



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:45 PM GMT

PDB ID : 4IXR  
Title : RT fs X-ray diffraction of Photosystem II, first illuminated state  
Authors : Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.  
Deposited on : 2013-01-27  
Resolution : 5.90 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](mailto: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.

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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

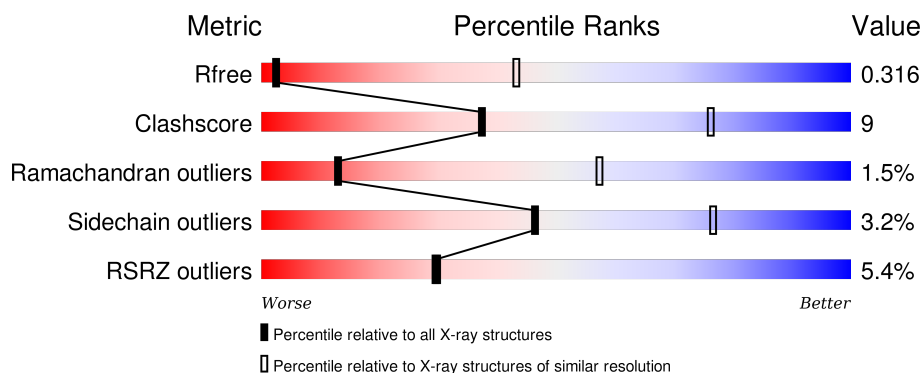
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.90 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	1000 (8.00-3.66)
Clashscore	102246	1048 (8.00-3.70)
Ramachandran outliers	100387	1021 (8.00-3.66)
Sidechain outliers	100360	1010 (8.00-3.64)
RSRZ outliers	91569	1015 (8.00-3.64)

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  $\geq 3$ , 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	360	<div> <div>3%</div> <div>61%</div> <div>31%</div> <div>7%</div> </div>
1	a	360	<div> <div>%</div> <div>91%</div> <div>7%</div> </div>
2	B	510	<div> <div>6%</div> <div>67%</div> <div>27%</div> <div>• •</div> </div>
2	b	510	<div> <div>7%</div> <div>93%</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	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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	BCT	d	401	-	-	-	X
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	X	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	X
23	CLA	B	601	X	-	-	X
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	X
23	CLA	B	604	X	-	-	X
23	CLA	B	605	X	-	-	X
23	CLA	B	606	X	-	-	X
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	X
23	CLA	B	609	X	-	-	X
23	CLA	B	610	X	-	-	X
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	X
23	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	X
23	CLA	B	616	X	-	-	X
23	CLA	C	501	X	-	-	X
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	X
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	X
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	X
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	X
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	X
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	X
23	CLA	b	605	X	-	-	X
23	CLA	b	606	X	-	-	X
23	CLA	b	607	X	-	-	X
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	X
23	CLA	b	610	X	-	-	X
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	X
23	CLA	b	613	X	-	-	X
23	CLA	b	614	X	-	-	X
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	X
23	CLA	b	620	X	-	-	X
23	CLA	c	501	X	-	-	X
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	X
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	X
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	X
23	CLA	c	510	X	-	-	X
23	CLA	c	511	X	-	-	X
23	CLA	c	512	X	-	-	X
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	X
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	a	410	-	-	-	X
25	PL9	j	101	-	-	-	X
26	OEC	A	409	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	514	-	-	-	X
27	BCR	C	515	-	-	-	X
27	BCR	C	516	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	622	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	h	101	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	y	101	-	-	-	X
27	BCR	z	101	-	-	-	X
28	DGD	B	627	-	-	-	X
28	DGD	C	519	-	-	-	X
28	DGD	D	409	-	-	-	X
28	DGD	b	602	-	-	-	X
28	DGD	d	409	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	414	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	D	408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	b	601	-	-	-	X
30	SQD	d	408	-	-	-	X
30	SQD	f	102	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	521	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	519	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	101	-	-	-	X
31	LMG	k	103	-	-	-	X
32	CL	A	416	-	-	-	X
32	CL	a	418	-	-	-	X
33	LMT	B	625	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	B	629	-	-	-	X
33	LMT	D	410	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	M	102	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	604	-	-	-	X
33	LMT	b	627	-	-	-	X
33	LMT	d	410	-	-	-	X
33	LMT	i	102	-	-	-	X
33	LMT	m	101	-	-	-	X
34	HEM	F	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	f	101	-	-	-	X
34	HEM	v	201	-	-	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 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
			2627	1720	432	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	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 Z.

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

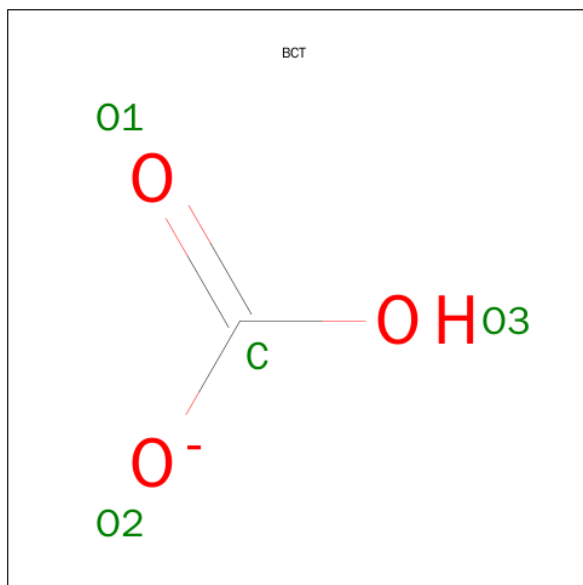
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

- 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 BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			4	1	3		
22	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ).



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

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

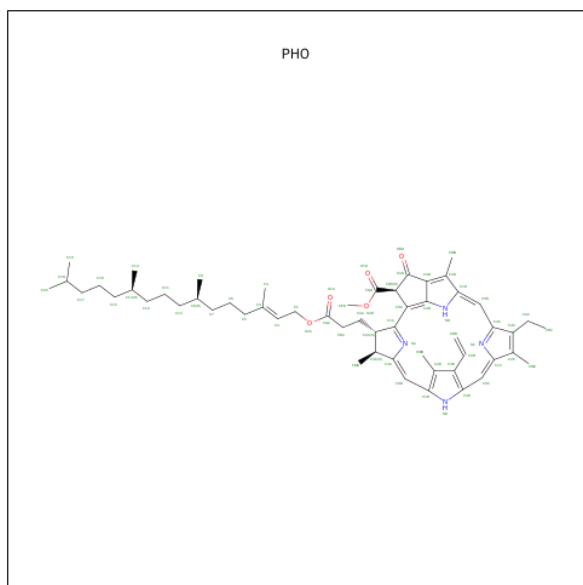
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total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

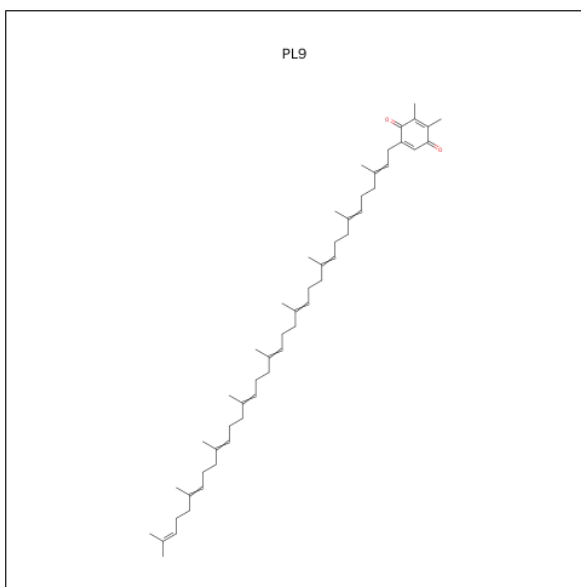
- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).





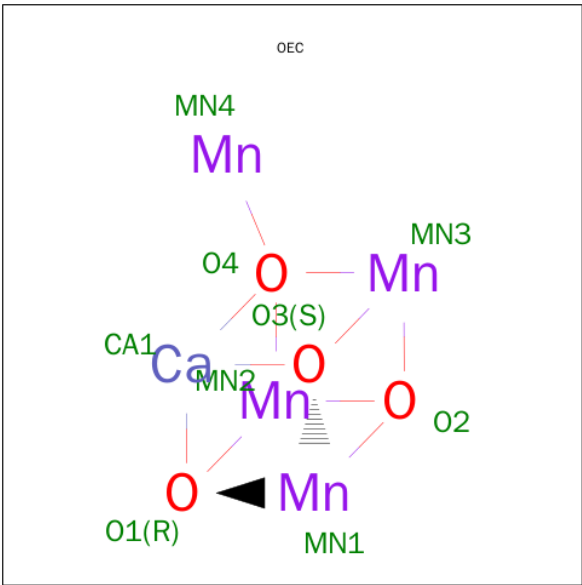
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 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:  $C_{53}H_{80}O_2$ ).



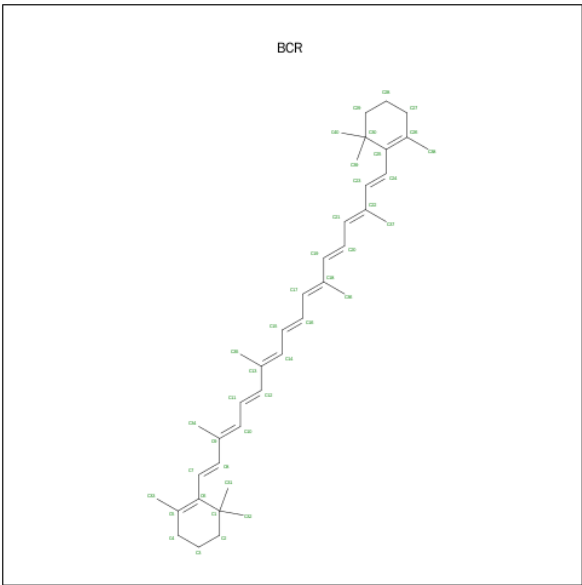
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	J	1	Total	C	O	0	0
			35	33	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			55	53	2		
25	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	Ca	Mn	0	0
			5	1	4		
26	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	1	Total	C	0	0
			40	40		
27	B	1	Total	C	0	0
			40	40		

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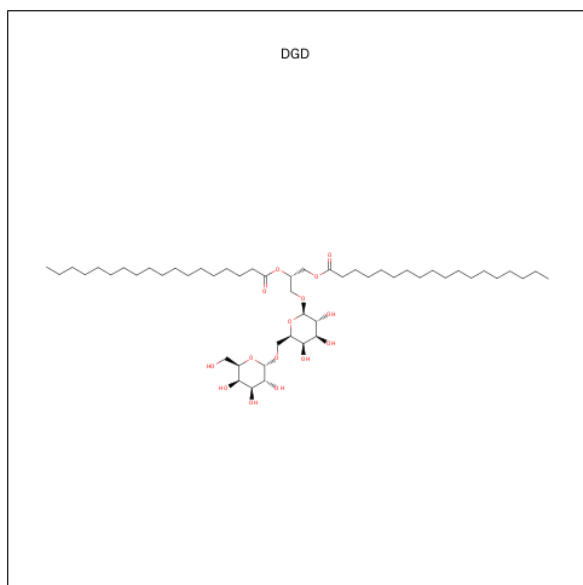
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	z	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



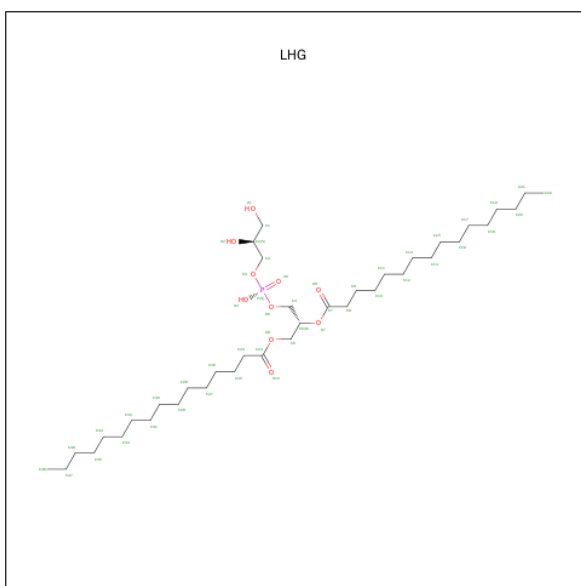
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52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

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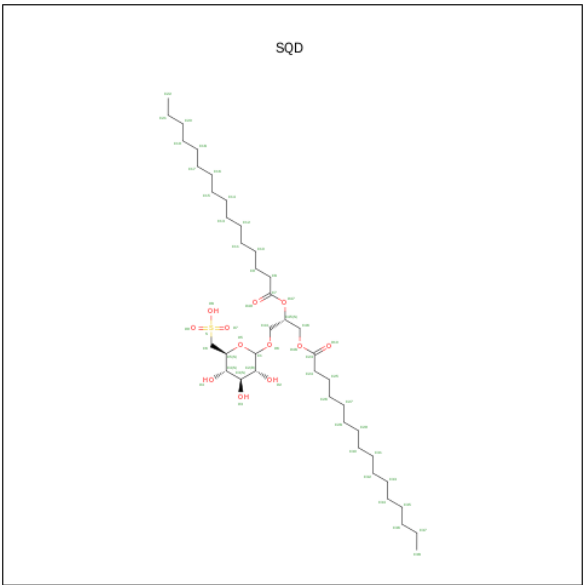
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	0
			53	38	15		
28	c	1	Total	C	O	0	0
			62	47	15		
28	c	1	Total	C	O	0	0
			66	51	15		
28	d	1	Total	C	O	0	0
			63	48	15		

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



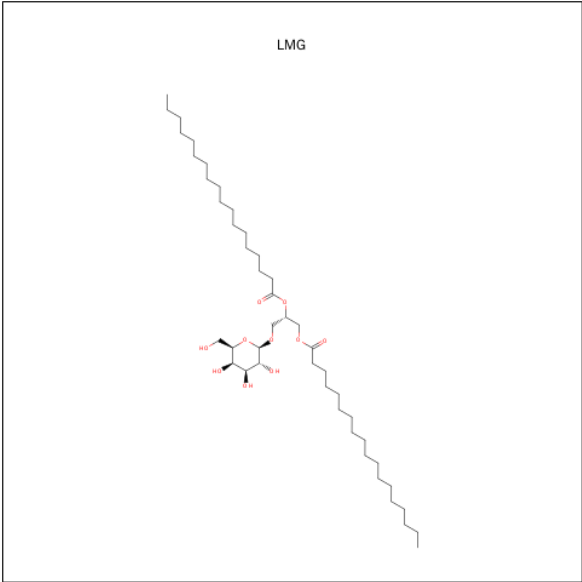
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

- 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 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



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

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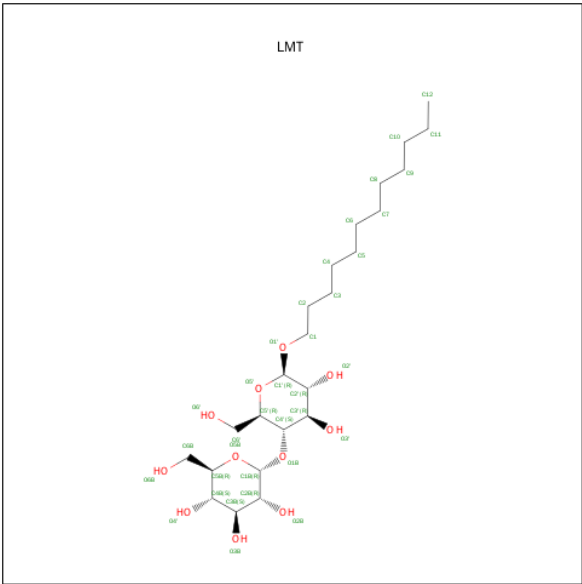
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	b	1	Total	C	O	0	0
			49	39	10		
31	c	1	Total	C	O	0	0
			45	35	10		
31	d	1	Total	C	O	0	0
			46	36	10		
31	d	1	Total	C	O	0	0
			48	38	10		
31	e	1	Total	C	O	0	0
			44	34	10		
31	i	1	Total	C	O	0	0
			43	33	10		
31	k	1	Total	C	O	0	0
			48	38	10		
31	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

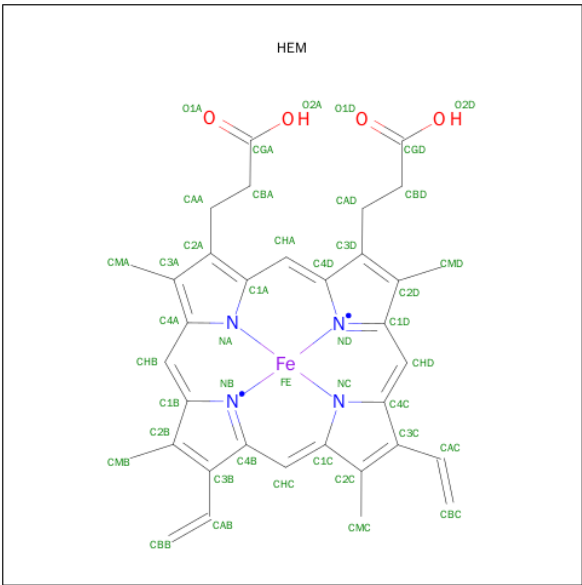
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Cl	0	0
			1	1		
32	a	1	Total	Cl	0	0
			1	1		

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



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

- 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 43	C 34	Fe 1	N 4	O 4	0	0
34	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

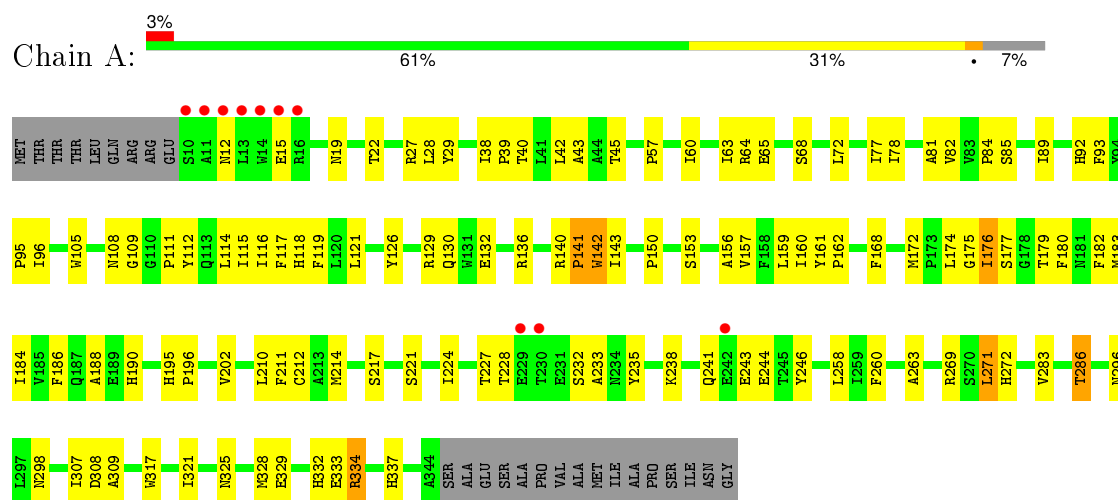
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

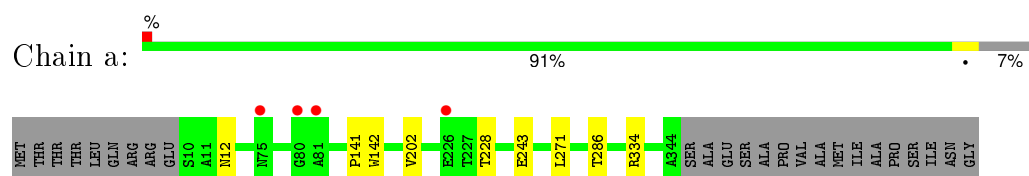
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

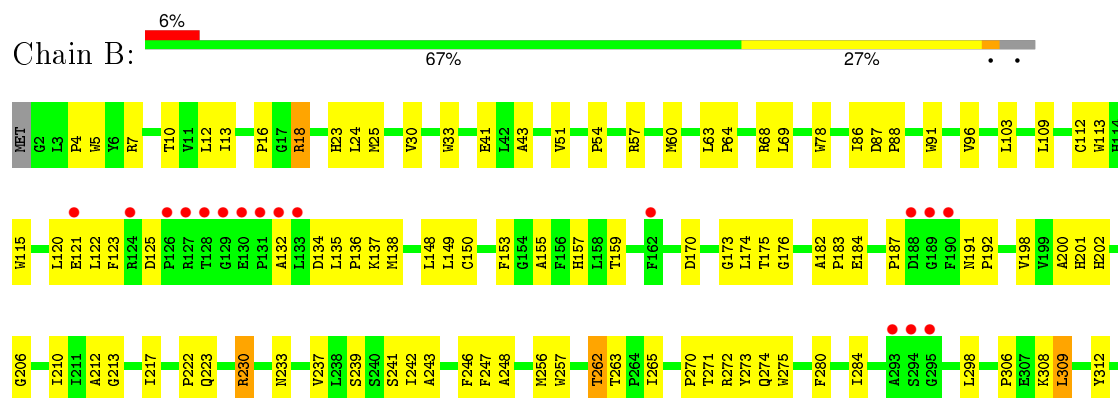
#### • Molecule 1: Photosystem Q(B) protein 1

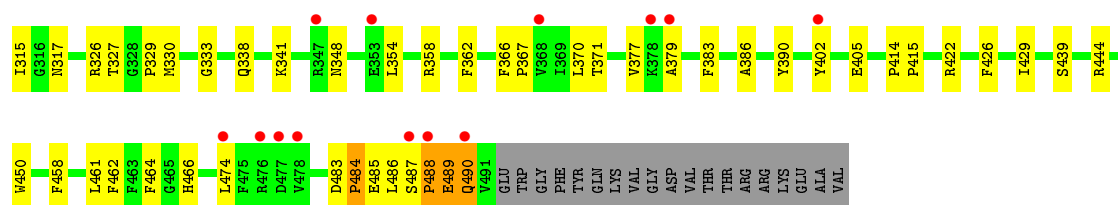


#### • Molecule 1: Photosystem Q(B) protein 1

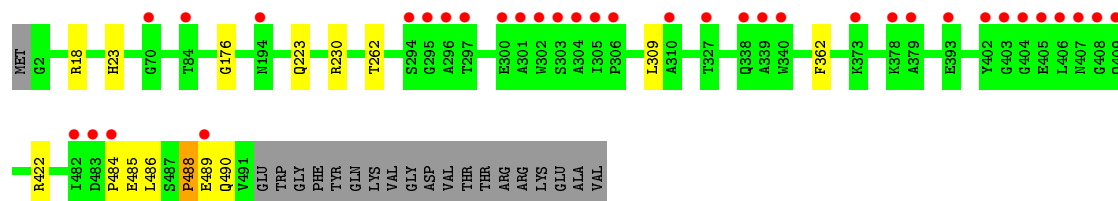
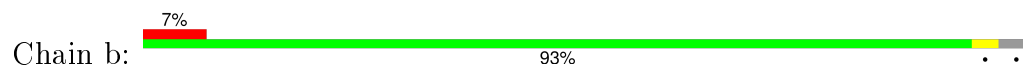


#### • Molecule 2: Photosystem II core light harvesting protein

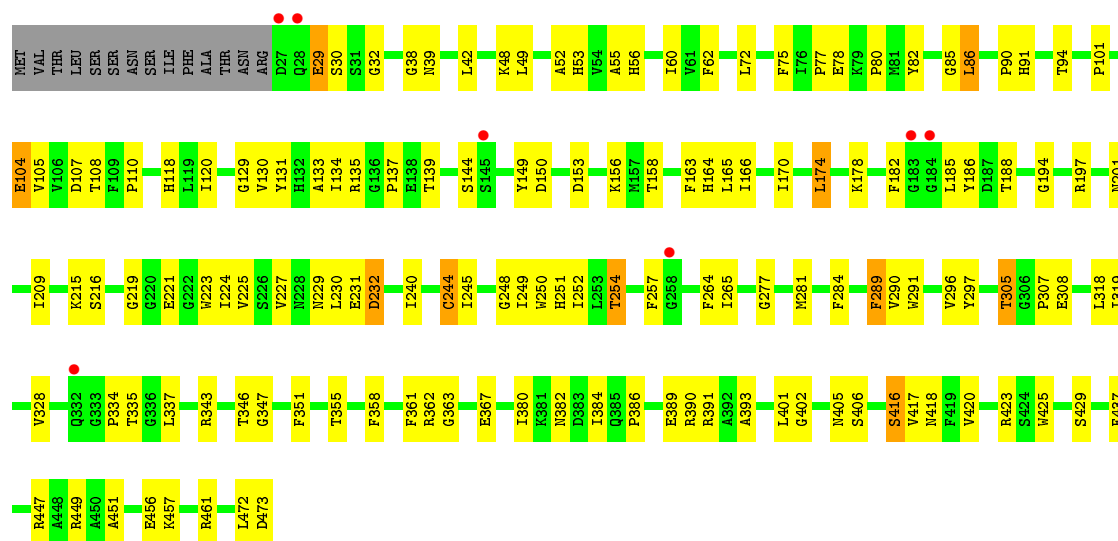




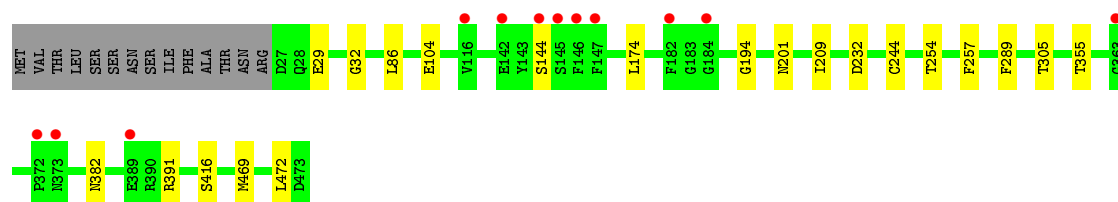
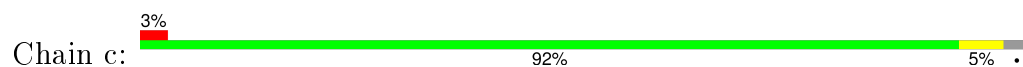
• Molecule 2: Photosystem II core light harvesting protein



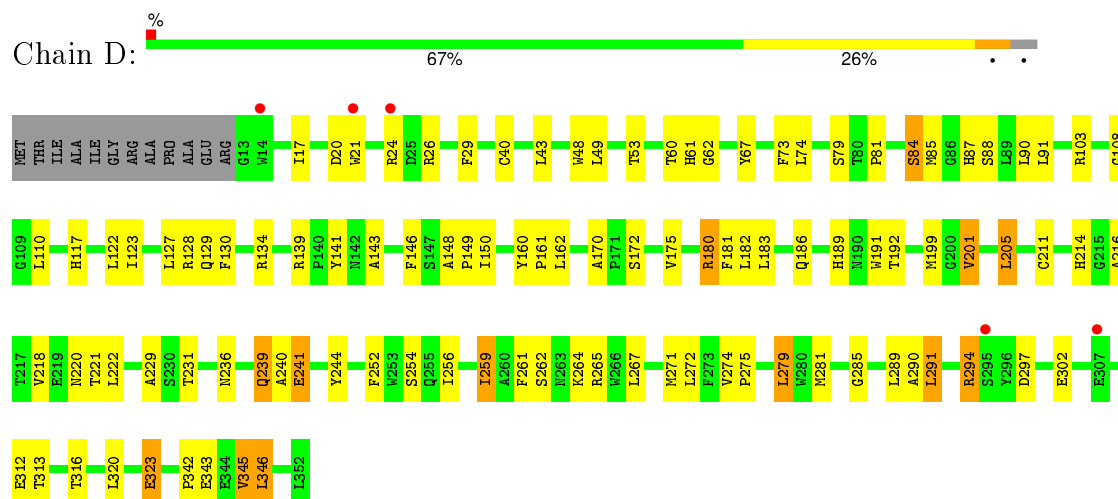
• Molecule 3: Photosystem II CP43 protein



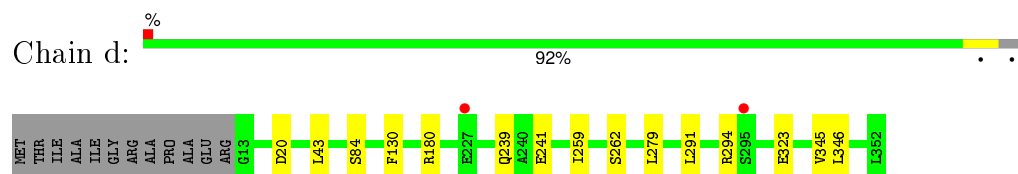
• Molecule 3: Photosystem II CP43 protein



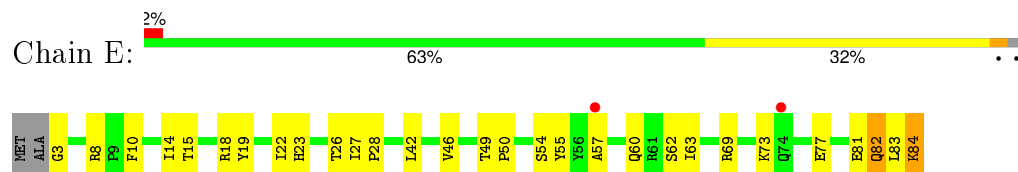
• Molecule 4: Photosystem II D2 protein



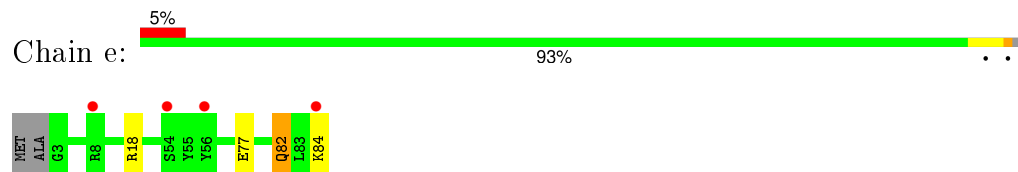
- Molecule 4: Photosystem II D2 protein



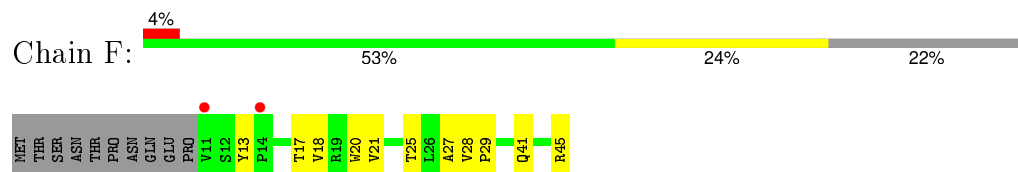
- Molecule 5: Cytochrome b559 subunit alpha



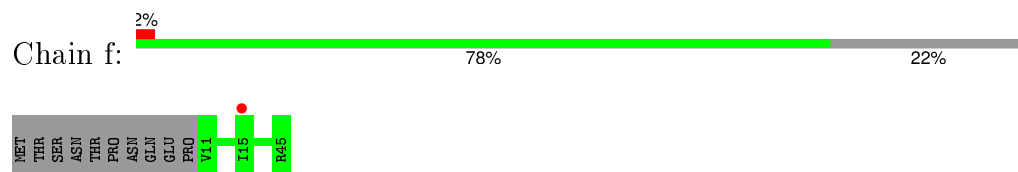
- Molecule 5: Cytochrome b559 subunit alpha



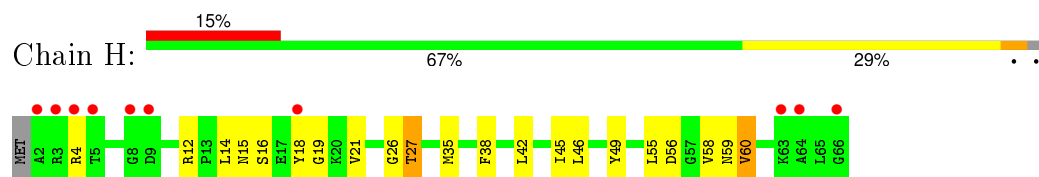
- Molecule 6: Cytochrome b559 subunit beta



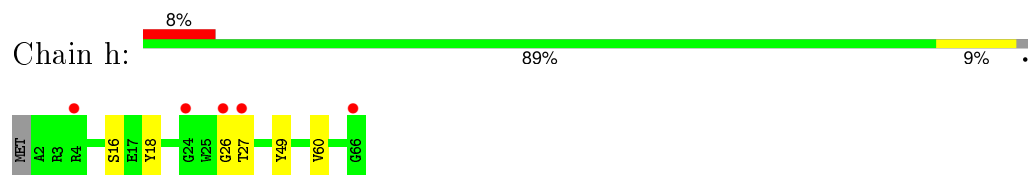
- Molecule 6: Cytochrome b559 subunit beta



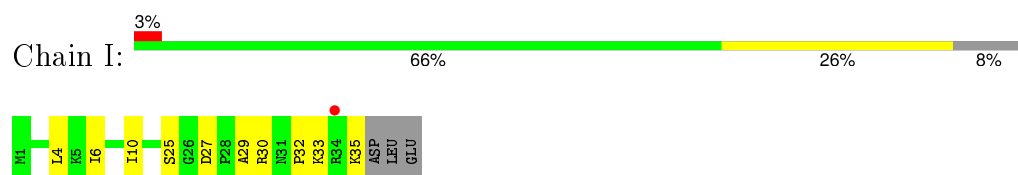
- Molecule 7: Photosystem II reaction center protein H



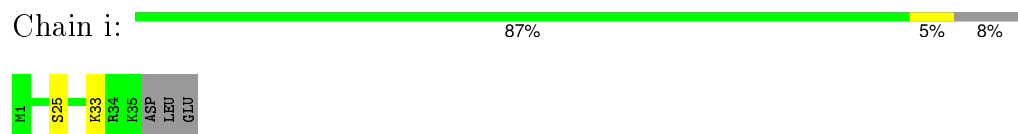
- Molecule 7: Photosystem II reaction center protein H



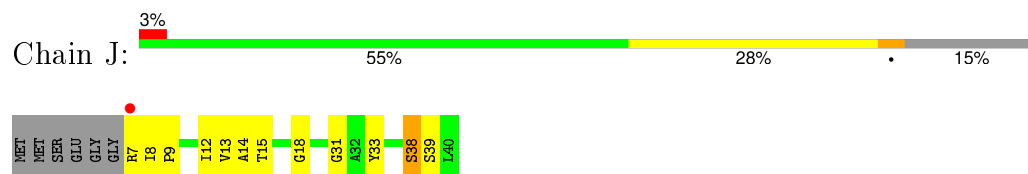
- Molecule 8: Photosystem II reaction center protein I



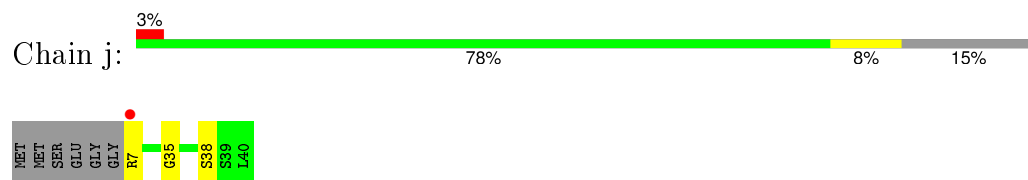
- Molecule 8: Photosystem II reaction center protein I



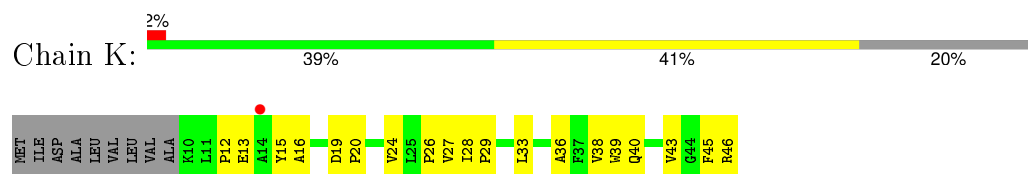
- Molecule 9: Photosystem II reaction center protein J



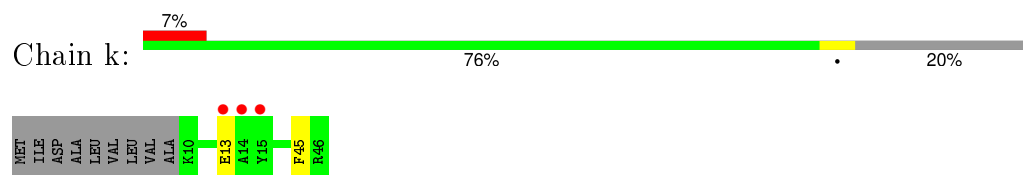
- Molecule 9: Photosystem II reaction center protein J



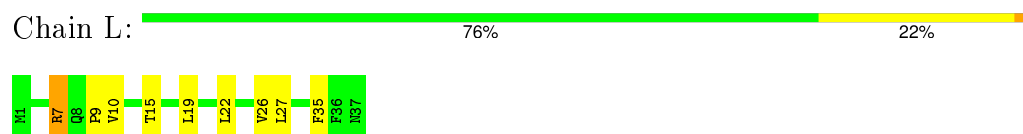
- Molecule 10: Photosystem II reaction center protein K



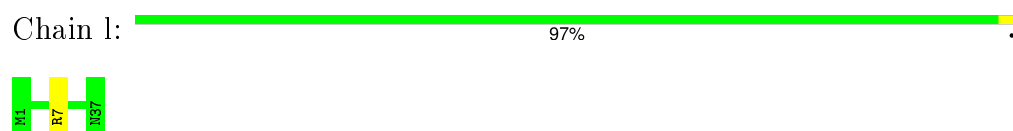
- Molecule 10: Photosystem II reaction center protein K



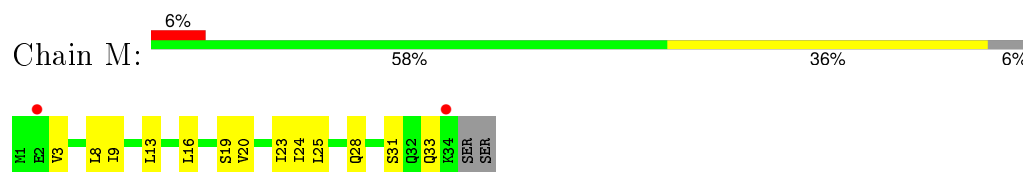
- Molecule 11: Photosystem II reaction center protein L



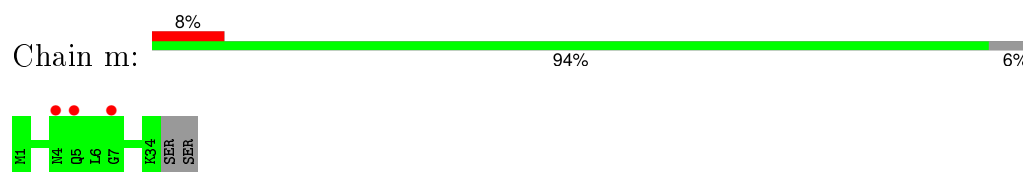
- Molecule 11: Photosystem II reaction center protein L



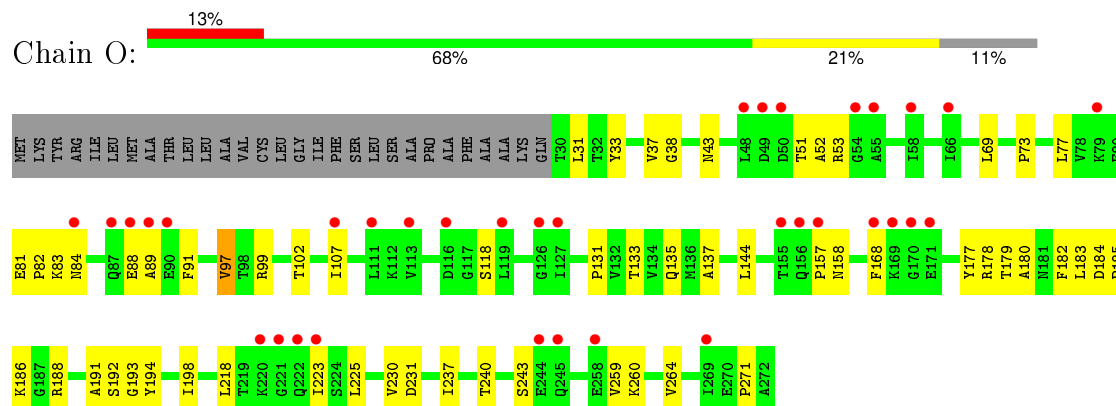
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

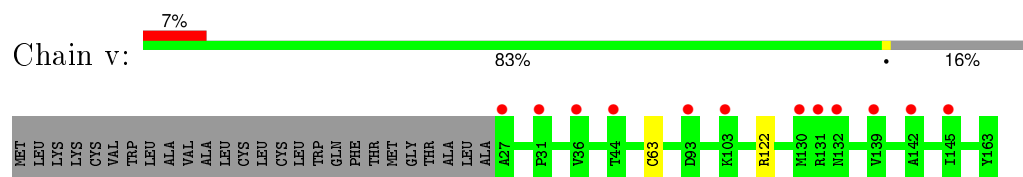


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

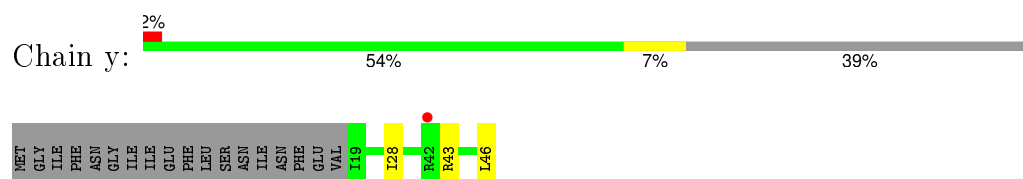




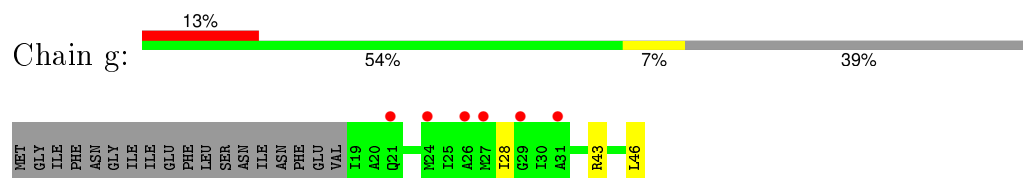
- Molecule 16: Cytochrome c-550



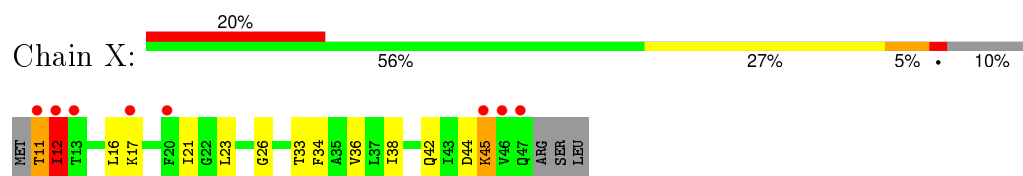
- Molecule 17: Photosystem II reaction center protein ycf12



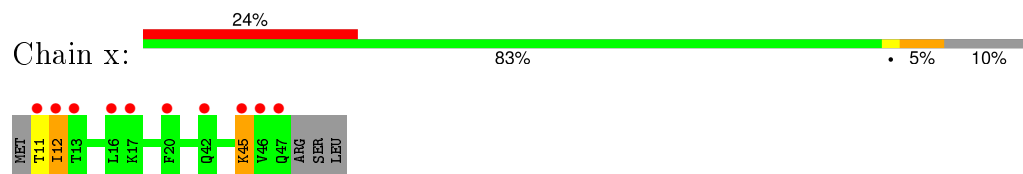
- Molecule 17: Photosystem II reaction center protein ycf12



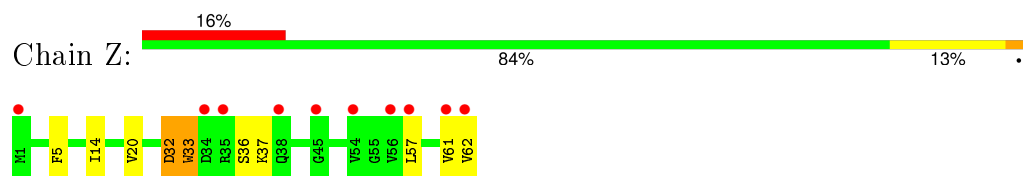
- Molecule 18: Photosystem II reaction center X protein



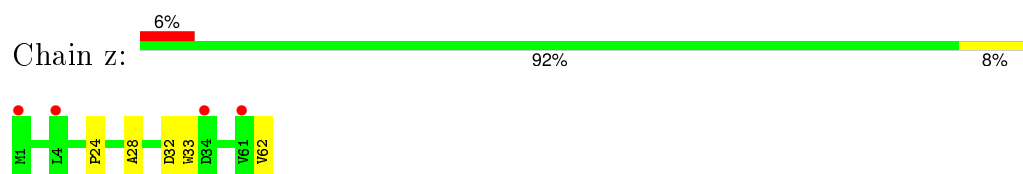
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z

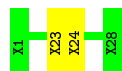


- Molecule 19: Photosystem II reaction center protein Z



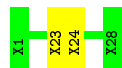
- Molecule 20: Photosystem II reaction center protein Y

Chain G:  93% 7%



- Molecule 20: Photosystem II reaction center protein Y

Chain Y:  93% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.98Å 227.57Å 306.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 5.90 82.97 – 5.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.97-5.90) 98.5 (82.97-5.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, $R_{free}$	0.285 , 0.313 0.308 , 0.316	Depositor DCC
$R_{free}$ test set	1200 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	1.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 24671 reflections	Xtriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.28	0/3986	0.46	0/5433
3	C	0.28	0/3556	0.46	0/4842
3	c	0.27	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.29	0/685	0.48	0/933
5	e	0.28	0/685	0.48	0/933
6	F	0.28	0/291	0.45	0/397
6	f	0.26	0/291	0.45	0/397
7	H	0.26	0/520	0.49	0/709
7	h	0.27	0/520	0.50	0/709
8	I	0.28	0/293	0.48	0/395
8	i	0.32	0/293	0.49	0/395
9	J	0.29	0/255	0.46	0/346
9	j	0.28	0/255	0.44	0/346
10	K	0.29	0/303	0.52	0/416
10	k	0.28	0/303	0.53	0/416
11	L	0.25	0/311	0.43	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.65	0/367
12	m	0.41	0/270	0.65	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.36	0/284	0.49	0/381
14	t	0.35	0/284	0.47	0/381
15	U	0.27	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.30	0/1081	0.52	0/1468
16	v	0.26	0/1081	0.46	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	g	0.24	0/202	0.51	0/272
17	y	0.25	0/202	0.52	0/272
18	X	0.30	0/273	0.52	0/370
18	x	0.32	0/273	0.50	0/370
19	Z	0.30	0/490	0.50	0/669
19	z	0.28	0/490	0.48	0/669
All	All	0.29	0/41948	0.48	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 ⓘ

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	2627	0	2524	105	0
1	a	2627	0	2524	0	0
2	B	3850	0	3718	137	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	116	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	95	0
4	d	2706	0	2608	0	0
5	E	666	0	651	24	0
5	e	666	0	651	0	0
6	F	282	0	291	11	0
6	f	282	0	291	0	0
7	H	507	0	521	20	0
7	h	507	0	521	0	0
8	I	286	0	308	5	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	16	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	10	0
11	l	304	0	316	0	0
12	M	267	0	289	13	0
12	m	267	0	289	0	0
13	O	1845	0	1801	39	0
13	o	1845	0	1801	0	0
14	T	275	0	288	17	0
14	t	275	0	288	0	0
15	U	774	0	773	13	0
15	u	774	0	773	0	0
16	V	1060	0	1068	13	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	12	0
18	x	270	0	299	0	0
19	Z	479	0	516	9	0
19	z	479	0	516	0	0
20	G	140	0	32	1	0
20	Y	140	0	32	1	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	1	0	0
22	d	4	0	1	0	0
23	A	260	0	288	48	0
23	B	1040	0	1152	131	0
23	C	845	0	936	66	0
23	D	130	0	144	10	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	5	0
24	D	64	0	74	6	0
24	a	128	0	148	0	0
25	A	45	0	61	2	0
25	D	55	0	80	12	0
25	J	35	0	45	1	0
25	a	45	0	61	0	0
25	d	55	0	80	0	0
25	j	35	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	5	0	0	0	0
26	a	5	0	0	0	0
27	A	40	0	56	7	0
27	B	160	0	224	21	0
27	C	120	0	168	22	0
27	D	40	0	56	3	0
27	H	40	0	56	7	0
27	J	40	0	56	4	0
27	T	80	0	112	11	0
27	a	40	0	56	0	0
27	b	80	0	112	0	0
27	c	80	0	112	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	j	40	0	56	0	0
27	k	40	0	56	0	0
27	y	40	0	56	0	0
27	z	40	0	56	0	0
28	A	56	0	70	1	0
28	B	110	0	136	2	0
28	C	181	0	245	21	0
28	D	63	0	87	2	0
28	a	56	0	70	0	0
28	b	110	0	136	0	0
28	c	181	0	244	0	0
28	d	63	0	87	0	0
29	A	76	0	95	7	0
29	a	76	0	95	0	0
30	A	105	0	147	12	0
30	B	47	0	61	2	0
30	D	43	0	50	5	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	A	93	0	125	5	0
31	B	98	0	135	8	0
31	C	93	0	126	5	0
31	D	94	0	126	8	0
31	E	44	0	58	1	0
31	I	43	0	55	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	M	42	0	53	2	0
31	a	93	0	124	0	0
31	b	98	0	135	0	0
31	c	45	0	59	0	0
31	d	94	0	126	0	0
31	e	44	0	58	0	0
31	i	43	0	55	0	0
31	k	48	0	66	0	0
31	m	42	0	53	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	B	140	0	184	5	0
33	D	31	0	35	1	0
33	I	35	0	46	2	0
33	M	35	0	46	1	0
33	b	140	0	184	0	0
33	d	31	0	35	0	0
33	i	35	0	46	0	0
33	m	35	0	46	0	0
34	F	43	0	30	5	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	50232	0	51361	801	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 9.

The worst 5 of 801 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)
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.58	0.88
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.57	0.86
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.86
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.59	0.83
27:B:617:BCR:H383	30:B:626:SQD:H92	1.62	0.82

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	333/360 (92%)	311 (93%)	17 (5%)	5 (2%)	13	57
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	16	61
2	B	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	19	65
2	b	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	19	65
3	C	445/461 (96%)	406 (91%)	33 (7%)	6 (1%)	15	60
3	c	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	15	60
4	D	338/352 (96%)	316 (94%)	20 (6%)	2 (1%)	30	74
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	30	74
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	60
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	60
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	31
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	31
8	I	33/38 (87%)	27 (82%)	4 (12%)	2 (6%)	2	25
8	i	33/38 (87%)	28 (85%)	4 (12%)	1 (3%)	5	42
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	42
9	j	32/40 (80%)	28 (88%)	2 (6%)	2 (6%)	2	25
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	27
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	27
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	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%)	206 (86%)	31 (13%)	4 (2%)	11	55
13	o	241/272 (89%)	208 (86%)	29 (12%)	4 (2%)	11	55
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	40
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	40
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	41
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	41
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	37
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4	37
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	27
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	27
19	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	55
19	z	60/62 (97%)	54 (90%)	3 (5%)	3 (5%)	3	31
All	All	5138/5650 (91%)	4681 (91%)	378 (7%)	79 (2%)	13	57

5 of 79 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	271/291 (93%)	266 (98%)	5 (2%)	66	87
1	a	271/291 (93%)	266 (98%)	5 (2%)	66	87
2	B	390/407 (96%)	380 (97%)	10 (3%)	54	80
2	b	390/407 (96%)	379 (97%)	11 (3%)	51	78
3	C	347/362 (96%)	333 (96%)	14 (4%)	38	71
3	c	347/362 (96%)	332 (96%)	15 (4%)	35	70
4	D	275/283 (97%)	260 (94%)	15 (6%)	27	64
4	d	275/283 (97%)	262 (95%)	13 (5%)	32	68
5	E	72/73 (99%)	68 (94%)	4 (6%)	26	63
5	e	72/73 (99%)	68 (94%)	4 (6%)	26	63
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	54
7	h	53/55 (96%)	50 (94%)	3 (6%)	25	62
8	I	32/35 (91%)	31 (97%)	1 (3%)	47	77
8	i	32/35 (91%)	31 (97%)	1 (3%)	47	77
9	J	24/28 (86%)	23 (96%)	1 (4%)	36	70
9	j	24/28 (86%)	23 (96%)	1 (4%)	36	70
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	78
11	l	35/35 (100%)	34 (97%)	1 (3%)	50	78
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	75
14	t	29/29 (100%)	28 (97%)	1 (3%)	44	75
15	U	84/112 (75%)	83 (99%)	1 (1%)	78	90
15	u	84/112 (75%)	82 (98%)	2 (2%)	57	82
16	V	116/138 (84%)	114 (98%)	2 (2%)	68	87
16	v	116/138 (84%)	114 (98%)	2 (2%)	68	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	g	20/37 (54%)	18 (90%)	2 (10%)	9	38
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	38
18	X	30/34 (88%)	27 (90%)	3 (10%)	9	38
18	x	30/34 (88%)	27 (90%)	3 (10%)	9	38
19	Z	52/52 (100%)	49 (94%)	3 (6%)	25	61
19	z	52/52 (100%)	50 (96%)	2 (4%)	40	73
All	All	4244/4616 (92%)	4107 (97%)	137 (3%)	46	76

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	y	28	ILE
2	b	223	GLN
15	u	103	GLN
18	X	11	THR
1	a	202	VAL

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

Mol	Chain	Res	Type
17	y	45	ASN
15	u	93	ASN
1	a	241	GLN
1	A	303	ASN
2	b	201	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	BCT	A	402	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	403	-	55,73,73	0.95	4 (7%)	61,113,113	1.19	9 (14%)
23	CLA	A	404	-	55,73,73	0.96	3 (5%)	61,113,113	1.22	8 (13%)
23	CLA	A	405	-	55,73,73	0.93	3 (5%)	61,113,113	1.27	8 (13%)
24	PHO	A	406	-	67,69,69	1.25	12 (17%)	84,99,99	1.09	6 (7%)
23	CLA	A	407	-	55,73,73	0.94	4 (7%)	61,113,113	1.18	6 (9%)
25	PL9	A	408	-	45,45,55	1.46	7 (15%)	56,57,69	1.74	14 (25%)
26	OEC	A	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	A	410	-	41,41,41	0.70	0	56,56,56	1.92	11 (19%)
28	DGD	A	411	-	57,57,67	1.20	7 (12%)	71,71,81	1.56	12 (16%)
29	LHG	A	412	-	38,38,48	1.01	2 (5%)	39,44,54	1.01	3 (7%)
30	SQD	A	413	-	50,51,54	0.97	3 (6%)	58,62,65	1.65	10 (17%)
31	LMG	A	414	-	51,51,55	1.12	6 (11%)	59,59,63	1.35	4 (6%)
29	LHG	A	415	-	36,36,48	1.04	2 (5%)	37,42,54	1.10	3 (8%)
30	SQD	A	417	-	53,54,54	1.00	4 (7%)	61,65,65	1.71	11 (18%)
31	LMG	A	418	-	42,42,55	1.20	6 (14%)	50,50,63	1.52	9 (18%)
23	CLA	B	601	-	55,73,73	0.98	4 (7%)	61,113,113	1.20	8 (13%)
23	CLA	B	602	-	55,73,73	0.95	3 (5%)	61,113,113	1.16	6 (9%)
23	CLA	B	603	-	55,73,73	0.96	3 (5%)	61,113,113	1.22	7 (11%)
23	CLA	B	604	-	55,73,73	0.97	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	B	605	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	9 (14%)
23	CLA	B	606	-	55,73,73	0.95	4 (7%)	61,113,113	1.23	7 (11%)
23	CLA	B	607	-	55,73,73	0.93	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	B	608	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	B	609	-	55,73,73	0.96	4 (7%)	61,113,113	1.20	7 (11%)
23	CLA	B	610	-	55,73,73	0.97	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
23	CLA	B	611	-	55,73,73	0.95	4 (7%)	61,113,113	1.22	7 (11%)
23	CLA	B	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	8 (13%)
23	CLA	B	613	-	55,73,73	0.93	4 (7%)	61,113,113	1.13	5 (8%)
23	CLA	B	614	-	55,73,73	0.96	3 (5%)	61,113,113	1.16	6 (9%)
23	CLA	B	615	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	5 (8%)
23	CLA	B	616	-	55,73,73	0.95	4 (7%)	61,113,113	1.21	8 (13%)
27	BCR	B	617	-	41,41,41	0.67	0	56,56,56	1.86	14 (25%)
27	BCR	B	618	-	41,41,41	0.64	0	56,56,56	2.31	18 (32%)
27	BCR	B	619	-	41,41,41	0.64	0	56,56,56	1.88	17 (30%)
27	BCR	B	620	-	41,41,41	0.70	0	56,56,56	2.18	15 (26%)
28	DGD	B	621	-	59,59,67	1.20	8 (13%)	73,73,81	1.12	4 (5%)
31	LMG	B	622	-	49,49,55	1.11	7 (14%)	57,57,63	1.33	6 (10%)
31	LMG	B	623	-	49,49,55	1.16	8 (16%)	57,57,63	1.42	8 (14%)
33	LMT	B	624	-	36,36,36	0.41	0	47,47,47	0.72	0
33	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.71	0
30	SQD	B	626	-	46,47,54	1.01	4 (8%)	54,58,65	1.72	9 (16%)
28	DGD	B	627	-	53,53,67	1.19	6 (11%)	67,67,81	1.48	10 (14%)
33	LMT	B	628	-	36,36,36	0.44	0	47,47,47	0.81	1 (2%)
33	LMT	B	629	-	36,36,36	0.44	0	47,47,47	0.66	0
23	CLA	C	501	-	55,73,73	0.94	3 (5%)	61,113,113	1.16	6 (9%)
23	CLA	C	502	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	7 (11%)
23	CLA	C	503	-	55,73,73	0.92	3 (5%)	61,113,113	1.22	8 (13%)
23	CLA	C	504	-	55,73,73	0.97	3 (5%)	61,113,113	1.21	7 (11%)
23	CLA	C	505	-	55,73,73	0.97	4 (7%)	61,113,113	1.21	8 (13%)
23	CLA	C	506	-	55,73,73	0.96	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	C	507	-	55,73,73	0.94	3 (5%)	61,113,113	1.26	7 (11%)
23	CLA	C	508	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	7 (11%)
23	CLA	C	509	-	55,73,73	0.96	4 (7%)	61,113,113	1.14	6 (9%)
23	CLA	C	510	-	55,73,73	0.97	3 (5%)	61,113,113	1.18	8 (13%)
23	CLA	C	511	3	55,73,73	0.97	4 (7%)	61,113,113	1.23	9 (14%)
23	CLA	C	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.25	9 (14%)
23	CLA	C	513	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
27	BCR	C	514	-	41,41,41	0.70	0	56,56,56	2.36	18 (32%)
27	BCR	C	515	-	41,41,41	0.64	0	56,56,56	1.92	15 (26%)
27	BCR	C	516	-	41,41,41	0.66	0	56,56,56	1.98	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	DGD	C	517	-	54,54,67	1.18	6 (11%)	68,68,81	1.31	7 (10%)
28	DGD	C	518	-	63,63,67	1.19	10 (15%)	77,77,81	1.31	7 (9%)
28	DGD	C	519	-	67,67,67	1.10	6 (8%)	81,81,81	1.45	10 (12%)
31	LMG	C	520	-	48,48,55	1.10	6 (12%)	56,56,63	1.32	7 (12%)
31	LMG	C	521	-	45,45,55	1.16	6 (13%)	53,53,63	1.40	9 (16%)
23	CLA	D	401	-	55,73,73	0.92	3 (5%)	61,113,113	1.26	8 (13%)
24	PHO	D	402	-	67,69,69	1.21	12 (17%)	84,99,99	1.07	7 (8%)
23	CLA	D	403	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
25	PL9	D	404	-	55,55,55	1.46	8 (14%)	68,69,69	1.82	20 (29%)
27	BCR	D	405	-	41,41,41	0.64	0	56,56,56	2.22	16 (28%)
31	LMG	D	406	-	46,46,55	1.15	5 (10%)	54,54,63	1.39	7 (12%)
31	LMG	D	407	-	48,48,55	1.16	8 (16%)	56,56,63	1.48	7 (12%)
30	SQD	D	408	-	42,43,54	1.09	4 (9%)	50,54,65	2.19	9 (18%)
28	DGD	D	409	-	64,64,67	1.12	6 (9%)	78,78,81	1.52	8 (10%)
33	LMT	D	410	-	32,32,36	0.49	0	43,43,47	0.72	2 (4%)
31	LMG	E	101	-	44,44,55	1.16	7 (15%)	52,52,63	1.35	7 (13%)
34	HEM	F	101	5,6	30,50,50	2.04	8 (26%)	24,82,82	2.38	10 (41%)
30	SQD	F	102	-	44,45,54	1.03	4 (9%)	52,56,65	1.82	10 (19%)
27	BCR	H	101	-	41,41,41	0.68	0	56,56,56	1.77	14 (25%)
31	LMG	I	101	-	43,43,55	1.23	8 (18%)	51,51,63	1.33	8 (15%)
33	LMT	I	102	-	36,36,36	0.41	0	47,47,47	0.70	2 (4%)
25	PL9	J	101	-	35,35,55	1.36	5 (14%)	44,45,69	1.66	8 (18%)
27	BCR	J	102	-	41,41,41	0.70	0	56,56,56	3.42	26 (46%)
31	LMG	M	101	-	42,42,55	1.25	7 (16%)	50,50,63	1.54	9 (18%)
33	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.69	0
27	BCR	T	101	-	41,41,41	0.66	0	56,56,56	1.79	12 (21%)
27	BCR	T	102	-	41,41,41	0.66	0	56,56,56	2.29	18 (32%)
34	HEM	V	201	16	30,50,50	2.29	8 (26%)	24,82,82	2.12	6 (25%)
30	SQD	a	401	-	53,54,54	0.98	4 (7%)	61,65,65	1.76	10 (16%)
31	LMG	a	402	-	42,42,55	1.20	6 (14%)	50,50,63	1.53	8 (16%)
23	CLA	a	404	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	CLA	a	405	-	55,73,73	0.95	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	a	406	-	55,73,73	0.93	3 (5%)	61,113,113	1.27	8 (13%)
24	PHO	a	407	-	67,69,69	1.22	11 (16%)	84,99,99	1.06	8 (9%)
24	PHO	a	408	-	67,69,69	1.23	9 (13%)	84,99,99	1.05	5 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	a	409	-	55,73,73	0.94	4 (7%)	61,113,113	1.19	8 (13%)
25	PL9	a	410	-	45,45,55	1.42	7 (15%)	56,57,69	1.82	16 (28%)
26	OEC	a	411	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	a	412	-	41,41,41	0.71	0	56,56,56	1.95	13 (23%)
28	DGD	a	413	-	57,57,67	1.17	7 (12%)	71,71,81	1.50	12 (16%)
29	LHG	a	414	-	38,38,48	1.03	2 (5%)	39,44,54	1.03	4 (10%)
30	SQD	a	415	-	50,51,54	0.96	4 (8%)	58,62,65	1.69	9 (15%)
31	LMG	a	416	-	51,51,55	1.09	6 (11%)	59,59,63	1.38	5 (8%)
29	LHG	a	417	-	36,36,48	1.05	2 (5%)	37,42,54	1.04	2 (5%)
30	SQD	b	601	-	46,47,54	1.00	4 (8%)	54,58,65	1.82	10 (18%)
28	DGD	b	602	-	53,53,67	1.20	5 (9%)	67,67,81	1.41	10 (14%)
33	LMT	b	603	-	36,36,36	0.43	0	47,47,47	0.78	1 (2%)
33	LMT	b	604	-	36,36,36	0.39	0	47,47,47	0.64	0
23	CLA	b	605	-	55,73,73	0.96	4 (7%)	61,113,113	1.25	8 (13%)
23	CLA	b	606	-	55,73,73	0.97	3 (5%)	61,113,113	1.23	7 (11%)
23	CLA	b	607	-	55,73,73	0.93	3 (5%)	61,113,113	1.25	8 (13%)
23	CLA	b	608	-	55,73,73	0.95	3 (5%)	61,113,113	1.16	6 (9%)
23	CLA	b	609	-	55,73,73	0.96	4 (7%)	61,113,113	1.16	8 (13%)
23	CLA	b	610	-	55,73,73	0.97	3 (5%)	61,113,113	1.23	8 (13%)
23	CLA	b	611	-	55,73,73	0.96	3 (5%)	61,113,113	1.14	6 (9%)
23	CLA	b	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.26	8 (13%)
23	CLA	b	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.18	8 (13%)
23	CLA	b	614	-	55,73,73	0.94	3 (5%)	61,113,113	1.24	6 (9%)
23	CLA	b	615	-	55,73,73	0.96	4 (7%)	61,113,113	1.22	7 (11%)
23	CLA	b	616	-	55,73,73	0.93	4 (7%)	61,113,113	1.24	7 (11%)
23	CLA	b	617	-	55,73,73	0.95	3 (5%)	61,113,113	1.27	8 (13%)
23	CLA	b	618	-	55,73,73	0.97	3 (5%)	61,113,113	1.17	6 (9%)
23	CLA	b	619	-	55,73,73	0.94	4 (7%)	61,113,113	1.21	8 (13%)
23	CLA	b	620	-	55,73,73	0.98	5 (9%)	61,113,113	1.15	7 (11%)
27	BCR	b	621	-	41,41,41	0.62	0	56,56,56	1.99	18 (32%)
27	BCR	b	622	-	41,41,41	0.69	0	56,56,56	2.25	15 (26%)
28	DGD	b	623	-	59,59,67	1.17	7 (11%)	73,73,81	1.16	5 (6%)
31	LMG	b	624	-	49,49,55	1.14	7 (14%)	57,57,63	1.31	8 (14%)
31	LMG	b	625	-	49,49,55	1.15	8 (16%)	57,57,63	1.45	10 (17%)
33	LMT	b	626	-	36,36,36	0.38	0	47,47,47	0.75	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMT	b	627	-	36,36,36	0.42	0	47,47,47	0.66	0
23	CLA	c	501	-	55,73,73	0.94	3 (5%)	61,113,113	1.24	9 (14%)
23	CLA	c	502	-	55,73,73	0.97	4 (7%)	61,113,113	1.22	8 (13%)
23	CLA	c	503	-	55,73,73	0.93	3 (5%)	61,113,113	1.18	7 (11%)
23	CLA	c	504	-	55,73,73	0.92	3 (5%)	61,113,113	1.25	7 (11%)
23	CLA	c	505	-	55,73,73	0.96	4 (7%)	61,113,113	1.23	8 (13%)
23	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.29	7 (11%)
23	CLA	c	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	8 (13%)
23	CLA	c	508	-	55,73,73	0.94	3 (5%)	61,113,113	1.27	8 (13%)
23	CLA	c	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.12	6 (9%)
23	CLA	c	510	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	8 (13%)
23	CLA	c	511	-	55,73,73	0.97	4 (7%)	61,113,113	1.16	7 (11%)
23	CLA	c	512	-	55,73,73	0.93	3 (5%)	61,113,113	1.26	9 (14%)
23	CLA	c	513	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
27	BCR	c	514	-	41,41,41	0.67	0	56,56,56	2.39	18 (32%)
27	BCR	c	515	-	41,41,41	0.66	0	56,56,56	2.02	16 (28%)
28	DGD	c	516	-	54,54,67	1.21	6 (11%)	68,68,81	1.31	8 (11%)
28	DGD	c	517	-	63,63,67	1.18	10 (15%)	77,77,81	1.36	7 (9%)
28	DGD	c	518	-	67,67,67	1.09	6 (8%)	81,81,81	1.49	12 (14%)
31	LMG	c	519	-	45,45,55	1.19	6 (13%)	53,53,63	1.36	6 (11%)
22	BCT	d	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	402	-	55,73,73	0.93	3 (5%)	61,113,113	1.28	8 (13%)
23	CLA	d	403	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	6 (9%)
25	PL9	d	404	-	55,55,55	1.46	8 (14%)	68,69,69	1.91	20 (29%)
27	BCR	d	405	-	41,41,41	0.64	0	56,56,56	2.19	16 (28%)
31	LMG	d	406	-	46,46,55	1.16	7 (15%)	54,54,63	1.33	6 (11%)
31	LMG	d	407	-	48,48,55	1.14	8 (16%)	56,56,63	1.55	6 (10%)
30	SQD	d	408	-	42,43,54	1.10	4 (9%)	50,54,65	2.17	9 (18%)
28	DGD	d	409	-	64,64,67	1.11	5 (7%)	78,78,81	1.53	10 (12%)
33	LMT	d	410	-	32,32,36	0.47	0	43,43,47	0.71	1 (2%)
31	LMG	e	101	-	44,44,55	1.19	8 (18%)	52,52,63	1.37	9 (17%)
34	HEM	f	101	5,6	30,50,50	2.04	9 (30%)	24,82,82	2.42	11 (45%)
30	SQD	f	102	-	44,45,54	1.02	3 (6%)	52,56,65	1.80	10 (19%)
27	BCR	h	101	-	41,41,41	0.70	0	56,56,56	1.77	14 (25%)
31	LMG	i	101	-	43,43,55	1.24	8 (18%)	51,51,63	1.32	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMT	i	102	-	36,36,36	0.46	1 (2%)	47,47,47	0.72	1 (2%)
25	PL9	j	101	-	35,35,55	1.35	5 (14%)	44,45,69	1.67	8 (18%)
27	BCR	j	102	-	41,41,41	0.68	0	56,56,56	3.41	25 (44%)
27	BCR	k	102	-	41,41,41	0.70	0	56,56,56	1.99	15 (26%)
31	LMG	k	103	-	48,48,55	1.11	6 (12%)	56,56,63	1.29	7 (12%)
33	LMT	m	101	-	36,36,36	0.41	0	47,47,47	0.68	0
31	LMG	m	102	-	42,42,55	1.30	7 (16%)	50,50,63	1.60	10 (20%)
34	HEM	v	201	16	30,50,50	2.21	7 (23%)	24,82,82	2.17	6 (25%)
27	BCR	y	101	-	41,41,41	0.69	0	56,56,56	1.97	16 (28%)
27	BCR	z	101	-	41,41,41	0.62	0	56,56,56	1.85	13 (23%)

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	BCT	A	402	21	-	0/0/0/0	0/0/0/0
23	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	406	-	-	0/53/103/103	0/1/6/6
23	CLA	A	407	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	A	408	-	-	0/41/61/73	0/1/1/1
26	OEC	A	409	1,3	-	0/0/0/54	0/0/0/5
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
28	DGD	A	411	-	-	0/45/85/95	0/2/2/2
29	LHG	A	412	-	-	0/43/43/53	0/0/0/0
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
31	LMG	A	414	-	-	0/46/66/70	0/1/1/1
29	LHG	A	415	-	-	0/41/41/53	0/0/0/0
30	SQD	A	417	-	-	0/49/69/69	0/1/1/1
31	LMG	A	418	-	-	0/37/57/70	0/1/1/1
23	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	DGD	B	621	-	-	0/47/87/95	0/2/2/2
31	LMG	B	622	-	-	0/44/64/70	0/1/1/1
31	LMG	B	623	-	-	0/44/64/70	0/1/1/1
33	LMT	B	624	-	-	0/21/61/61	0/2/2/2
33	LMT	B	625	-	-	0/21/61/61	0/2/2/2
30	SQD	B	626	-	-	0/42/62/69	0/1/1/1
28	DGD	B	627	-	-	0/41/81/95	0/2/2/2
33	LMT	B	628	-	-	0/21/61/61	0/2/2/2
33	LMT	B	629	-	-	0/21/61/61	0/2/2/2
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	BCR	C	516	-	-	0/29/63/63	0/2/2/2
28	DGD	C	517	-	-	0/42/82/95	0/2/2/2
28	DGD	C	518	-	-	2/51/91/95	0/2/2/2
28	DGD	C	519	-	-	0/55/95/95	0/2/2/2
31	LMG	C	520	-	-	0/43/63/70	0/1/1/1
31	LMG	C	521	-	-	0/40/60/70	0/1/1/1
23	CLA	D	401	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	D	404	-	-	0/53/73/73	0/1/1/1
27	BCR	D	405	-	-	0/29/63/63	0/2/2/2
31	LMG	D	406	-	-	0/41/61/70	0/1/1/1
31	LMG	D	407	-	-	0/43/63/70	0/1/1/1
30	SQD	D	408	-	-	2/38/58/69	0/1/1/1
28	DGD	D	409	-	-	1/52/92/95	0/2/2/2
33	LMT	D	410	-	-	0/17/57/61	0/2/2/2
31	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
27	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	LMG	I	101	-	-	0/38/58/70	0/1/1/1
33	LMT	I	102	-	-	0/21/61/61	0/2/2/2
25	PL9	J	101	-	-	0/29/49/73	0/1/1/1
27	BCR	J	102	-	-	0/29/63/63	0/2/2/2
31	LMG	M	101	-	-	1/37/57/70	0/1/1/1
33	LMT	M	102	-	-	0/21/61/61	0/2/2/2
27	BCR	T	101	-	-	0/29/63/63	0/2/2/2
27	BCR	T	102	-	-	0/29/63/63	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
31	LMG	a	402	-	-	0/37/57/70	0/1/1/1
23	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6
23	CLA	a	409	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	a	410	-	-	0/41/61/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	OEC	a	411	1,3	-	0/0/0/54	0/0/0/5
27	BCR	a	412	-	-	0/29/63/63	0/2/2/2
28	DGD	a	413	-	-	0/45/85/95	0/2/2/2
29	LHG	a	414	-	-	0/43/43/53	0/0/0/0
30	SQD	a	415	-	-	0/46/66/69	0/1/1/1
31	LMG	a	416	-	-	0/46/66/70	0/1/1/1
29	LHG	a	417	-	-	0/41/41/53	0/0/0/0
30	SQD	b	601	-	-	0/42/62/69	0/1/1/1
28	DGD	b	602	-	-	0/41/81/95	0/2/2/2
33	LMT	b	603	-	-	0/21/61/61	0/2/2/2
33	LMT	b	604	-	-	0/21/61/61	0/2/2/2
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	BCR	b	622	-	-	0/29/63/63	0/2/2/2
28	DGD	b	623	-	-	0/47/87/95	0/2/2/2
31	LMG	b	624	-	-	0/44/64/70	0/1/1/1
31	LMG	b	625	-	-	0/44/64/70	0/1/1/1
33	LMT	b	626	-	-	0/21/61/61	0/2/2/2
33	LMT	b	627	-	-	0/21/61/61	0/2/2/2
23	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
28	DGD	c	516	-	-	0/42/82/95	0/2/2/2
28	DGD	c	517	-	-	2/51/91/95	0/2/2/2
28	DGD	c	518	-	-	0/55/95/95	0/2/2/2
31	LMG	c	519	-	-	0/40/60/70	0/1/1/1
22	BCT	d	401	21	-	0/0/0/0	0/0/0/0
23	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	d	404	-	-	0/53/73/73	0/1/1/1
27	BCR	d	405	-	-	0/29/63/63	0/2/2/2
31	LMG	d	406	-	-	0/41/61/70	0/1/1/1
31	LMG	d	407	-	-	0/43/63/70	0/1/1/1
30	SQD	d	408	-	-	2/38/58/69	0/1/1/1
28	DGD	d	409	-	-	1/52/92/95	0/2/2/2
33	LMT	d	410	-	-	0/17/57/61	0/2/2/2
31	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
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
31	LMG	i	101	-	-	0/38/58/70	0/1/1/1
33	LMT	i	102	-	-	0/21/61/61	0/2/2/2
25	PL9	j	101	-	-	0/29/49/73	0/1/1/1
27	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
31	LMG	k	103	-	-	0/43/63/70	0/1/1/1
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
31	LMG	m	102	-	-	1/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/10/54/54	0/0/8/8
27	BCR	y	101	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	z	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 643 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-8.34	1.44	1.51
34	v	201	HEM	C3B-C4B	-7.51	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.01	1.46	1.51
34	f	101	HEM	C3B-C4B	-5.99	1.46	1.51
34	F	101	HEM	C3D-C4D	-5.17	1.44	1.51

The worst 5 of 1453 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	j	102	BCR	C32-C1-C6	-14.13	88.14	110.30
27	J	102	BCR	C32-C1-C6	-13.83	88.62	110.30
27	T	102	BCR	C7-C8-C9	-8.70	112.96	126.22
27	B	618	BCR	C7-C8-C9	-8.55	113.18	126.22
27	J	102	BCR	C32-C1-C31	-8.06	82.55	108.37

5 of 210 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	D	409	DGD	C3G-O3G-C1D-O6D
28	d	409	DGD	C3G-O3G-C1D-O6D
31	m	102	LMG	C8-O7-C10-C11
31	M	101	LMG	C8-O7-C10-C11
28	c	517	DGD	C2G-O2G-C1B-O1B

There are no ring outliers.

85 monomers are involved in 396 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	403	CLA	12	0
23	A	404	CLA	23	0
23	A	405	CLA	15	0
24	A	406	PHO	5	0
23	A	407	CLA	2	0
25	A	408	PL9	2	0
27	A	410	BCR	7	0
28	A	411	DGD	1	0
29	A	412	LHG	4	0
30	A	413	SQD	5	0
31	A	414	LMG	3	0
29	A	415	LHG	3	0
30	A	417	SQD	7	0
31	A	418	LMG	2	0
23	B	601	CLA	2	0
23	B	602	CLA	6	0
23	B	603	CLA	14	0
23	B	604	CLA	9	0
23	B	605	CLA	13	0
23	B	606	CLA	12	0
23	B	607	CLA	19	0
23	B	608	CLA	12	0
23	B	609	CLA	16	0
23	B	610	CLA	6	0
23	B	611	CLA	9	0
23	B	612	CLA	13	0
23	B	613	CLA	13	0
23	B	614	CLA	5	0
23	B	615	CLA	2	0
23	B	616	CLA	7	0
27	B	617	BCR	4	0
27	B	618	BCR	10	0
27	B	619	BCR	6	0
27	B	620	BCR	4	0
31	B	622	LMG	3	0
31	B	623	LMG	5	0
33	B	624	LMT	1	0
30	B	626	SQD	2	0
28	B	627	DGD	2	0
33	B	628	LMT	2	0
33	B	629	LMT	2	0
23	C	501	CLA	7	0
23	C	502	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	503	CLA	6	0
23	C	504	CLA	7	0
23	C	505	CLA	6	0
23	C	506	CLA	4	0
23	C	507	CLA	9	0
23	C	508	CLA	4	0
23	C	509	CLA	3	0
23	C	510	CLA	9	0
23	C	511	CLA	11	0
23	C	512	CLA	5	0
23	C	513	CLA	4	0
27	C	514	BCR	9	0
27	C	515	BCR	8	0
27	C	516	BCR	5	0
28	C	517	DGD	8	0
28	C	518	DGD	8	0
28	C	519	DGD	5	0
31	C	520	LMG	3	0
31	C	521	LMG	2	0
23	D	401	CLA	7	0
24	D	402	PHO	6	0
23	D	403	CLA	3	0
25	D	404	PL9	12	0
27	D	405	BCR	3	0
31	D	406	LMG	2	0
31	D	407	LMG	6	0
30	D	408	SQD	5	0
28	D	409	DGD	2	0
33	D	410	LMT	1	0
31	E	101	LMG	1	0
34	F	101	HEM	5	0
30	F	102	SQD	2	0
27	H	101	BCR	7	0
31	I	101	LMG	2	0
33	I	102	LMT	2	0
25	J	101	PL9	1	0
27	J	102	BCR	4	0
31	M	101	LMG	2	0
33	M	102	LMT	1	0
27	T	101	BCR	6	0
27	T	102	BCR	6	0
34	V	201	HEM	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/360 (93%)	0.16	10 (2%) 54 48	43, 64, 104, 149	0
1	a	335/360 (93%)	-0.07	4 (1%) 81 75	44, 65, 106, 149	0
2	B	490/510 (96%)	0.40	30 (6%) 25 25	46, 69, 103, 159	0
2	b	490/510 (96%)	0.36	35 (7%) 19 21	47, 71, 104, 159	0
3	C	447/461 (96%)	0.11	7 (1%) 74 68	54, 79, 106, 132	0
3	c	447/461 (96%)	0.26	12 (2%) 58 53	56, 81, 105, 135	0
4	D	340/352 (96%)	0.01	5 (1%) 76 70	44, 66, 103, 137	0
4	d	340/352 (96%)	-0.04	2 (0%) 90 87	45, 66, 102, 134	0
5	E	82/84 (97%)	0.12	2 (2%) 62 57	68, 92, 125, 130	0
5	e	82/84 (97%)	0.44	4 (4%) 33 32	70, 92, 125, 129	0
6	F	35/45 (77%)	0.08	2 (5%) 27 27	68, 84, 119, 139	0
6	f	35/45 (77%)	0.40	1 (2%) 55 50	73, 85, 120, 141	0
7	H	65/66 (98%)	0.87	10 (15%) 3 8	77, 94, 122, 138	0
7	h	65/66 (98%)	0.65	5 (7%) 16 19	73, 93, 120, 144	0
8	I	35/38 (92%)	0.21	1 (2%) 55 50	65, 79, 107, 118	0
8	i	35/38 (92%)	0.09	0 100 100	66, 81, 106, 120	0
9	J	34/40 (85%)	0.06	1 (2%) 55 50	69, 85, 95, 112	0
9	j	34/40 (85%)	-0.21	1 (2%) 55 50	74, 88, 95, 116	0
10	K	37/46 (80%)	0.19	1 (2%) 58 53	77, 87, 101, 122	0
10	k	37/46 (80%)	0.33	3 (8%) 15 18	73, 88, 108, 123	0
11	L	37/37 (100%)	0.04	0 100 100	48, 62, 128, 156	0
11	l	37/37 (100%)	-0.08	0 100 100	52, 60, 126, 158	0
12	M	34/36 (94%)	0.14	2 (5%) 26 26	56, 71, 110, 164	0
12	m	34/36 (94%)	0.30	3 (8%) 12 16	55, 69, 108, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	0.91	35 (14%) 3 9	50, 78, 122, 169	0
13	o	243/272 (89%)	0.67	22 (9%) 11 15	52, 78, 121, 167	0
14	T	32/32 (100%)	0.32	5 (15%) 3 8	55, 67, 158, 174	0
14	t	32/32 (100%)	-0.04	0 100 100	54, 69, 159, 168	0
15	U	97/134 (72%)	1.02	12 (12%) 5 11	56, 71, 92, 108	0
15	u	97/134 (72%)	0.83	6 (6%) 24 24	55, 71, 91, 111	0
16	V	137/163 (84%)	0.39	8 (5%) 26 27	53, 71, 86, 101	0
16	v	137/163 (84%)	0.81	12 (8%) 12 16	59, 72, 88, 95	0
17	g	28/46 (60%)	0.88	6 (21%) 1 6	95, 108, 126, 132	0
17	y	28/46 (60%)	0.35	1 (3%) 46 43	89, 107, 126, 131	0
18	X	37/41 (90%)	1.04	8 (21%) 1 6	76, 93, 124, 140	0
18	x	37/41 (90%)	1.03	10 (27%) 1 5	75, 90, 126, 141	0
19	Z	62/62 (100%)	1.18	10 (16%) 3 8	87, 104, 168, 185	0
19	z	62/62 (100%)	0.79	4 (6%) 22 23	88, 105, 172, 187	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.33	280 (5%) 29 30	43, 75, 115, 187	0

The worst 5 of 280 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	170	GLY	6.1
2	B	129	GLY	5.7
10	k	14	ALA	4.4
13	o	84	ASN	4.4
15	U	54	LYS	4.3

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
33	LMT	i	102	35/35	0.38	1.07	8.40	99,137,146,152	0
25	PL9	J	101	35/55	0.29	0.53	6.13	119,157,178,182	0
27	BCR	B	620	40/40	0.57	0.94	5.94	75,86,98,103	0
32	CL	A	416	1/1	0.44	1.00	5.65	49,49,49,49	0
27	BCR	C	514	40/40	0.84	1.01	4.74	73,80,87,94	0
27	BCR	c	514	40/40	0.80	1.11	4.58	76,82,88,89	0
27	BCR	z	101	40/40	0.67	1.31	4.55	86,96,112,115	0
31	LMG	C	521	45/55	0.33	1.12	4.29	84,119,143,175	0
33	LMT	B	629	35/35	0.48	0.67	4.22	70,137,165,168	0
28	DGD	D	409	63/66	0.56	0.74	4.05	104,127,181,188	0
23	CLA	b	605	65/65	0.50	0.91	4.01	88,108,124,137	0
31	LMG	c	519	45/55	0.55	0.97	3.91	86,119,142,171	0
33	LMT	b	627	35/35	0.56	0.88	3.73	100,140,152,154	0
23	CLA	C	513	65/65	0.75	0.92	3.68	95,109,142,149	0
27	BCR	C	515	40/40	0.80	1.03	3.65	85,92,115,116	0
23	CLA	c	511	65/65	0.82	0.69	3.57	75,91,102,108	0
28	DGD	d	409	63/66	0.59	0.62	3.54	106,128,181,190	0
22	BCT	d	401	4/4	0.86	0.48	3.49	87,91,92,94	0
27	BCR	j	102	40/40	0.49	0.51	3.47	110,128,180,184	0
33	LMT	I	102	35/35	0.65	0.68	3.46	99,135,144,145	0
23	CLA	B	612	65/65	0.90	0.51	3.44	61,72,82,86	0
23	CLA	c	507	65/65	0.82	0.66	3.40	83,93,105,111	0
23	CLA	b	607	65/65	0.83	0.78	3.37	68,82,92,103	0
27	BCR	b	622	40/40	0.66	0.65	3.37	72,83,94,96	0
23	CLA	c	501	65/65	0.85	0.81	3.36	67,82,92,94	0
23	CLA	c	513	65/65	0.66	1.06	3.31	93,109,142,148	0
23	CLA	D	403	65/65	0.86	0.87	3.30	74,87,123,124	0
31	LMG	E	101	44/55	0.45	0.66	3.29	87,123,132,139	0
27	BCR	y	101	40/40	0.68	0.78	3.25	79,86,106,109	0
33	LMT	D	410	31/35	0.60	0.95	3.25	83,133,154,159	0
33	LMT	B	625	35/35	0.72	0.76	3.21	95,139,149,152	0
23	CLA	c	503	65/65	0.83	0.81	3.14	77,89,97,103	0
23	CLA	B	601	65/65	0.53	1.00	3.09	92,108,131,137	0
23	CLA	B	604	65/65	0.83	0.58	3.07	59,67,104,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	DGD	B	627	52/66	0.72	0.50	3.05	75,105,178,180	0
23	CLA	B	609	65/65	0.90	0.73	3.05	74,89,104,106	0
23	CLA	c	512	65/65	0.77	1.05	2.97	83,104,146,152	0
23	CLA	C	512	65/65	0.83	0.84	2.97	89,101,144,149	0
27	BCR	c	515	40/40	0.78	0.79	2.93	75,86,95,101	0
27	BCR	H	101	40/40	0.70	1.03	2.90	83,96,130,131	0
23	CLA	B	605	65/65	0.87	0.66	2.89	58,78,86,92	0
31	LMG	i	101	43/55	0.72	0.67	2.78	84,120,162,177	0
30	SQD	d	408	43/54	0.64	0.74	2.73	67,109,152,157	0
33	LMT	B	628	35/35	0.39	0.62	2.70	72,126,141,144	0
23	CLA	b	613	65/65	0.81	0.73	2.68	65,93,104,114	0
33	LMT	d	410	31/35	0.39	0.87	2.68	83,134,157,157	0
23	CLA	C	509	65/65	0.86	0.63	2.60	62,81,95,98	0
31	LMG	a	402	42/55	0.66	0.51	2.56	72,100,119,143	0
23	CLA	B	610	65/65	0.84	0.68	2.44	69,81,88,92	0
23	CLA	A	407	65/65	0.84	0.49	2.31	56,66,127,129	0
23	CLA	B	603	65/65	0.89	0.66	2.27	65,81,94,109	0
33	LMT	b	603	35/35	0.61	0.48	2.26	73,119,136,138	0
31	LMG	I	101	43/55	0.74	0.56	2.24	73,118,166,178	0
33	LMT	b	604	35/35	0.68	0.49	2.24	69,133,158,160	0
25	PL9	j	101	35/55	0.32	0.43	2.21	120,160,178,182	0
32	CL	a	418	1/1	0.78	0.48	2.20	49,49,49,49	0
23	CLA	b	612	65/65	0.80	0.51	2.18	63,75,95,98	0
23	CLA	b	619	65/65	0.81	0.59	2.18	85,97,108,116	0
23	CLA	b	609	65/65	0.87	0.51	2.17	61,76,84,88	0
27	BCR	k	102	40/40	0.63	0.78	2.15	72,80,109,111	0
23	CLA	d	403	65/65	0.83	0.67	2.13	72,88,121,128	0
23	CLA	B	608	65/65	0.79	0.64	2.12	64,75,93,97	0
27	BCR	a	412	40/40	0.73	0.42	2.10	54,71,84,87	0
23	CLA	c	509	65/65	0.85	0.53	2.08	67,85,91,97	0
27	BCR	D	405	40/40	0.63	0.53	2.08	68,81,105,110	0
30	SQD	B	626	47/54	0.68	0.42	2.07	75,100,144,148	0
23	CLA	C	501	65/65	0.86	0.47	2.05	69,82,90,95	0
23	CLA	b	608	65/65	0.84	0.40	1.91	61,68,107,117	0
29	LHG	A	415	37/49	0.61	0.59	1.89	104,133,190,202	0
27	BCR	h	101	40/40	0.73	0.94	1.86	85,94,124,127	0
23	CLA	b	614	65/65	0.84	0.60	1.84	66,82,88,91	0
23	CLA	C	507	65/65	0.74	0.66	1.81	79,93,100,104	0
23	CLA	a	409	65/65	0.81	0.46	1.80	55,67,129,133	0
29	LHG	a	417	37/49	0.70	0.38	1.79	110,135,197,206	0
23	CLA	B	606	65/65	0.79	0.72	1.70	67,81,110,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	SQD	F	102	45/54	0.69	0.77	1.70	87,127,149,152	0
30	SQD	f	102	45/54	0.75	0.59	1.69	88,133,148,152	0
30	SQD	D	408	43/54	0.72	0.67	1.67	71,103,148,152	0
25	PL9	a	410	45/55	0.64	0.46	1.65	82,103,121,125	0
30	SQD	b	601	47/54	0.68	0.41	1.65	81,103,147,151	0
31	LMG	A	418	42/55	0.62	0.44	1.61	81,105,123,147	0
23	CLA	b	620	65/65	0.71	0.59	1.60	75,98,145,147	0
24	PHO	A	406	64/64	0.84	0.37	1.58	50,69,77,81	0
25	PL9	A	408	45/55	0.67	0.48	1.57	89,101,119,127	0
30	SQD	A	413	51/54	0.73	0.40	1.50	81,99,128,131	0
23	CLA	c	502	65/65	0.68	0.61	1.49	63,75,100,106	0
23	CLA	B	615	65/65	0.82	0.83	1.47	83,96,106,116	0
27	BCR	C	516	40/40	0.75	0.57	1.43	74,86,95,100	0
27	BCR	J	102	40/40	0.58	0.45	1.39	108,125,177,180	0
23	CLA	B	602	65/65	0.79	0.63	1.35	68,87,95,96	0
28	DGD	C	519	66/66	0.66	0.44	1.31	55,72,100,114	0
23	CLA	C	502	65/65	0.79	0.50	1.24	59,75,108,111	0
23	CLA	C	503	65/65	0.87	0.50	1.22	71,88,99,105	0
23	CLA	C	506	65/65	0.67	0.61	1.17	79,91,125,133	0
23	CLA	b	616	65/65	0.91	0.34	1.16	61,73,83,86	0
23	CLA	b	606	65/65	0.86	0.47	1.14	70,87,96,97	0
23	CLA	c	506	65/65	0.79	0.49	1.14	78,92,122,128	0
23	CLA	C	510	65/65	0.79	0.38	1.10	67,74,83,93	0
27	BCR	A	410	40/40	0.70	0.47	1.09	52,68,85,90	0
31	LMG	M	101	42/55	0.74	0.35	1.07	83,111,135,144	0
31	LMG	d	407	48/55	0.82	0.36	1.00	58,70,85,120	0
27	BCR	d	405	40/40	0.77	0.38	1.00	69,82,102,106	0
27	BCR	B	618	40/40	0.62	0.36	0.98	75,82,94,95	0
28	DGD	a	413	56/66	0.75	0.38	0.97	76,100,145,148	0
28	DGD	A	411	56/66	0.71	0.38	0.95	77,102,146,153	0
30	SQD	A	417	54/54	0.78	0.37	0.94	77,113,147,154	0
23	CLA	C	504	65/65	0.77	0.36	0.89	62,83,138,145	0
23	CLA	c	510	65/65	0.90	0.42	0.89	67,75,84,89	0
23	CLA	c	508	65/65	0.90	0.36	0.87	70,85,118,134	0
23	CLA	C	511	65/65	0.80	0.55	0.87	74,88,102,109	0
23	CLA	d	402	65/65	0.84	0.36	0.84	49,57,81,95	0
28	DGD	B	621	58/66	0.85	0.38	0.80	46,71,101,105	0
23	CLA	B	616	65/65	0.69	0.72	0.80	79,93,147,152	0
27	BCR	B	619	40/40	0.71	0.34	0.80	62,75,83,86	0
23	CLA	b	610	65/65	0.87	0.53	0.79	70,83,112,126	0
29	LHG	a	414	39/49	0.79	0.41	0.79	60,78,94,102	0
23	CLA	c	504	65/65	0.82	0.34	0.79	75,83,133,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	HEM	V	201	43/43	0.85	0.47	0.76	58,69,74,76	0
30	SQD	a	401	54/54	0.75	0.42	0.75	76,114,149,152	0
34	HEM	F	101	43/43	0.88	0.45	0.74	89,105,127,130	0
23	CLA	c	505	65/65	0.82	0.35	0.72	70,77,83,85	0
27	BCR	B	617	40/40	0.78	0.33	0.63	67,74,81,84	0
31	LMG	m	102	42/55	0.77	0.38	0.61	73,111,128,138	0
28	DGD	c	518	66/66	0.76	0.34	0.61	54,73,105,118	0
33	LMT	M	102	35/35	0.82	0.51	0.60	69,96,112,115	0
28	DGD	b	602	52/66	0.80	0.41	0.57	79,107,180,186	0
26	OEC	A	409	5/9	0.94	0.43	0.55	35,44,57,62	0
23	CLA	C	505	65/65	0.78	0.41	0.53	69,77,86,91	0
24	PHO	a	408	64/64	0.86	0.33	0.52	58,68,79,86	0
28	DGD	b	623	58/66	0.80	0.36	0.52	57,74,99,107	0
23	CLA	B	614	65/65	0.73	0.41	0.51	63,83,125,129	0
23	CLA	a	406	65/65	0.79	0.36	0.48	55,71,140,147	0
23	CLA	a	404	65/65	0.90	0.33	0.44	53,60,67,74	0
34	HEM	f	101	43/43	0.89	0.50	0.43	89,105,124,126	0
23	CLA	b	618	65/65	0.82	0.32	0.43	60,82,123,130	0
31	LMG	k	103	48/55	0.74	0.43	0.43	79,100,112,115	0
28	DGD	c	517	62/66	0.84	0.31	0.40	64,84,132,141	0
29	LHG	A	412	39/49	0.82	0.29	0.39	59,79,89,93	0
27	BCR	T	102	40/40	0.72	0.33	0.38	71,79,86,86	0
34	HEM	v	201	43/43	0.84	0.51	0.35	57,68,75,76	0
30	SQD	a	415	51/54	0.71	0.39	0.32	88,101,128,129	0
31	LMG	e	101	44/55	0.66	0.44	0.32	91,122,132,136	0
23	CLA	B	613	65/65	0.86	0.30	0.31	46,64,88,93	0
31	LMG	D	406	46/55	0.80	0.33	0.30	58,73,116,129	0
25	PL9	d	404	55/55	0.75	0.32	0.29	45,65,78,85	0
31	LMG	a	416	51/55	0.80	0.33	0.28	62,80,93,100	0
28	DGD	C	518	62/66	0.82	0.34	0.27	58,81,134,144	0
23	CLA	b	617	65/65	0.92	0.27	0.22	57,67,91,93	0
23	CLA	A	403	65/65	0.91	0.28	0.18	52,58,66,70	0
25	PL9	D	404	55/55	0.77	0.32	0.15	42,61,71,77	0
31	LMG	B	622	49/55	0.75	0.33	0.15	61,79,105,117	0
28	DGD	C	517	53/66	0.87	0.29	0.14	61,79,96,101	0
28	DGD	c	516	53/66	0.82	0.31	0.14	63,77,96,103	0
23	CLA	B	611	65/65	0.87	0.31	0.09	63,72,80,87	0
31	LMG	C	520	48/55	0.80	0.30	0.09	89,100,109,112	0
23	CLA	b	615	65/65	0.90	0.28	0.06	54,72,80,87	0
23	CLA	C	508	65/65	0.86	0.32	0.05	71,86,117,132	0
27	BCR	b	621	40/40	0.72	0.28	0.02	63,73,84,87	0
23	CLA	A	405	65/65	0.85	0.30	0.02	44,69,140,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	PHO	D	402	64/64	0.88	0.29	0.01	51,62,72,74	0
23	CLA	a	405	65/65	0.87	0.31	-0.03	44,53,69,73	0
26	OEC	a	411	5/9	0.92	0.35	-0.04	35,44,62,68	0
31	LMG	D	407	48/55	0.86	0.26	-0.08	54,72,81,120	0
27	BCR	T	101	40/40	0.79	0.32	-0.08	68,75,82,83	0
31	LMG	B	623	49/55	0.83	0.31	-0.15	58,76,84,87	0
22	BCT	A	402	4/4	0.87	0.33	-0.16	85,90,90,94	0
24	PHO	a	407	64/64	0.87	0.28	-0.19	53,63,70,73	0
23	CLA	D	401	65/65	0.88	0.27	-0.20	49,59,87,97	0
23	CLA	b	611	65/65	0.87	0.33	-0.21	54,64,89,92	0
31	LMG	b	624	49/55	0.85	0.27	-0.26	59,82,102,113	0
33	LMT	m	101	35/35	0.81	0.41	-0.35	68,93,112,114	0
31	LMG	b	625	49/55	0.81	0.32	-0.39	51,75,86,89	0
23	CLA	A	404	65/65	0.90	0.29	-0.42	44,54,67,74	0
23	CLA	B	607	65/65	0.86	0.28	-0.42	52,66,82,85	0
31	LMG	A	414	51/55	0.84	0.26	-0.45	63,77,92,95	0
31	LMG	d	406	46/55	0.89	0.24	-0.59	63,73,116,130	0
21	FE2	A	401	1/1	0.78	0.17	-1.38	64,64,64,64	0
21	FE2	a	403	1/1	0.87	0.16	-2.83	72,72,72,72	0
33	LMT	B	624	35/35	0.50	0.82	-	80,142,170,171	0
35	CA	K	101	1/1	0.62	0.53	-	86,86,86,86	0
35	CA	o	301	1/1	0.64	0.47	-	98,98,98,98	0
35	CA	O	301	1/1	0.35	0.47	-	112,112,112,112	0
33	LMT	b	626	35/35	0.62	0.67	-	76,139,174,176	0
35	CA	k	101	1/1	0.32	0.54	-	103,103,103,103	0

## 6.5 Other polymers

There are no such residues in this entry.