



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:42 PM GMT

PDB ID : 4TNH
Title : RT XFEL structure of Photosystem II in the dark state at 4.9 Å 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 : 4.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

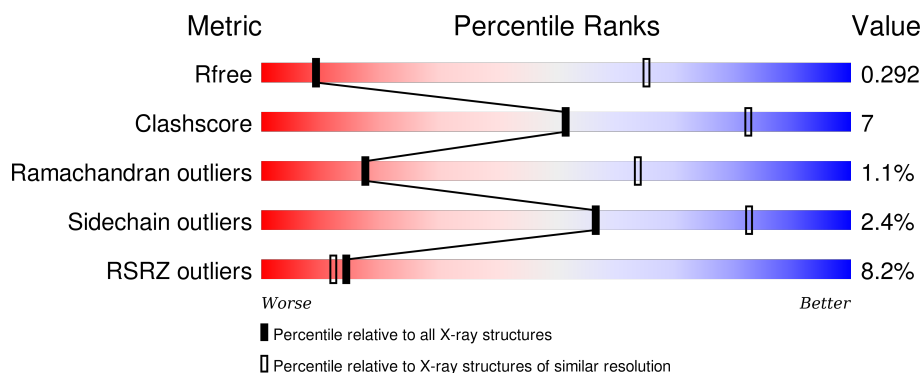
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.90 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	1118 (6.10-3.60)
Clashscore	102246	1018 (6.10-3.66)
Ramachandran outliers	100387	1157 (6.10-3.60)
Sidechain outliers	100360	1135 (6.10-3.60)
RSRZ outliers	91569	1121 (6.10-3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>9%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div>
1	a	344	<div> <div>13%</div> <div>95%</div> <div>• •</div> </div>
2	B	510	<div> <div>8%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
2	b	510	<div> <div>9%</div> <div>94%</div> <div>• •</div> </div>




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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	-	-	-
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	-	-	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	-	-	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
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	-	-	-
22	CLA	D	405	X	-	-	X
22	CLA	H	101	X	-	-	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	-	-	X
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	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	D	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	619	-	-	-	X
24	BCR	C	513	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	F	102	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	410	-	-	-	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	b	601	-	-	-	X
25	DGD	d	409	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	D	411	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	M	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	a	402	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	e	101	-	-	-	X
27	LMG	l	101	-	-	-	X
27	LMG	m	101	-	-	-	X
29	OEX	A	412	-	-	-	X
29	OEX	a	414	-	-	-	X
30	SQD	B	622	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	103	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	d	402	-	-	-	X
30	SQD	f	103	-	-	-	X
31	LMT	B	624	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	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	410	-	-	-	X
31	LMT	i	102	-	-	-	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	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	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				

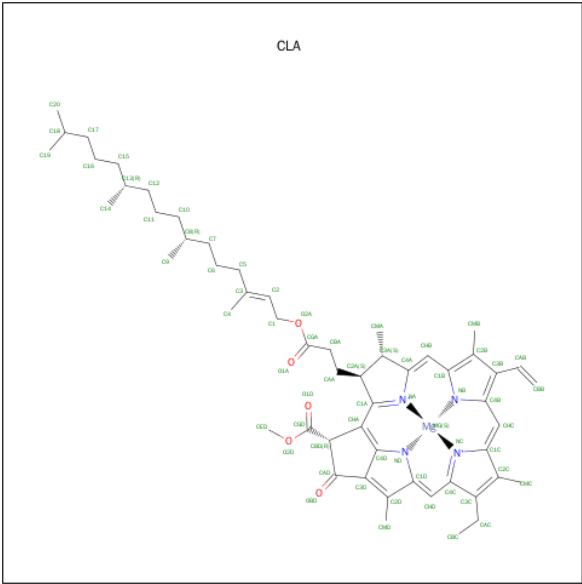
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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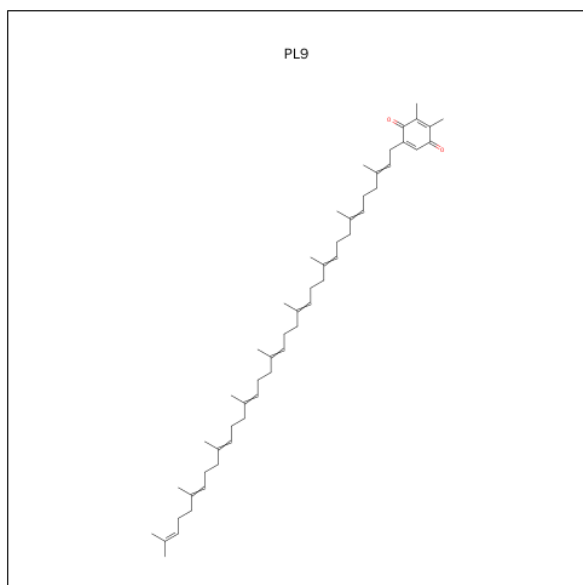
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N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

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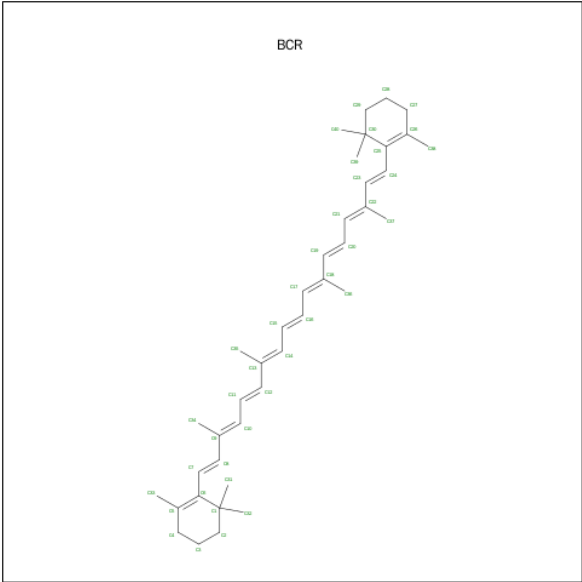
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- 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: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	a	1	Total	C	O	0	0
			45	43	2		
23	d	1	Total	C	O	0	0
			55	53	2		
23	j	1	Total	C	O	0	0
			35	33	2		

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



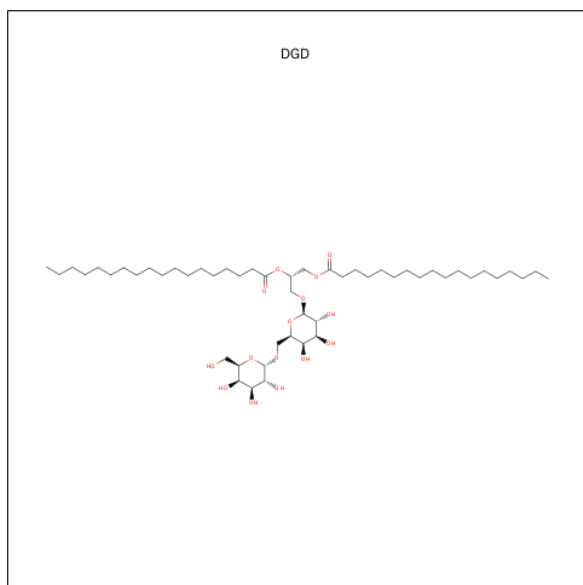
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total 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: $C_{51}H_{96}O_{15}$).



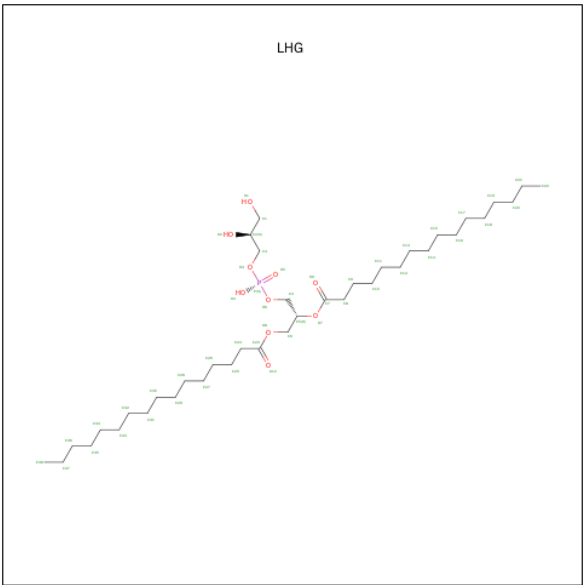
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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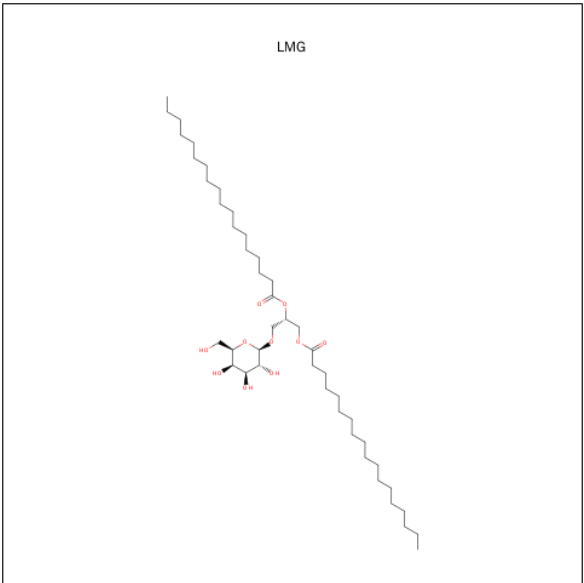
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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: C₄₅H₈₆O₁₀).

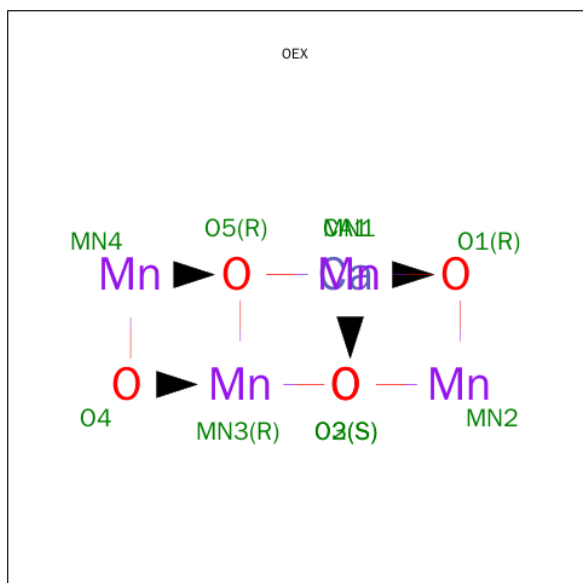


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total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

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

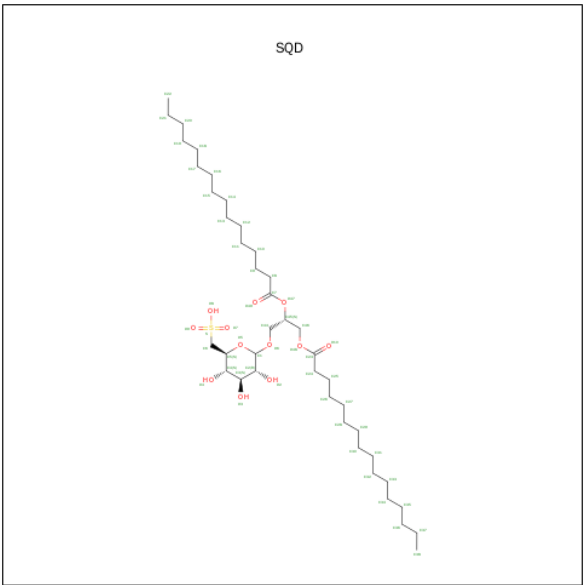
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

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



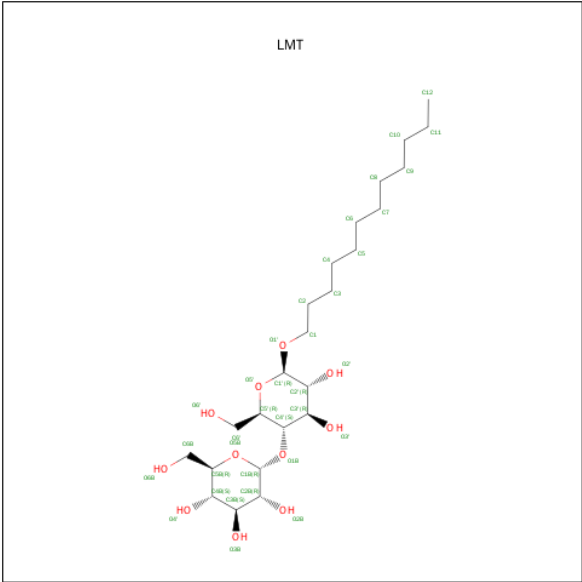
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



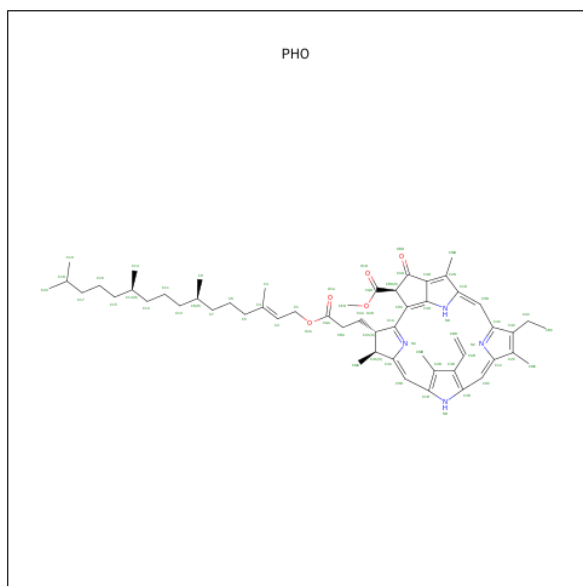
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			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: C₂₄H₄₆O₁₁).



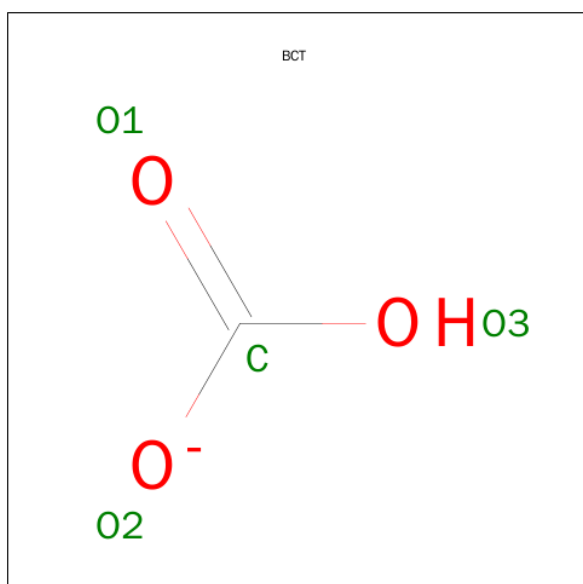
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total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

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



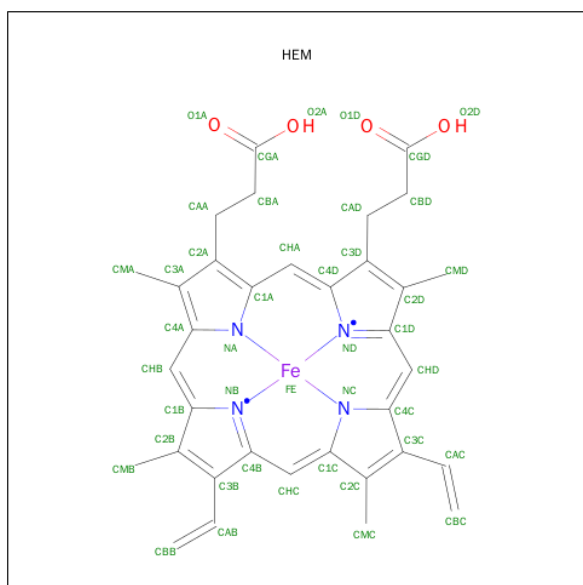
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- 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

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

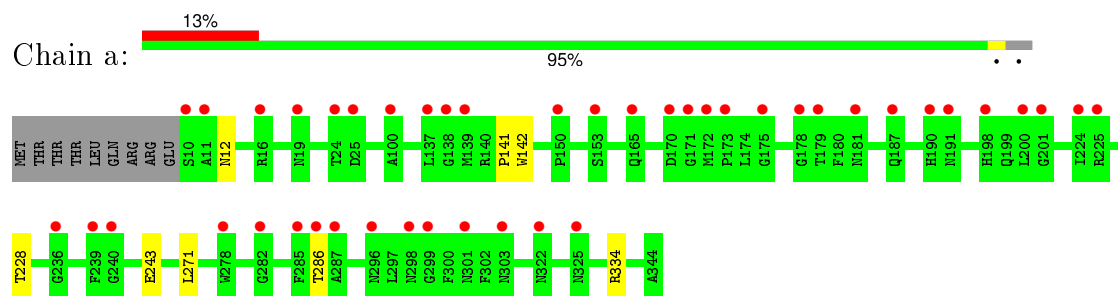
3 Residue-property plots

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.

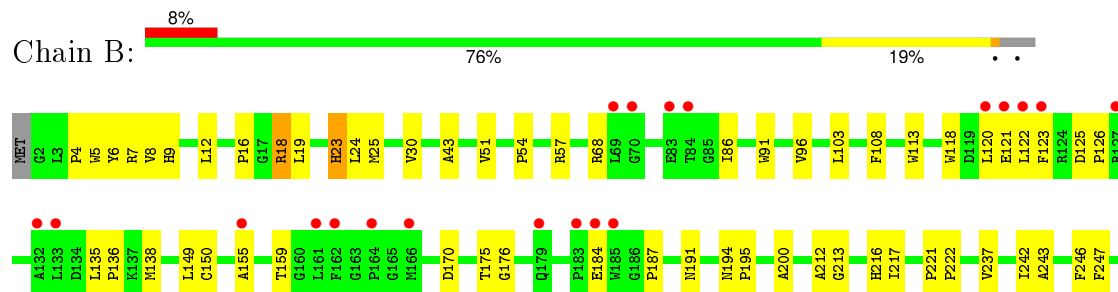
• Molecule 1: Photosystem Q(B) protein 1

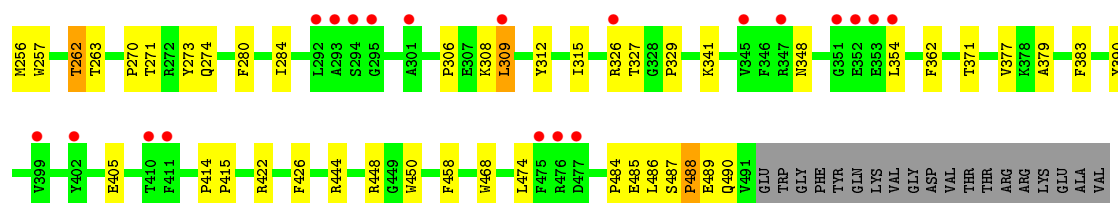


• Molecule 1: Photosystem Q(B) protein 1



• Molecule 2: Photosystem II core light harvesting protein

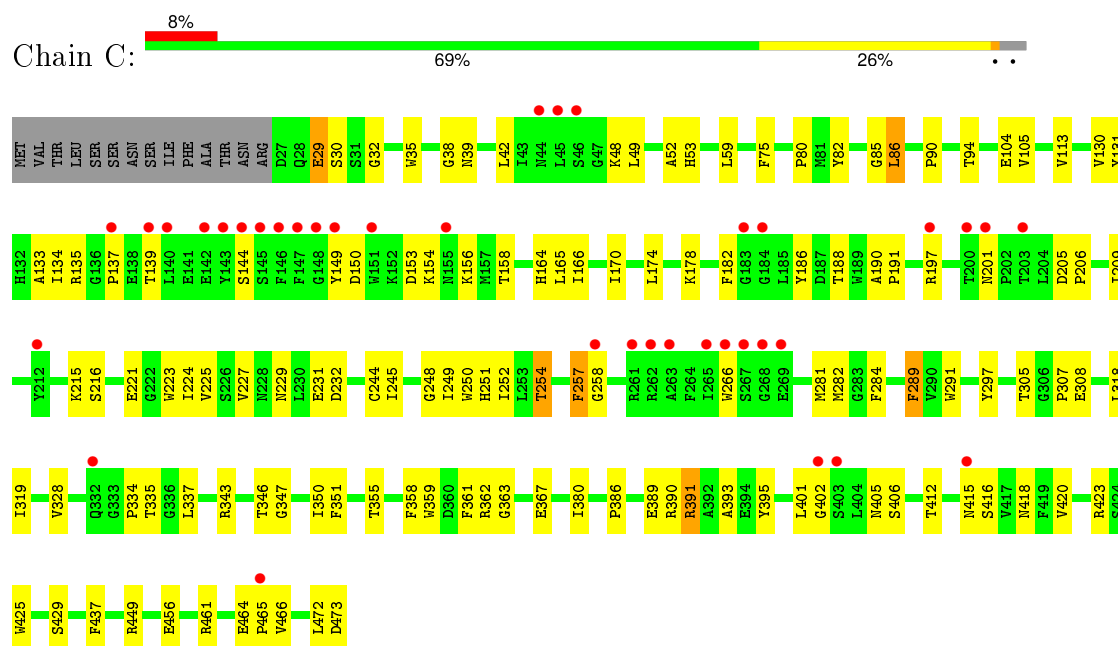




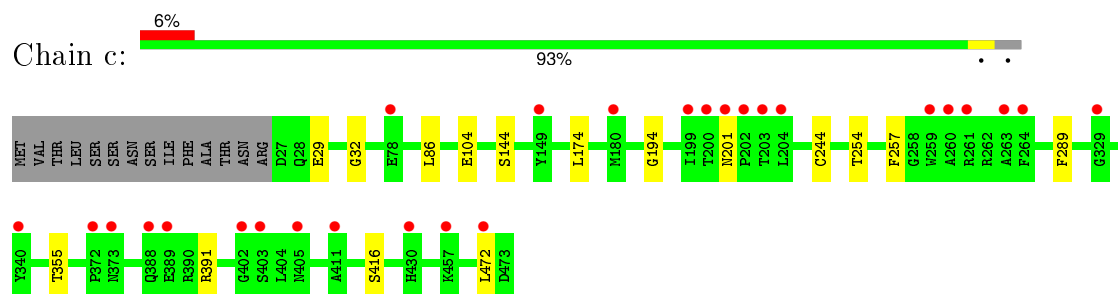
• Molecule 2: Photosystem II core light harvesting protein



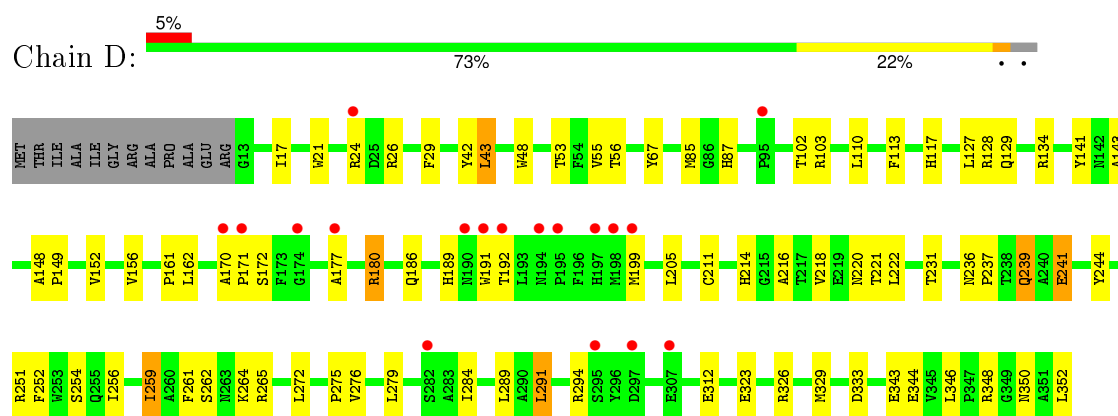
• Molecule 3: Photosystem II CP43 protein



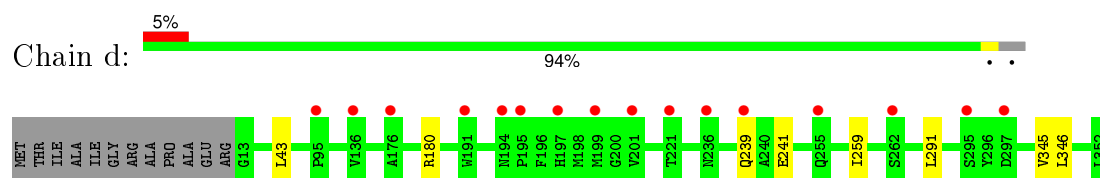
• Molecule 3: Photosystem II CP43 protein



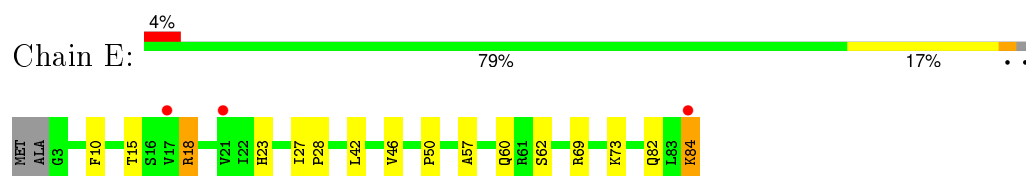
• Molecule 4: Photosystem II D2 protein



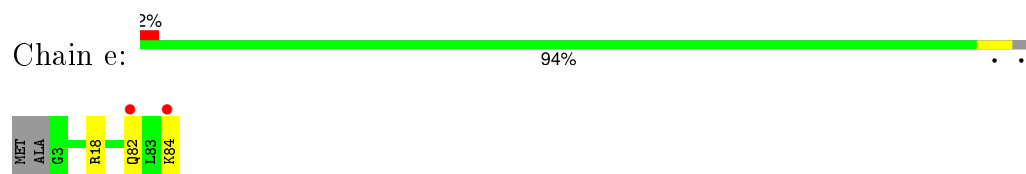
- Molecule 4: Photosystem II D2 protein



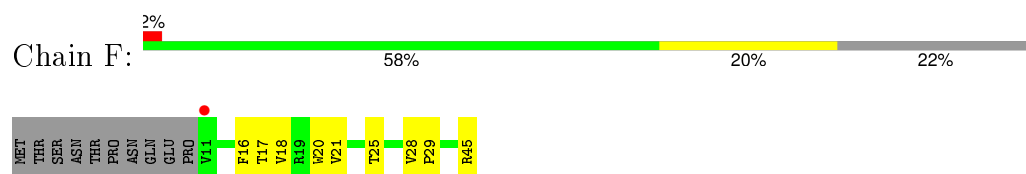
- Molecule 5: Cytochrome b559 subunit alpha



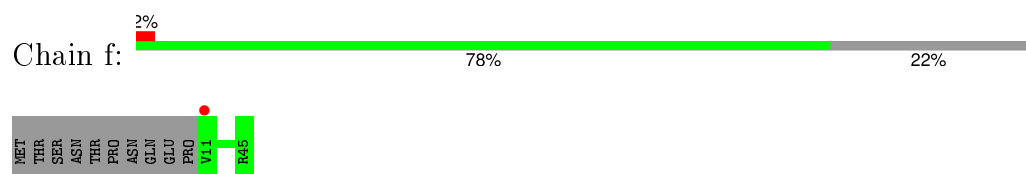
- Molecule 5: Cytochrome b559 subunit alpha



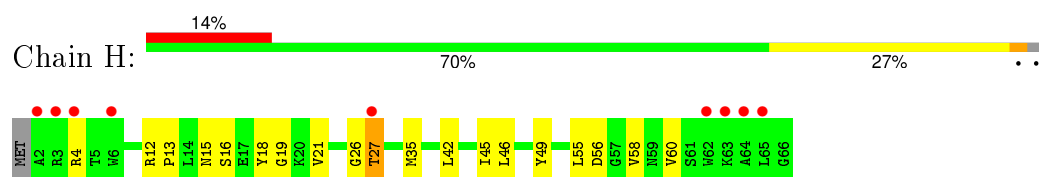
- Molecule 6: Cytochrome b559 subunit beta



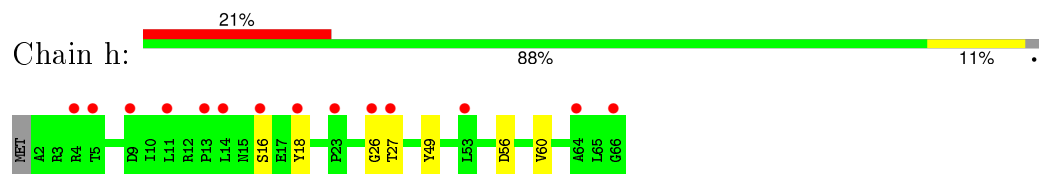
- Molecule 6: Cytochrome b559 subunit beta



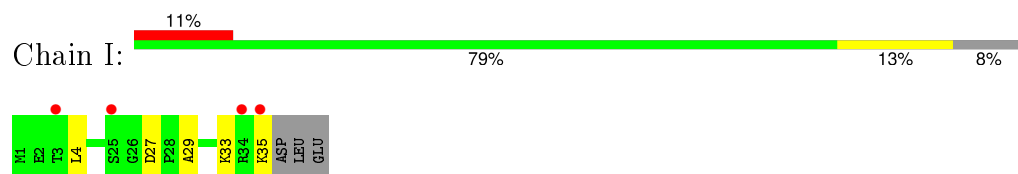
- Molecule 7: Photosystem II reaction center protein H



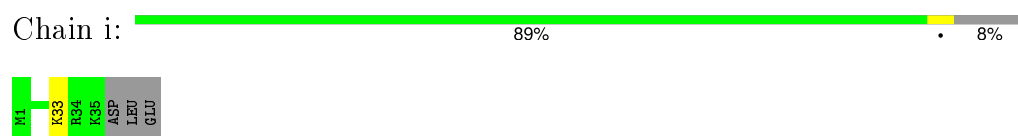
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



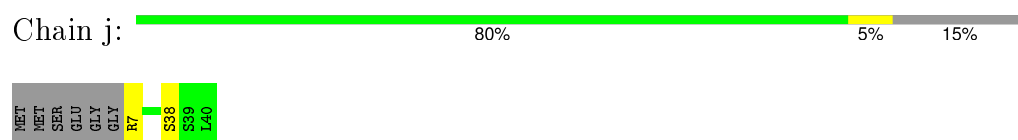
- Molecule 8: Photosystem II reaction center protein I



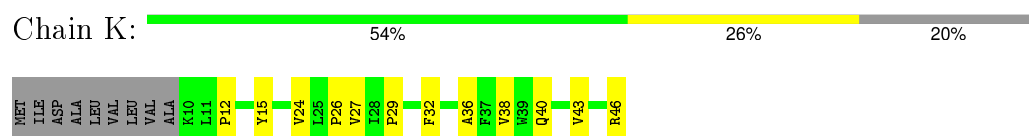
- Molecule 9: Photosystem II reaction center protein J



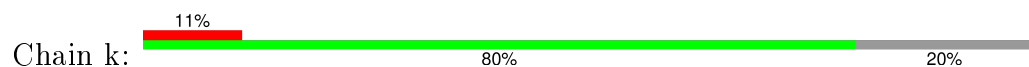
- Molecule 9: Photosystem II reaction center protein J

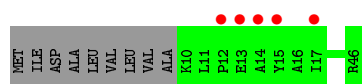


- Molecule 10: Photosystem II reaction center protein K

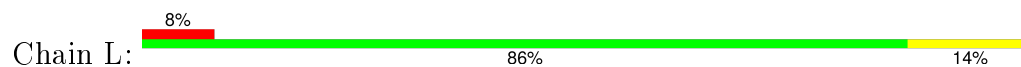


- Molecule 10: Photosystem II reaction center protein K

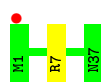




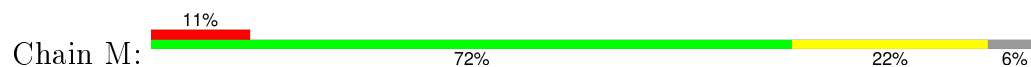
- Molecule 11: Photosystem II reaction center protein L



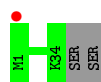
- Molecule 11: Photosystem II reaction center protein L



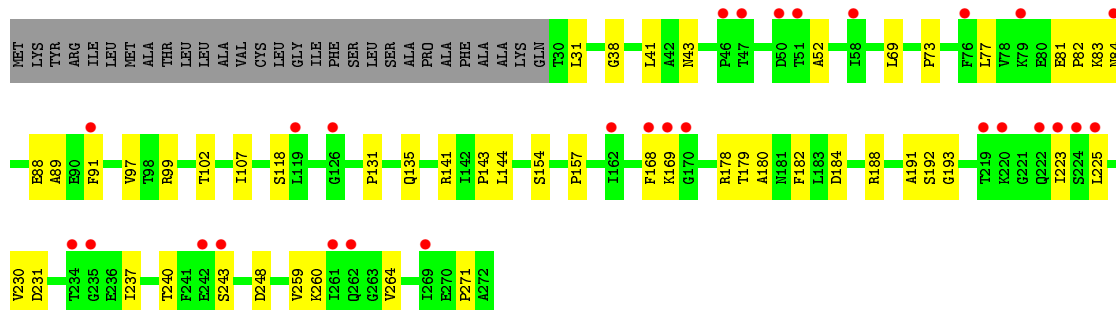
- Molecule 12: Photosystem II reaction center protein M



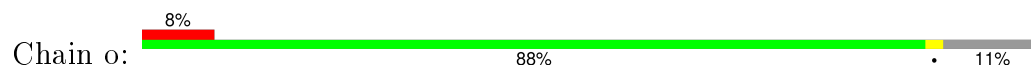
- Molecule 12: Photosystem II reaction center protein M

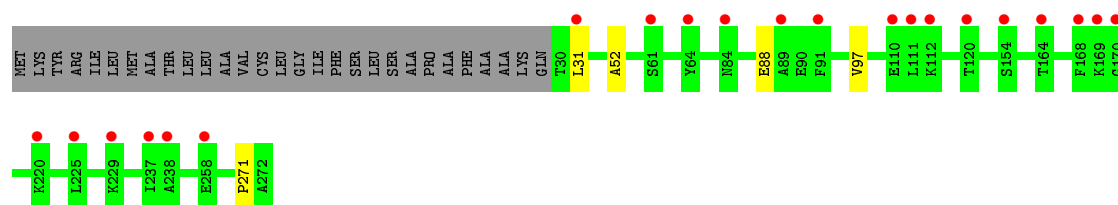


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

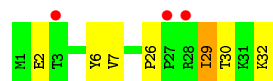
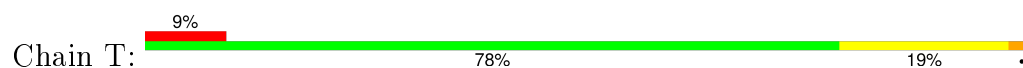


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

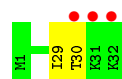




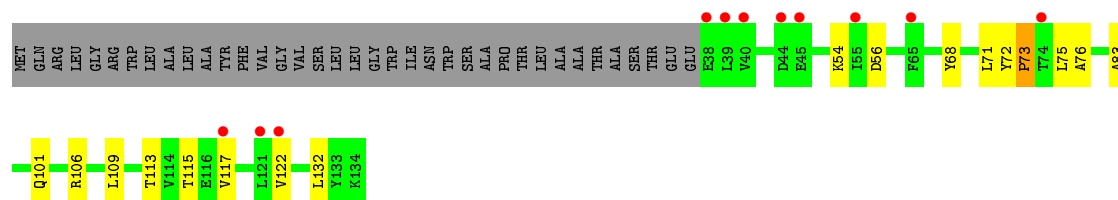
- Molecule 14: Photosystem II reaction center protein T



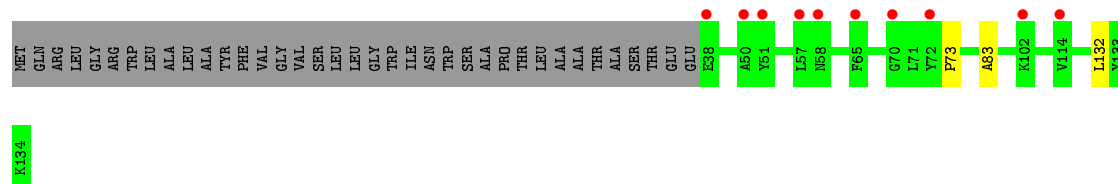
- Molecule 14: Photosystem II reaction center protein T



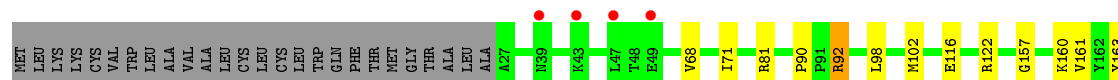
- Molecule 15: Photosystem II 12 kDa extrinsic protein



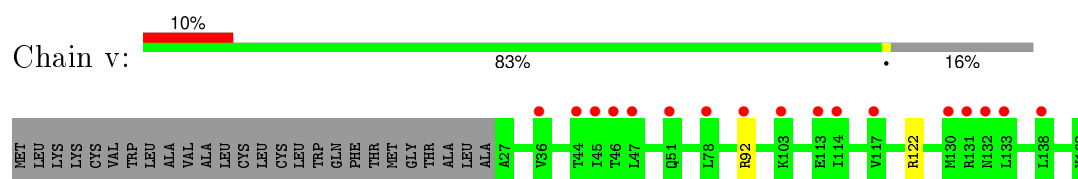
- Molecule 15: Photosystem II 12 kDa extrinsic protein



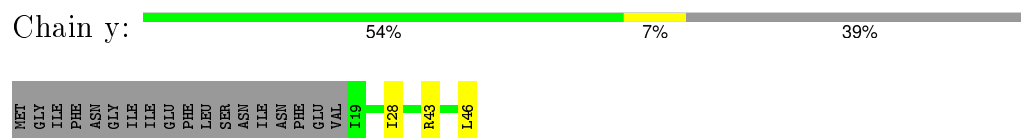
- Molecule 16: Cytochrome c-550



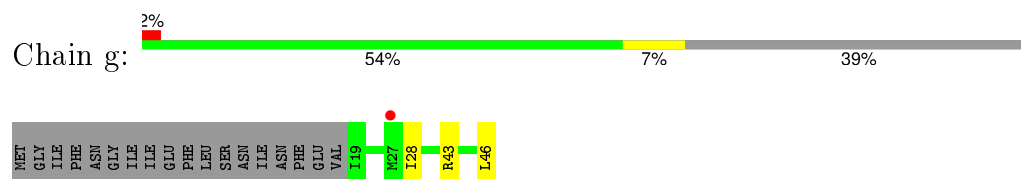
- Molecule 16: Cytochrome c-550



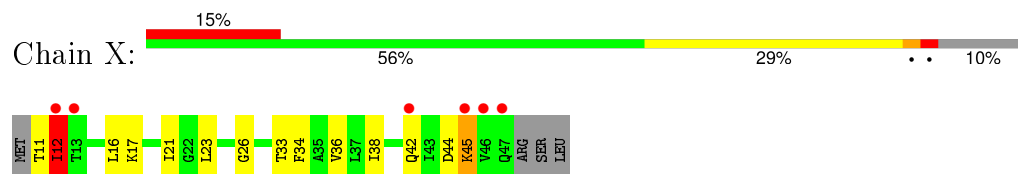
- Molecule 17: Photosystem II reaction center protein Ycf12



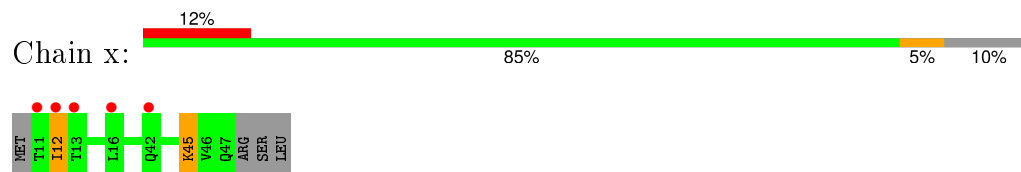
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



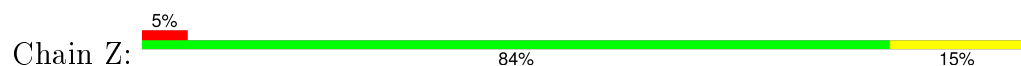
There are no outlier residues recorded for this chain.

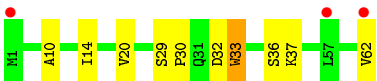
- Molecule 19: Photosystem II reaction center protein Y



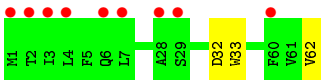
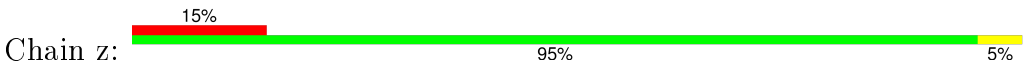
There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.88Å 229.03Å 307.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 4.90 72.93 – 4.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (72.93-4.90) 97.8 (72.93-4.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.281 , 0.292 0.296 , 0.292	Depositor DCC
R_{free} test set	2096 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	173.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 154.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 42966 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, PHO, DGD, CL, 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	0.46	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.21	0/255	0.40	0/346
9	j	0.21	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	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.24	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.43	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	0.21	0/202	0.46	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	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	85	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	89	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	88	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	12	0
5	e	666	0	651	0	0
6	F	282	0	291	7	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	3	0
8	i	286	0	308	0	0
9	J	249	0	262	7	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	5	0
11	l	304	0	316	0	0
12	M	267	0	289	8	0
12	m	267	0	289	0	0
13	O	1845	0	1801	31	0
13	o	1845	0	1801	0	0
14	T	275	0	288	6	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	10	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	6	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	46	0
22	B	975	0	1080	97	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	5	0
23	D	55	0	80	12	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	12	0
24	C	80	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	40	0	56	3	0
24	H	40	0	56	1	0
24	J	40	0	56	2	0
24	K	40	0	56	3	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	1	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	3	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	3	0
27	D	143	0	196	11	0
27	E	44	0	58	2	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	42	0	54	0	0
27	b	49	0	68	0	0
27	c	93	0	126	0	0
27	d	143	0	196	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	l	51	0	72	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	10	0	0	0	0
30	A	105	0	147	8	0
30	B	90	0	111	5	0
30	F	45	0	54	3	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	183	0	0
31	d	31	0	35	0	0
31	i	35	0	46	0	0
32	D	128	0	148	13	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	51373	595	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 595 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	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.82
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.53	0.80
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.80

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	312 (94%)	17 (5%)	4 (1%)	16	62
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	16	62
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	24	69
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	30	74
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	21	67
3	c	445/461 (96%)	405 (91%)	35 (8%)	5 (1%)	17	64
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%)	27 (82%)	6 (18%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	43
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	43
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	51
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9	51
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	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%)	4678 (91%)	404 (8%)	56 (1%)	17	64

5 of 56 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
13	O	52	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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%)	269 (98%)	6 (2%)	60	84
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	55
7	h	53/55 (96%)	49 (92%)	4 (8%)	17	55
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	71
9	j	24/28 (86%)	23 (96%)	1 (4%)	36	71
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	92
13	o	202/228 (89%)	200 (99%)	2 (1%)	82	92
14	T	29/29 (100%)	28 (97%)	1 (3%)	44	76
14	t	29/29 (100%)	28 (97%)	1 (3%)	44	76
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%)	4141 (98%)	103 (2%)	57	83

5 of 103 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	243	GLU

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

Mol	Chain	Res	Type
1	A	241	GLN
4	D	117	HIS
4	d	117	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	0.94	3 (5%)	61,113,113	1.18	6 (9%)
22	CLA	A	403	-	55,73,73	0.95	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	1.18	7 (11%)
23	PL9	A	406	-	45,45,55	1.10	3 (6%)	56,57,69	1.60	11 (19%)
24	BCR	A	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	7 (12%)
25	DGD	A	408	-	57,57,67	0.91	0	71,71,81	1.43	8 (11%)
26	LHG	A	409	-	38,38,48	0.68	0	39,44,54	1.19	3 (7%)
27	LMG	A	410	-	51,51,55	0.74	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	0.95	3 (6%)	58,62,65	1.99	9 (15%)
30	SQD	A	414	-	53,54,54	0.94	3 (5%)	61,65,65	1.66	9 (14%)
27	LMG	A	415	-	42,42,55	0.82	0	50,50,63	1.27	4 (8%)
22	CLA	B	601	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	8 (13%)
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	6 (9%)
22	CLA	B	605	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	6 (9%)
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	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	B	608	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	B	609	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	6 (9%)
22	CLA	B	610	-	55,73,73	1.03	4 (7%)	61,113,113	1.35	7 (11%)
22	CLA	B	611	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	8 (13%)
22	CLA	B	612	-	55,73,73	0.92	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	B	613	-	55,73,73	0.93	3 (5%)	61,113,113	1.22	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	0.95	4 (7%)	61,113,113	1.20	7 (11%)
22	CLA	B	615	-	55,73,73	0.95	4 (7%)	61,113,113	1.18	6 (9%)
24	BCR	B	616	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	6 (10%)
24	BCR	B	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	9 (16%)
24	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	10 (17%)
24	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	8 (14%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	7 (9%)
27	LMG	B	621	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	6 (10%)
30	SQD	B	622	-	42,43,54	1.04	3 (7%)	50,54,65	1.92	9 (18%)
31	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	1.01	2 (4%)
31	LMT	B	624	-	36,36,36	1.08	4 (11%)	47,47,47	1.04	3 (6%)
25	DGD	B	625	-	53,53,67	1.06	4 (7%)	67,67,81	1.34	7 (10%)
30	SQD	B	626	-	46,47,54	1.01	3 (6%)	54,58,65	1.97	9 (16%)
31	LMT	B	627	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
31	LMT	B	628	-	36,36,36	1.11	5 (13%)	47,47,47	1.07	1 (2%)
22	CLA	C	501	-	55,73,73	0.95	3 (5%)	61,113,113	1.16	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	0.94	3 (5%)	61,113,113	1.25	7 (11%)
22	CLA	C	504	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	8 (13%)
22	CLA	C	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	C	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	C	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.26	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	0.96	3 (5%)	61,113,113	1.19	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	8 (13%)
22	CLA	C	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	8 (13%)
24	BCR	C	513	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	10 (17%)
24	BCR	C	514	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	8 (14%)
25	DGD	C	515	-	54,54,67	0.95	2 (3%)	68,68,81	1.28	8 (11%)
25	DGD	C	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.46	13 (16%)
25	DGD	C	517	-	67,67,67	0.88	2 (2%)	81,81,81	1.42	11 (13%)
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	1.27	4 (10%)
22	CLA	C	520	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	C	521	-	48,48,55	0.75	0	56,56,63	1.30	6 (10%)
32	PHO	D	401	-	67,69,69	1.21	9 (13%)	84,99,99	1.01	5 (5%)
32	PHO	D	402	-	67,69,69	1.22	9 (13%)	84,99,99	1.00	4 (4%)
33	BCT	D	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	D	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	D	406	-	55,55,55	1.15	3 (5%)	68,69,69	1.58	15 (22%)
27	LMG	D	407	-	49,49,55	0.75	0	57,57,63	1.32	5 (8%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.38	4 (7%)
25	DGD	D	409	-	64,64,67	0.90	0	78,78,81	1.35	10 (12%)
31	LMT	D	410	-	32,32,36	1.16	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	D	411	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	5 (9%)
27	LMG	E	101	-	44,44,55	0.75	1 (2%)	52,52,63	1.29	5 (9%)
34	HEM	F	101	5,6	30,50,50	2.12	11 (36%)	24,82,82	2.32	9 (37%)
24	BCR	F	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
30	SQD	F	103	-	44,45,54	1.02	3 (6%)	52,56,65	1.77	9 (17%)
22	CLA	H	101	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
24	BCR	H	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	4 (7%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.27	5 (9%)
31	LMT	I	102	-	36,36,36	1.09	5 (13%)	47,47,47	1.08	2 (4%)
23	PL9	J	101	-	35,35,55	1.17	2 (5%)	44,45,69	1.55	6 (13%)
24	BCR	J	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.59	13 (23%)
24	BCR	K	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	9 (16%)
27	LMG	M	101	-	42,42,55	0.85	2 (4%)	50,50,63	1.23	4 (8%)
31	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	2 (4%)
31	LMT	M	103	-	36,36,36	1.11	5 (13%)	47,47,47	1.03	3 (6%)
34	HEM	V	201	16	30,50,50	2.24	11 (36%)	24,82,82	2.23	6 (25%)
30	SQD	a	401	-	53,54,54	0.94	3 (5%)	61,65,65	1.66	9 (14%)
27	LMG	a	402	-	42,42,55	0.82	0	50,50,63	1.26	5 (10%)
22	CLA	a	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	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	1.22	9 (13%)	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	1.18	3 (6%)	56,57,69	1.60	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	a	410	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	7 (12%)
25	DGD	a	411	-	57,57,67	0.91	1 (1%)	71,71,81	1.41	7 (9%)
26	LHG	a	412	-	38,38,48	0.68	1 (2%)	39,44,54	1.20	3 (7%)
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	1.99	9 (15%)
25	DGD	b	601	-	53,53,67	1.04	4 (7%)	67,67,81	1.36	7 (10%)
30	SQD	b	602	-	46,47,54	1.01	4 (8%)	54,58,65	1.98	9 (16%)
31	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	0.98	1 (2%)
31	LMT	b	604	-	36,36,36	1.11	5 (13%)	47,47,47	1.06	1 (2%)
22	CLA	b	605	-	55,73,73	0.95	4 (7%)	61,113,113	1.21	8 (13%)
22	CLA	b	606	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	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	7 (11%)
22	CLA	b	609	-	55,73,73	0.93	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	b	610	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
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	0.95	3 (5%)	61,113,113	1.18	8 (13%)
22	CLA	b	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	b	614	-	55,73,73	1.03	4 (7%)	61,113,113	1.34	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	0.94	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	3 (5%)	61,113,113	1.20	9 (14%)
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	1.08	2 (4%)	56,56,56	1.22	6 (10%)
24	BCR	b	621	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	9 (16%)
24	BCR	b	622	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	11 (19%)
24	BCR	b	623	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
25	DGD	b	624	-	59,59,67	0.89	0	73,73,81	1.36	6 (8%)
27	LMG	b	625	-	49,49,55	0.76	1 (2%)	57,57,63	1.33	6 (10%)
31	LMT	b	626	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
31	LMT	b	627	-	36,36,36	1.07	4 (11%)	47,47,47	1.03	2 (4%)
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	0.96	4 (7%)	61,113,113	1.22	8 (13%)
22	CLA	c	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.23	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	504	-	55,73,73	0.95	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	7 (11%)
22	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	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	1.18	6 (9%)
22	CLA	c	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	c	510	3	55,73,73	0.93	3 (5%)	61,113,113	1.21	6 (9%)
22	CLA	c	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	c	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	7 (11%)
24	BCR	c	513	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	11 (19%)
24	BCR	c	514	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	8 (14%)
25	DGD	c	515	-	54,54,67	0.94	1 (1%)	68,68,81	1.29	7 (10%)
25	DGD	c	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.45	13 (16%)
25	DGD	c	517	-	67,67,67	0.87	2 (2%)	81,81,81	1.42	8 (9%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.29	6 (11%)
26	LHG	c	519	-	36,36,48	0.72	0	37,42,54	1.26	4 (10%)
22	CLA	c	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
24	BCR	c	521	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	9 (16%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
32	PHO	d	401	-	67,69,69	1.20	9 (13%)	84,99,99	1.00	3 (3%)
30	SQD	d	402	-	42,43,54	1.03	3 (7%)	50,54,65	1.92	10 (20%)
33	BCT	d	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	404	-	55,73,73	0.96	4 (7%)	61,113,113	1.19	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	1.15	3 (5%)	68,69,69	1.59	15 (22%)
27	LMG	d	407	-	49,49,55	0.76	0	57,57,63	1.30	4 (7%)
27	LMG	d	408	-	48,48,55	0.75	0	56,56,63	1.38	4 (7%)
25	DGD	d	409	-	64,64,67	0.91	1 (1%)	78,78,81	1.36	10 (12%)
31	LMT	d	410	-	32,32,36	1.15	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	d	411	-	46,46,55	0.77	0	54,54,63	1.30	5 (9%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.29	5 (9%)
34	HEM	f	101	5,6	30,50,50	2.10	12 (40%)	24,82,82	2.33	9 (37%)
24	BCR	f	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
30	SQD	f	103	-	44,45,54	1.02	3 (6%)	52,56,65	1.78	9 (17%)
24	BCR	g	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.31	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	h	101	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
27	LMG	i	101	-	43,43,55	0.81	0	51,51,63	1.27	5 (9%)
31	LMT	i	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.06	2 (4%)
23	PL9	j	101	-	35,35,55	1.13	1 (2%)	44,45,69	1.55	6 (13%)
24	BCR	j	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.58	13 (23%)
27	LMG	l	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.34	6 (10%)
27	LMG	m	101	-	42,42,55	0.85	2 (4%)	50,50,63	1.25	4 (8%)
34	HEM	v	201	16	30,50,50	2.23	11 (36%)	24,82,82	2.24	6 (25%)
24	BCR	x	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	5 (8%)
24	BCR	y	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.30	7 (12%)

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
30	SQD	B	622	-	-	1/38/58/69	0/1/1/1
31	LMT	B	623	-	-	0/21/61/61	0/2/2/2
31	LMT	B	624	-	-	0/21/61/61	0/2/2/2
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
27	LMG	C	521	-	-	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
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	-	-	0/44/64/70	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
27	LMG	D	411	-	-	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
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
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
27	LMG	M	101	-	-	1/37/57/70	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
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PL9	d	406	-	-	0/53/73/73	0/1/1/1
27	LMG	d	407	-	-	0/44/64/70	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
27	LMG	d	411	-	-	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	l	101	-	-	0/46/66/70	0/1/1/1
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 496 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-7.31	1.45	1.51
34	v	201	HEM	C3B-C4B	-7.09	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.15	1.46	1.51
34	f	101	HEM	C3B-C4B	-6.09	1.46	1.51
34	F	101	HEM	C3D-C4D	-5.29	1.44	1.51

The worst 5 of 1177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	101	PL9	C7-C3-C2	-6.13	118.34	123.42
23	J	101	PL9	C7-C3-C2	-6.12	118.35	123.42
23	d	406	PL9	C7-C3-C2	-5.83	118.58	123.42
23	A	406	PL9	C7-C3-C2	-5.77	118.63	123.42
23	a	409	PL9	C7-C3-C2	-5.62	118.76	123.42

5 of 209 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C8-O7-C10-C11
25	c	516	DGD	C2G-O2G-C1B-C2B
25	C	516	DGD	C2G-O2G-C1B-C2B
30	B	622	SQD	C45-O47-C7-C8
30	d	402	SQD	C45-O47-C7-C8

There are no ring outliers.

79 monomers are involved in 311 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	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	405	CLA	12	0
23	A	406	PL9	5	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	5	0
27	A	415	LMG	1	0
22	B	601	CLA	1	0
22	B	602	CLA	11	0
22	B	603	CLA	4	0
22	B	604	CLA	9	0
22	B	605	CLA	7	0
22	B	606	CLA	16	0
22	B	607	CLA	11	0
22	B	608	CLA	15	0
22	B	609	CLA	3	0
22	B	610	CLA	5	0
22	B	611	CLA	10	0
22	B	612	CLA	9	0
22	B	613	CLA	5	0
22	B	614	CLA	4	0
22	B	615	CLA	6	0
24	B	616	BCR	6	0
24	B	617	BCR	2	0
24	B	618	BCR	4	0
24	B	619	BCR	1	0
25	B	620	DGD	2	0
27	B	621	LMG	3	0
30	B	622	SQD	3	0
31	B	623	LMT	2	0
25	B	625	DGD	2	0
30	B	626	SQD	2	0
31	B	627	LMT	2	0
31	B	628	LMT	2	0
22	C	501	CLA	7	0
22	C	503	CLA	5	0
22	C	504	CLA	4	0
22	C	505	CLA	3	0
22	C	506	CLA	6	0
22	C	507	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	508	CLA	3	0
22	C	509	CLA	6	0
22	C	510	CLA	9	0
22	C	511	CLA	1	0
22	C	512	CLA	3	0
24	C	513	BCR	7	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	3	0
26	C	519	LHG	3	0
22	C	520	CLA	5	0
32	D	401	PHO	8	0
32	D	402	PHO	5	0
22	D	404	CLA	10	0
22	D	405	CLA	4	0
23	D	406	PL9	12	0
27	D	407	LMG	4	0
27	D	408	LMG	6	0
25	D	409	DGD	1	0
27	D	411	LMG	1	0
27	E	101	LMG	2	0
34	F	101	HEM	4	0
24	F	102	BCR	3	0
30	F	103	SQD	3	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
24	K	102	BCR	3	0
27	M	101	LMG	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.59	31 (9%) 11 10	205, 207, 208, 208	0
1	a	335/344 (97%)	0.61	44 (13%) 5 6	204, 207, 208, 209	0
2	B	490/510 (96%)	0.37	40 (8%) 14 12	205, 207, 208, 208	0
2	b	490/510 (96%)	0.48	47 (9%) 10 9	205, 207, 208, 209	0
3	C	447/461 (96%)	0.41	37 (8%) 14 12	205, 207, 208, 209	0
3	c	447/461 (96%)	0.25	27 (6%) 25 20	206, 207, 208, 209	0
4	D	340/352 (96%)	0.44	18 (5%) 30 25	204, 207, 208, 209	0
4	d	340/352 (96%)	0.40	16 (4%) 35 29	204, 207, 208, 208	0
5	E	82/84 (97%)	0.26	3 (3%) 45 37	205, 207, 208, 208	0
5	e	82/84 (97%)	0.15	2 (2%) 62 54	206, 207, 208, 208	0
6	F	35/45 (77%)	0.03	1 (2%) 55 45	206, 207, 208, 208	0
6	f	35/45 (77%)	-0.37	1 (2%) 55 45	206, 207, 208, 208	0
7	H	65/66 (98%)	0.53	9 (13%) 4 5	206, 207, 208, 209	0
7	h	65/66 (98%)	0.90	14 (21%) 1 3	206, 207, 208, 208	0
8	I	35/38 (92%)	0.62	4 (11%) 7 7	206, 207, 208, 208	0
8	i	35/38 (92%)	-0.04	0 100 100	206, 207, 208, 208	0
9	J	34/40 (85%)	0.11	1 (2%) 55 45	205, 207, 207, 208	0
9	j	34/40 (85%)	-0.42	0 100 100	206, 207, 208, 209	0
10	K	37/46 (80%)	-0.05	0 100 100	206, 207, 208, 208	0
10	k	37/46 (80%)	0.46	5 (13%) 4 6	206, 207, 208, 209	0
11	L	37/37 (100%)	0.68	3 (8%) 15 13	205, 207, 208, 208	0
11	l	37/37 (100%)	0.26	1 (2%) 58 49	206, 207, 208, 209	0
12	M	34/36 (94%)	0.67	4 (11%) 6 7	205, 206, 207, 208	0
12	m	34/36 (94%)	0.32	1 (2%) 55 45	205, 207, 207, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.70	28 (11%) 6 7	205, 207, 208, 209	0
13	o	243/272 (89%)	0.68	21 (8%) 13 12	205, 207, 208, 209	0
14	T	32/32 (100%)	0.24	3 (9%) 11 10	206, 207, 208, 209	0
14	t	32/32 (100%)	0.62	3 (9%) 11 10	205, 206, 208, 208	0
15	U	97/134 (72%)	0.92	11 (11%) 7 7	205, 207, 208, 208	0
15	u	97/134 (72%)	0.78	10 (10%) 9 9	205, 207, 208, 208	0
16	V	137/163 (84%)	0.29	4 (2%) 55 45	205, 207, 208, 208	0
16	v	137/163 (84%)	0.78	17 (12%) 5 7	206, 207, 208, 208	0
17	g	28/46 (60%)	0.27	1 (3%) 46 39	206, 207, 208, 209	0
17	y	28/46 (60%)	-0.01	0 100 100	206, 207, 208, 208	0
18	X	37/41 (90%)	0.73	6 (16%) 3 4	205, 207, 208, 209	0
18	x	37/41 (90%)	1.03	5 (13%) 4 6	206, 207, 208, 208	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.28	3 (4%) 34 28	205, 207, 208, 209	0
20	z	62/62 (100%)	0.87	9 (14%) 3 5	206, 207, 208, 209	0
All	All	5214/5674 (91%)	0.47	430 (8%) 14 12	204, 207, 208, 209	0

The worst 5 of 430 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	7.6
18	x	11	THR	7.2
13	o	169	LYS	6.5
1	a	239	PHE	6.1
7	H	64	ALA	5.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	LMT	i	102	35/35	0.31	1.62	13.57	206,208,209,210	0
27	LMG	C	518	45/55	0.61	0.98	6.09	205,206,208,208	0
23	PL9	J	101	35/55	0.24	0.59	5.85	204,207,208,209	0
24	BCR	C	513	40/40	0.89	0.83	5.85	205,206,207,208	0
23	PL9	j	101	35/55	0.26	0.49	5.81	205,208,209,209	0
24	BCR	a	410	40/40	0.81	0.70	5.59	205,206,207,207	0
24	BCR	c	521	40/40	0.79	1.36	5.43	205,207,208,209	0
24	BCR	b	623	40/40	0.69	0.82	5.26	204,206,207,207	0
24	BCR	B	619	40/40	0.73	0.94	4.84	205,206,207,207	0
33	BCT	d	403	4/4	0.77	1.00	4.36	207,207,207,208	0
24	BCR	y	101	40/40	0.73	0.81	4.08	205,206,207,207	0
27	LMG	c	518	45/55	0.66	0.96	3.91	206,207,208,208	0
22	CLA	a	408	65/65	0.78	0.76	3.85	205,206,207,209	0
24	BCR	c	513	40/40	0.78	1.04	3.83	204,206,207,208	0
25	DGD	D	409	63/66	0.68	0.82	3.61	205,208,209,211	0
22	CLA	b	605	65/65	0.50	1.07	3.60	205,208,209,209	0
31	LMT	I	102	35/35	0.38	0.89	3.50	205,207,209,210	0
22	CLA	B	601	65/65	0.61	1.07	3.47	206,207,208,209	0
31	LMT	b	627	35/35	0.69	1.25	3.32	205,208,210,210	0
24	BCR	g	101	40/40	0.51	0.74	3.29	204,206,207,207	0
22	CLA	B	609	65/65	0.90	0.68	3.09	205,206,208,208	0
22	CLA	D	405	65/65	0.86	0.62	3.09	205,206,207,207	0
24	BCR	H	102	40/40	0.69	1.01	3.02	206,207,208,208	0
31	LMT	D	410	31/35	0.74	0.76	2.76	206,208,208,209	0
25	DGD	B	625	52/66	0.71	0.65	2.75	205,208,210,210	0
24	BCR	f	102	40/40	0.60	0.47	2.74	206,206,207,208	0
31	LMT	B	624	35/35	0.79	0.56	2.72	205,207,210,210	0
30	SQD	B	626	47/54	0.66	0.68	2.64	204,207,209,211	0
22	CLA	b	607	65/65	0.80	0.56	2.63	205,206,207,209	0
22	CLA	B	603	65/65	0.74	0.55	2.56	204,206,207,208	0
25	DGD	d	409	63/66	0.70	0.77	2.52	205,208,210,211	0
22	CLA	b	606	65/65	0.83	0.77	2.51	205,206,207,207	0
24	BCR	F	102	40/40	0.58	0.52	2.44	205,206,207,208	0
22	CLA	B	611	65/65	0.88	0.51	2.34	204,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	B	604	65/65	0.86	0.66	2.33	205,207,208,208	0
22	CLA	c	501	65/65	0.84	0.63	2.31	205,207,208,209	0
22	CLA	c	512	65/65	0.75	0.72	2.28	205,207,208,208	0
24	BCR	K	102	40/40	0.77	0.95	2.26	204,207,208,209	0
22	CLA	A	405	65/65	0.79	0.65	2.24	204,206,208,208	0
30	SQD	d	402	43/54	0.65	1.13	2.19	205,207,209,211	0
27	LMG	e	101	44/55	0.74	0.42	2.17	204,207,208,209	0
27	LMG	M	101	42/55	0.74	0.49	2.04	205,207,209,210	0
24	BCR	A	407	40/40	0.78	0.56	2.01	205,206,207,208	0
27	LMG	D	411	46/55	0.75	0.42	1.99	205,206,207,208	0
24	BCR	c	514	40/40	0.72	0.86	1.98	205,206,207,208	0
27	LMG	E	101	44/55	0.39	0.77	1.97	204,207,209,210	0
22	CLA	b	613	65/65	0.77	0.87	1.95	205,207,208,209	0
22	CLA	c	511	65/65	0.86	0.75	1.90	205,207,208,209	0
30	SQD	a	401	54/54	0.85	0.50	1.88	205,207,209,211	0
22	CLA	B	608	65/65	0.88	0.62	1.84	205,207,208,209	0
22	CLA	c	506	65/65	0.86	0.73	1.79	206,207,208,208	0
22	CLA	B	614	65/65	0.86	0.89	1.77	205,206,207,208	0
22	CLA	C	506	65/65	0.74	0.86	1.77	204,207,207,208	0
22	CLA	b	608	65/65	0.86	0.61	1.76	205,206,207,208	0
22	CLA	c	510	65/65	0.71	0.61	1.75	206,207,208,209	0
22	CLA	c	508	65/65	0.80	0.55	1.70	205,207,208,208	0
22	CLA	C	511	65/65	0.84	1.13	1.69	205,207,208,208	0
24	BCR	C	514	40/40	0.70	0.86	1.66	205,206,207,207	0
27	LMG	a	402	42/55	0.56	0.47	1.62	204,207,209,209	0
27	LMG	m	101	42/55	0.74	0.58	1.55	203,207,208,209	0
22	CLA	c	503	65/65	0.77	0.59	1.55	205,207,208,208	0
25	DGD	b	601	52/66	0.79	0.46	1.49	204,207,208,209	0
31	LMT	d	410	31/35	0.52	0.72	1.45	206,208,209,210	0
30	SQD	F	103	45/54	0.70	0.85	1.41	205,207,209,210	0
34	HEM	F	101	43/43	0.90	0.54	1.41	205,207,208,209	0
31	LMT	B	627	35/35	0.76	0.60	1.37	205,207,209,209	0
22	CLA	C	512	65/65	0.77	0.93	1.34	205,207,208,209	0
22	CLA	d	405	65/65	0.81	0.51	1.33	204,206,207,208	0
31	LMT	b	603	35/35	0.67	0.56	1.33	205,207,208,209	0
22	CLA	B	605	65/65	0.83	0.80	1.33	205,206,207,208	0
22	CLA	c	502	65/65	0.54	0.65	1.33	205,207,208,208	0
24	BCR	B	616	40/40	0.60	0.54	1.32	205,206,207,207	0
22	CLA	b	609	65/65	0.86	0.64	1.30	205,207,208,209	0
24	BCR	B	617	40/40	0.71	0.43	1.28	204,206,207,208	0
22	CLA	C	503	65/65	0.84	0.45	1.28	205,207,207,208	0
22	CLA	C	501	65/65	0.90	0.46	1.25	205,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	SQD	f	103	45/54	0.86	0.60	1.24	205,207,208,210	0
22	CLA	h	101	65/65	0.87	0.52	1.23	204,207,208,209	0
27	LMG	A	415	42/55	0.60	0.45	1.22	204,207,208,209	0
22	CLA	b	615	65/65	0.89	0.37	1.21	205,206,207,208	0
23	PL9	A	406	45/55	0.52	0.53	1.14	205,206,207,208	0
22	CLA	C	508	65/65	0.79	0.85	1.13	205,206,207,208	0
31	LMT	b	604	35/35	0.69	0.48	1.08	205,207,209,209	0
22	CLA	C	502	65/65	0.73	0.50	1.04	205,206,207,208	0
31	LMT	B	628	35/35	0.65	0.51	1.01	204,207,209,209	0
24	BCR	J	102	40/40	0.52	0.37	0.97	205,207,208,209	0
22	CLA	B	615	65/65	0.86	0.80	0.97	205,206,208,208	0
34	HEM	V	201	43/43	0.88	0.50	0.95	203,206,207,208	0
25	DGD	A	408	56/66	0.63	0.50	0.93	206,207,209,210	0
27	LMG	d	411	46/55	0.88	0.30	0.91	204,206,207,208	0
22	CLA	B	613	65/65	0.72	0.50	0.90	205,206,207,208	0
22	CLA	b	616	65/65	0.95	0.34	0.90	204,206,208,209	0
22	CLA	B	602	65/65	0.92	0.52	0.86	204,206,208,209	0
34	HEM	v	201	43/43	0.87	0.71	0.84	205,207,207,208	0
22	CLA	B	607	65/65	0.86	0.43	0.83	205,206,207,209	0
22	CLA	b	619	65/65	0.69	0.78	0.82	205,207,208,209	0
27	LMG	l	101	51/55	0.70	0.40	0.81	205,206,208,208	0
22	CLA	c	505	65/65	0.85	0.56	0.78	204,206,208,208	0
24	BCR	x	101	40/40	0.62	0.88	0.78	205,207,208,208	0
22	CLA	b	618	65/65	0.83	0.77	0.76	205,207,208,208	0
26	LHG	c	519	37/49	0.66	0.36	0.69	205,207,211,214	0
30	SQD	B	622	43/54	0.80	0.46	0.68	205,207,209,212	0
22	CLA	b	611	65/65	0.86	0.43	0.68	205,206,207,208	0
23	PL9	a	409	45/55	0.73	0.36	0.67	204,206,207,208	0
30	SQD	b	602	47/54	0.77	0.39	0.67	205,207,209,212	0
22	CLA	C	505	65/65	0.79	0.56	0.65	205,206,207,208	0
30	SQD	A	414	54/54	0.83	0.40	0.64	204,207,208,210	0
22	CLA	b	612	65/65	0.87	0.60	0.63	205,206,207,209	0
22	CLA	b	617	65/65	0.81	0.41	0.59	205,206,208,209	0
22	CLA	C	510	65/65	0.83	0.49	0.56	205,206,207,208	0
34	HEM	f	101	43/43	0.92	0.30	0.40	206,207,207,208	0
24	BCR	b	621	40/40	0.78	0.34	0.40	204,206,207,207	0
24	BCR	b	622	40/40	0.83	0.31	0.38	204,206,207,207	0
24	BCR	B	618	40/40	0.87	0.29	0.38	204,205,207,207	0
27	LMG	C	521	48/55	0.73	0.34	0.36	204,206,207,208	0
24	BCR	j	102	40/40	0.68	0.29	0.34	206,207,209,209	0
22	CLA	H	101	65/65	0.84	0.41	0.29	205,206,207,208	0
22	CLA	b	614	65/65	0.91	0.30	0.29	205,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	a	404	65/65	0.83	0.58	0.26	205,206,207,208	0
27	LMG	d	408	48/55	0.75	0.40	0.25	204,206,207,208	0
22	CLA	A	403	65/65	0.89	0.58	0.24	204,206,207,207	0
22	CLA	a	405	65/65	0.81	0.58	0.20	202,206,207,208	0
25	DGD	a	411	56/66	0.74	0.36	0.14	205,207,209,209	0
22	CLA	c	509	65/65	0.86	0.37	0.14	204,206,208,209	0
30	SQD	A	413	51/54	0.76	0.33	0.12	205,207,208,208	0
22	CLA	C	504	65/65	0.83	0.39	0.10	205,206,207,207	0
24	BCR	b	620	40/40	0.92	0.34	0.09	205,206,207,208	0
22	CLA	c	504	65/65	0.85	0.33	0.08	205,207,208,208	0
25	DGD	b	624	58/66	0.85	0.34	0.06	205,206,207,208	0
27	LMG	c	522	48/55	0.81	0.29	0.02	205,206,207,208	0
23	PL9	D	406	55/55	0.57	0.43	-0.05	204,206,207,207	0
32	PHO	d	401	64/64	0.70	0.43	-0.06	204,206,207,207	0
22	CLA	A	402	65/65	0.90	0.45	-0.06	205,206,207,208	0
22	CLA	c	507	65/65	0.89	0.31	-0.10	205,207,208,208	0
25	DGD	c	515	53/66	0.88	0.37	-0.16	205,207,208,209	0
22	CLA	C	509	65/65	0.87	0.35	-0.17	205,206,207,208	0
30	SQD	a	415	51/54	0.81	0.30	-0.18	205,206,208,208	0
22	CLA	C	507	65/65	0.88	0.30	-0.26	205,206,208,210	0
33	BCT	D	403	4/4	0.93	0.38	-0.31	206,206,206,206	0
25	DGD	C	517	66/66	0.67	0.36	-0.33	205,206,207,208	0
23	PL9	d	406	55/55	0.68	0.37	-0.36	204,206,207,208	0
32	PHO	D	402	64/64	0.77	0.34	-0.37	205,206,207,208	0
27	LMG	A	410	51/55	0.80	0.32	-0.41	204,206,207,208	0
25	DGD	B	620	58/66	0.87	0.31	-0.45	203,206,208,209	0
26	LHG	A	409	39/49	0.90	0.28	-0.46	205,206,208,209	0
29	OEX	A	412	10/10	0.96	0.44	-0.46	198,204,206,206	0
29	OEX	a	414	10/10	0.95	0.48	-0.46	198,203,205,207	0
26	LHG	C	519	37/49	0.73	0.38	-0.50	204,207,210,212	0
27	LMG	D	408	48/55	0.90	0.26	-0.50	202,206,208,208	0
32	PHO	a	407	64/64	0.82	0.28	-0.55	205,207,207,208	0
22	CLA	d	404	65/65	0.82	0.40	-0.55	204,206,207,207	0
32	PHO	D	401	64/64	0.82	0.32	-0.56	203,206,207,208	0
22	CLA	B	610	65/65	0.86	0.33	-0.59	205,206,207,207	0
25	DGD	c	517	66/66	0.77	0.31	-0.63	204,206,207,208	0
22	CLA	B	612	65/65	0.91	0.28	-0.63	204,206,207,207	0
22	CLA	c	520	65/65	0.90	0.27	-0.66	205,207,207,208	0
22	CLA	a	406	65/65	0.79	0.35	-0.67	205,207,208,209	0
26	LHG	a	412	39/49	0.81	0.28	-0.69	205,207,208,210	0
22	CLA	D	404	65/65	0.90	0.38	-0.69	203,206,207,208	0
22	CLA	A	404	65/65	0.86	0.35	-0.71	204,206,207,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	DGD	C	515	53/66	0.89	0.27	-0.76	204,206,207,208	0
22	CLA	C	520	65/65	0.81	0.30	-0.77	205,207,208,209	0
31	LMT	M	103	35/35	0.79	0.40	-0.81	205,206,208,210	0
31	LMT	M	102	35/35	0.68	0.39	-0.82	205,207,208,209	0
22	CLA	b	610	65/65	0.86	0.30	-0.91	205,206,207,208	0
27	LMG	b	625	49/55	0.78	0.29	-1.02	205,206,207,208	0
25	DGD	C	516	62/66	0.84	0.26	-1.13	204,206,208,208	0
22	CLA	B	606	65/65	0.90	0.28	-1.14	205,206,207,208	0
25	DGD	c	516	62/66	0.88	0.25	-1.16	205,207,208,209	0
27	LMG	D	407	49/55	0.78	0.27	-1.17	205,206,207,208	0
27	LMG	d	407	49/55	0.92	0.24	-1.22	205,206,207,207	0
28	CL	A	411	1/1	0.85	0.27	-1.26	207,207,207,207	0
21	FE2	a	403	1/1	0.78	0.28	-1.31	211,211,211,211	0
27	LMG	B	621	49/55	0.85	0.26	-1.46	204,206,207,208	0
28	CL	a	413	1/1	0.81	0.20	-3.00	204,204,204,204	0
21	FE2	A	401	1/1	0.88	0.17	-3.33	206,206,206,206	0
27	LMG	i	101	43/55	0.77	0.79	-	205,207,209,209	0
31	LMT	b	626	35/35	0.62	0.61	-	205,208,210,210	0
31	LMT	B	623	35/35	0.64	0.79	-	205,208,209,210	0
35	CA	k	101	1/1	0.55	0.23	-	204,204,204,204	0
35	CA	K	101	1/1	0.51	0.36	-	210,210,210,210	0
35	CA	o	301	1/1	0.55	1.07	-	209,209,209,209	0
35	CA	O	301	1/1	0.44	0.28	-	207,207,207,207	0
27	LMG	I	101	43/55	0.68	0.94	-	204,207,209,210	0

6.5 Other polymers [i](#)

There are no such residues in this entry.