,176	0
22	CLA	c	508	65/65	0.84	0.56	2.21	172,174,175,175	0
22	CLA	b	606	65/65	0.85	0.61	2.20	172,173,174,174	0
24	BCR	C	521	40/40	0.78	0.82	2.06	172,174,175,176	0
24	BCR	b	622	40/40	0.77	0.37	2.00	171,172,173,173	0
22	CLA	b	613	65/65	0.81	0.67	1.79	172,174,175,175	0
31	LMT	B	627	35/35	0.75	0.55	1.78	172,175,177,177	0
24	BCR	D	411	40/40	0.67	0.44	1.72	171,173,174,175	0
22	CLA	b	609	65/65	0.81	0.55	1.70	172,174,175,175	0
22	CLA	B	611	65/65	0.92	0.36	1.70	171,173,174,174	0
22	CLA	B	603	65/65	0.81	0.49	1.68	171,173,175,175	0
27	LMG	D	412	46/55	0.77	0.39	1.65	172,174,175,175	0
22	CLA	b	608	65/65	0.88	0.50	1.64	172,173,175,176	0
22	CLA	c	511	65/65	0.89	0.61	1.62	172,174,175,176	0
22	CLA	C	508	65/65	0.88	0.86	1.61	172,174,175,175	0
22	CLA	c	503	65/65	0.82	0.56	1.61	172,174,175,175	0
22	CLA	B	604	65/65	0.87	0.68	1.59	172,173,175,175	0
22	CLA	c	506	65/65	0.86	0.55	1.53	173,174,175,175	0
22	CLA	C	506	65/65	0.77	0.72	1.51	172,174,175,175	0
22	CLA	C	502	65/65	0.69	0.53	1.51	173,174,174,175	0
27	LMG	a	402	42/55	0.66	0.49	1.49	171,174,176,176	0
24	BCR	c	514	40/40	0.68	0.70	1.42	172,173,175,175	0
22	CLA	b	615	65/65	0.92	0.40	1.39	172,173,174,175	0
31	LMT	b	603	35/35	0.80	0.44	1.39	172,174,175,176	0
22	CLA	h	101	65/65	0.78	0.54	1.39	171,174,175,175	0
31	LMT	d	409	31/35	0.53	0.66	1.36	172,175,177,177	0
24	BCR	B	616	40/40	0.71	0.43	1.31	172,173,174,175	0
22	CLA	C	511	65/65	0.90	0.91	1.30	172,174,175,175	0
30	SQD	F	102	45/54	0.78	0.69	1.28	172,175,177,178	0
31	LMT	b	604	35/35	0.69	0.48	1.26	172,174,176,176	0
30	SQD	B	626	47/54	0.79	0.46	1.25	170,174,176,178	0
25	DGD	b	624	58/66	0.76	0.41	1.24	171,173,174,175	0
22	CLA	c	501	65/65	0.85	0.45	1.22	172,174,175,175	0
25	DGD	A	408	56/66	0.71	0.45	1.22	172,174,175,176	0
22	CLA	B	609	65/65	0.86	0.53	1.20	172,174,175,175	0
22	CLA	c	510	65/65	0.86	0.53	1.19	173,174,175,176	0
27	LMG	C	522	48/55	0.73	0.36	1.14	172,174,174,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	BCR	A	407	40/40	0.79	0.47	1.13	171,173,174,174	0
22	CLA	b	619	65/65	0.64	0.77	1.12	172,174,175,175	0
22	CLA	b	612	65/65	0.84	0.66	1.09	171,174,175,176	0
24	BCR	j	102	40/40	0.62	0.34	1.08	173,175,177,178	0
27	LMG	E	101	44/55	0.62	0.57	1.08	170,174,176,177	0
27	LMG	a	413	51/55	0.69	0.42	1.04	172,173,175,176	0
22	CLA	B	608	65/65	0.90	0.50	1.01	172,174,175,175	0
22	CLA	c	502	65/65	0.66	0.54	1.00	173,174,175,175	0
23	PL9	a	409	45/55	0.76	0.38	0.97	171,173,174,175	0
30	SQD	A	414	54/54	0.85	0.41	0.96	171,174,176,179	0
22	CLA	d	405	65/65	0.86	0.45	0.95	172,174,175,175	0
24	BCR	x	101	40/40	0.71	0.86	0.93	173,174,175,175	0
25	DGD	a	411	56/66	0.74	0.43	0.92	173,174,175,176	0
22	CLA	C	512	65/65	0.83	0.88	0.91	172,174,176,177	0
22	CLA	B	614	65/65	0.89	0.62	0.87	172,174,175,175	0
34	HEM	F	101	43/43	0.91	0.48	0.86	173,174,175,176	0
22	CLA	b	618	65/65	0.82	0.67	0.86	172,174,175,175	0
31	LMT	B	628	35/35	0.67	0.46	0.85	172,174,177,178	0
34	HEM	V	201	43/43	0.88	0.45	0.81	172,173,175,175	0
27	LMG	m	101	42/55	0.79	0.44	0.80	170,174,175,175	0
22	CLA	B	605	65/65	0.86	0.72	0.78	172,173,175,176	0
30	SQD	b	602	47/54	0.80	0.38	0.73	171,174,176,178	0
22	CLA	C	503	65/65	0.85	0.41	0.71	172,174,175,176	0
22	CLA	C	505	65/65	0.79	0.45	0.68	172,174,175,176	0
22	CLA	B	602	65/65	0.92	0.52	0.62	171,173,174,175	0
22	CLA	B	615	65/65	0.85	0.66	0.57	172,174,175,175	0
22	CLA	B	613	65/65	0.76	0.45	0.56	172,174,174,175	0
27	LMG	e	101	44/55	0.75	0.39	0.54	171,174,175,176	0
22	CLA	C	501	65/65	0.87	0.40	0.53	172,174,174,175	0
22	CLA	c	504	65/65	0.89	0.33	0.53	172,174,175,175	0
22	CLA	b	617	65/65	0.82	0.45	0.47	173,173,175,176	0
22	CLA	B	607	65/65	0.85	0.42	0.43	172,174,174,175	0
34	HEM	f	101	43/43	0.93	0.34	0.41	173,174,175,175	0
22	CLA	A	404	65/65	0.87	0.46	0.41	170,173,174,175	0
22	CLA	a	405	65/65	0.84	0.58	0.39	170,172,174,175	0
22	CLA	b	616	65/65	0.95	0.29	0.39	171,173,174,175	0
25	DGD	C	515	53/66	0.83	0.36	0.38	172,173,174,174	0
22	CLA	C	510	65/65	0.83	0.47	0.37	172,173,175,175	0
34	HEM	v	201	43/43	0.90	0.55	0.37	171,174,175,175	0
22	CLA	C	507	65/65	0.77	0.40	0.33	173,174,175,177	0
22	CLA	c	505	65/65	0.85	0.45	0.33	172,174,175,175	0
22	CLA	C	509	65/65	0.85	0.34	0.33	173,173,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	C	504	65/65	0.84	0.41	0.32	171,173,175,175	0
22	CLA	A	403	65/65	0.93	0.54	0.29	171,173,174,175	0
23	PL9	A	406	45/55	0.70	0.43	0.29	172,174,175,175	0
22	CLA	H	101	65/65	0.85	0.35	0.28	172,174,175,175	0
30	SQD	D	403	43/54	0.82	0.41	0.26	172,174,177,180	0
25	DGD	c	515	53/66	0.86	0.37	0.25	171,174,175,177	0
32	PHO	D	402	64/64	0.79	0.37	0.20	171,173,175,175	0
27	LMG	A	410	51/55	0.79	0.35	0.19	171,173,174,175	0
22	CLA	a	404	65/65	0.88	0.55	0.17	172,173,174,176	0
30	SQD	A	413	51/54	0.73	0.37	0.13	172,174,175,176	0
28	CL	A	411	1/1	0.75	0.46	0.09	172,172,172,172	0
24	BCR	b	621	40/40	0.86	0.33	0.09	171,173,174,174	0
32	PHO	D	401	64/64	0.84	0.40	0.09	171,173,174,175	0
31	LMT	M	103	35/35	0.77	0.47	0.07	172,173,175,176	0
26	LHG	c	519	37/49	0.75	0.35	0.05	172,174,178,181	0
22	CLA	B	610	65/65	0.84	0.34	0.04	172,174,174,175	0
32	PHO	d	401	64/64	0.72	0.42	0.04	172,173,174,174	0
22	CLA	b	611	65/65	0.92	0.31	0.02	172,174,175,175	0
24	BCR	b	620	40/40	0.90	0.32	0.01	172,173,174,175	0
27	LMG	D	408	48/55	0.86	0.28	0.01	170,173,175,175	0
23	PL9	D	407	55/55	0.68	0.39	-0.02	171,173,174,175	0
27	LMG	d	410	46/55	0.91	0.23	-0.07	172,173,175,175	0
22	CLA	d	404	65/65	0.84	0.46	-0.08	172,173,174,174	0
22	CLA	b	614	65/65	0.88	0.30	-0.11	172,173,174,175	0
22	CLA	A	402	65/65	0.90	0.43	-0.12	172,173,174,175	0
27	LMG	c	522	48/55	0.81	0.30	-0.14	172,174,175,176	0
23	PL9	d	406	55/55	0.69	0.38	-0.16	172,173,175,175	0
25	DGD	B	620	58/66	0.84	0.33	-0.16	171,173,175,176	0
30	SQD	a	415	51/54	0.85	0.29	-0.18	173,174,175,176	0
22	CLA	C	520	65/65	0.82	0.33	-0.19	172,174,175,176	0
22	CLA	c	509	65/65	0.88	0.32	-0.21	172,173,175,175	0
27	LMG	b	625	49/55	0.78	0.34	-0.23	172,174,175,175	0
26	LHG	C	519	37/49	0.64	0.48	-0.24	172,174,179,183	0
22	CLA	c	520	65/65	0.87	0.35	-0.27	173,174,174,175	0
22	CLA	b	610	65/65	0.90	0.33	-0.34	172,173,175,175	0
31	LMT	M	102	35/35	0.77	0.46	-0.36	172,174,175,175	0
22	CLA	a	406	65/65	0.85	0.36	-0.38	172,174,175,176	0
25	DGD	c	517	66/66	0.79	0.35	-0.45	172,173,175,176	0
26	LHG	A	409	39/49	0.85	0.28	-0.46	172,173,175,176	0
22	CLA	B	606	65/65	0.88	0.34	-0.47	172,173,174,175	0
22	CLA	D	405	65/65	0.89	0.37	-0.49	172,173,174,175	0
27	LMG	d	407	48/55	0.87	0.27	-0.50	171,173,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	DGD	C	517	66/66	0.77	0.34	-0.54	172,173,174,175	0
26	LHG	a	412	39/49	0.83	0.28	-0.56	171,174,176,177	0
22	CLA	c	507	65/65	0.91	0.25	-0.58	172,174,175,176	0
22	CLA	B	612	65/65	0.91	0.28	-0.60	171,173,175,175	0
27	LMG	B	624	49/55	0.78	0.30	-0.66	171,173,174,175	0
29	OEX	A	412	10/10	0.93	0.43	-0.70	165,169,172,173	0
32	PHO	a	407	64/64	0.86	0.26	-0.72	173,174,175,175	0
29	OEX	a	414	10/10	0.96	0.45	-0.77	168,171,173,177	0
25	DGD	C	516	62/66	0.84	0.29	-0.78	171,174,175,176	0
33	BCT	D	404	4/4	0.95	0.25	-0.92	173,174,174,174	0
25	DGD	c	516	62/66	0.87	0.30	-0.94	172,174,175,175	0
27	LMG	b	628	49/55	0.93	0.23	-1.28	172,174,175,175	0
27	LMG	B	621	49/55	0.88	0.26	-1.49	172,173,174,174	0
28	CL	a	416	1/1	0.91	0.34	-2.14	173,173,173,173	0
21	FE2	A	401	1/1	0.91	0.19	-2.52	170,170,170,170	0
21	FE2	a	403	1/1	0.85	0.18	-3.12	175,175,175,175	0
35	CA	K	101	1/1	0.81	0.35	-	177,177,177,177	0
35	CA	O	301	1/1	0.53	0.38	-	177,177,177,177	0
35	CA	k	101	1/1	0.78	0.20	-	172,172,172,172	0
27	LMG	i	101	43/55	0.75	0.80	-	172,174,177,178	0
27	LMG	I	101	43/55	0.65	1.04	-	172,174,177,177	0
31	LMT	b	626	35/35	0.59	0.69	-	172,175,176,177	0
31	LMT	B	622	35/35	0.65	0.86	-	171,175,177,177	0
35	CA	o	301	1/1	0.31	0.73	-	180,180,180,180	0

6.5 Other polymers (i)

There are no such residues in this entry.