



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:46 PM GMT

PDB ID : 4TNI
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 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 : 4.60 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)

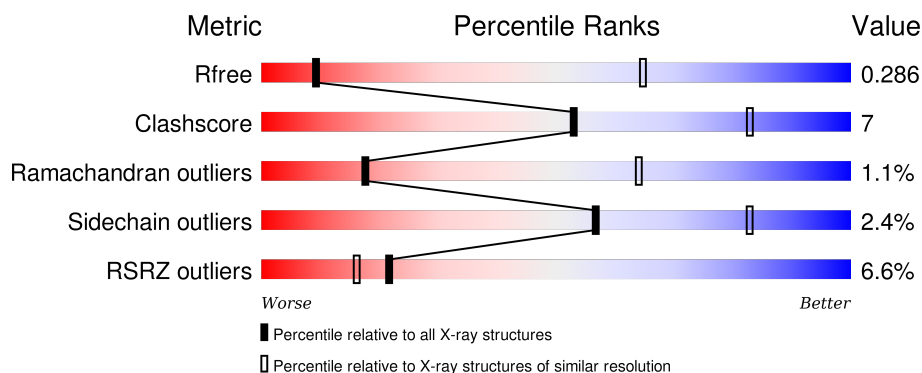
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1089 (5.52-3.60)
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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>70%</div> <div>25%</div> <div>• •</div> </div>
1	a	344	<div> <div>10%</div> <div>95%</div> <div>• •</div> </div>
2	B	510	<div> <div>5%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
2	b	510	<div> <div>7%</div> <div>94%</div> <div>• •</div> </div>

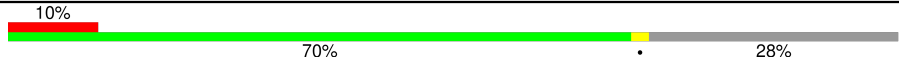

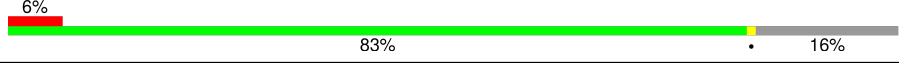

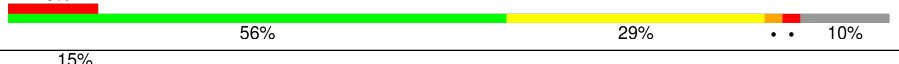
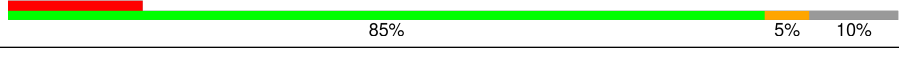
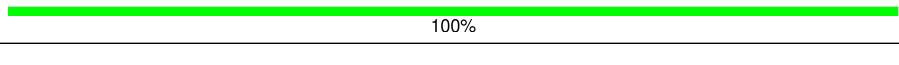

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Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

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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	-	-	-
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	405	X	-	-	-
22	CLA	D	406	X	-	-	X
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	X	-	-	-
22	CLA	a	407	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
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	405	X	-	-	X
22	CLA	d	406	X	-	-	X
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	d	407	-	-	-	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	J	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	409	-	-	-	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	C	517	-	-	-	X
25	DGD	D	410	-	-	-	X
25	DGD	a	410	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	410	-	-	-	X
27	LMG	A	414	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	m	101	-	-	-	X
28	OEX	A	411	-	-	-	X
28	OEX	a	414	-	-	-	X
29	SQD	B	622	-	-	-	X
29	SQD	B	626	-	-	-	X
29	SQD	F	103	-	-	-	X
29	SQD	a	401	-	-	-	X
29	SQD	b	602	-	-	-	X
29	SQD	d	403	-	-	-	X
29	SQD	f	103	-	-	-	X
30	LMT	B	624	-	-	-	X
30	LMT	B	627	-	-	-	X
30	LMT	B	628	-	-	-	X
30	LMT	D	411	-	-	-	X
30	LMT	I	102	-	-	-	X
30	LMT	M	103	-	-	-	X
30	LMT	b	603	-	-	-	X
30	LMT	b	604	-	-	-	X
30	LMT	b	627	-	-	-	X
30	LMT	d	411	-	-	-	X
30	LMT	i	102	-	-	-	X
31	PHO	d	401	-	-	-	X
32	CL	a	413	-	-	-	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 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				

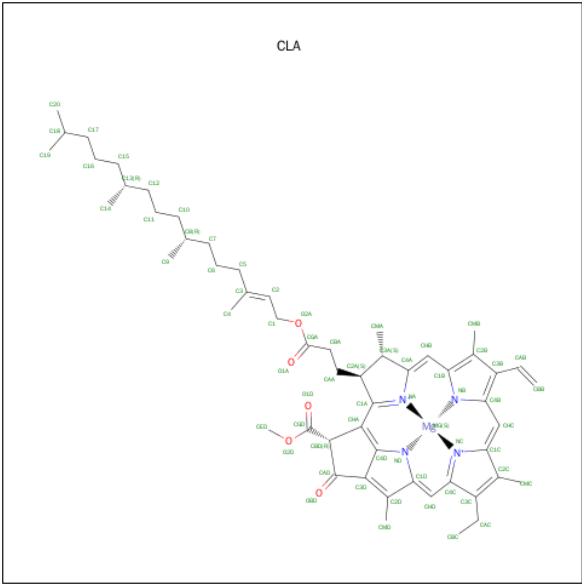
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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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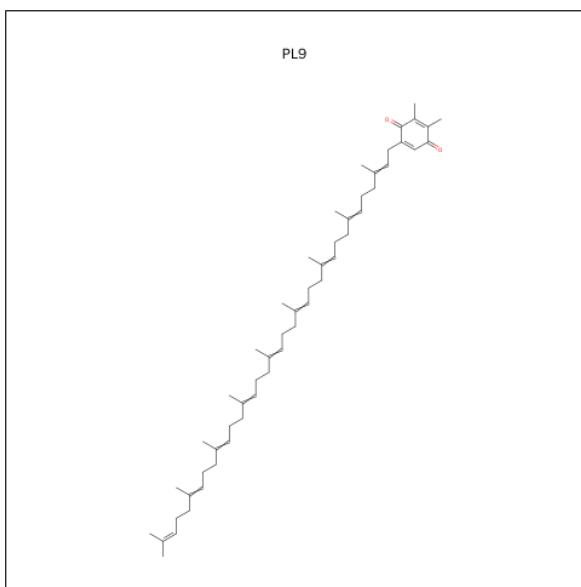
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 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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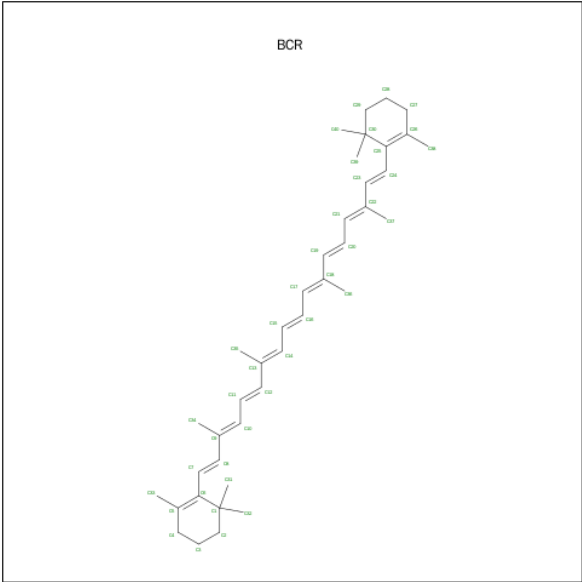
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: $C_{53}H_{80}O_2$).



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: $C_{40}H_{56}$).



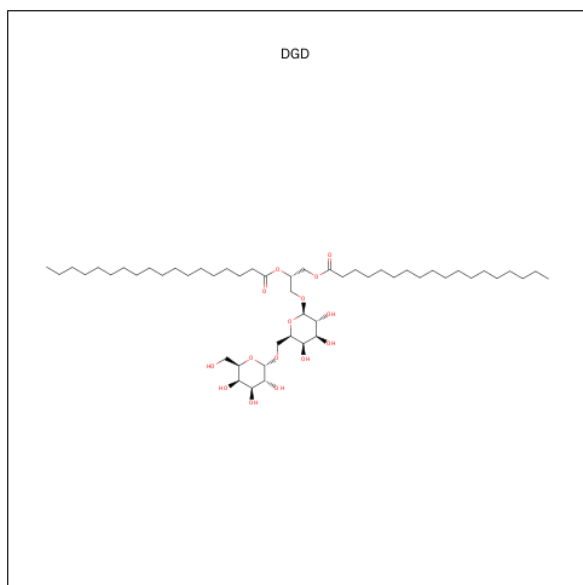
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total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



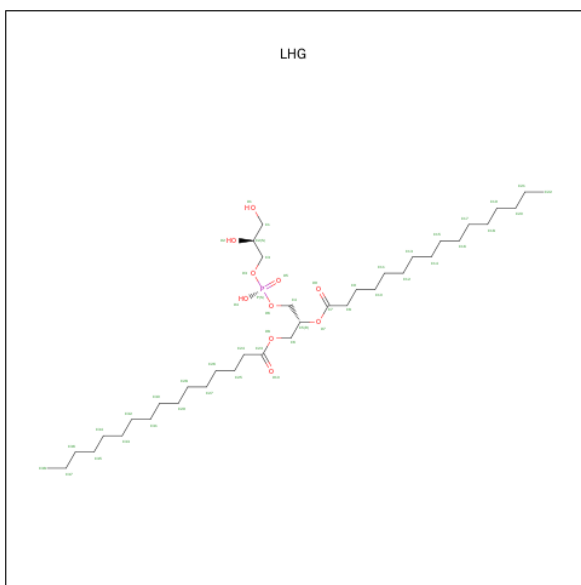
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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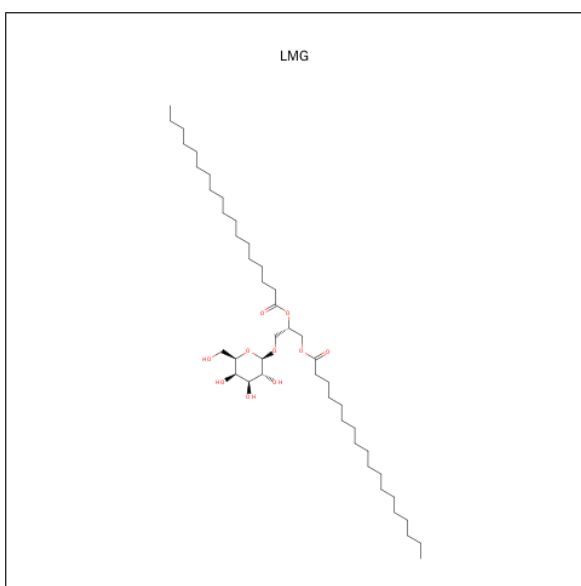
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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



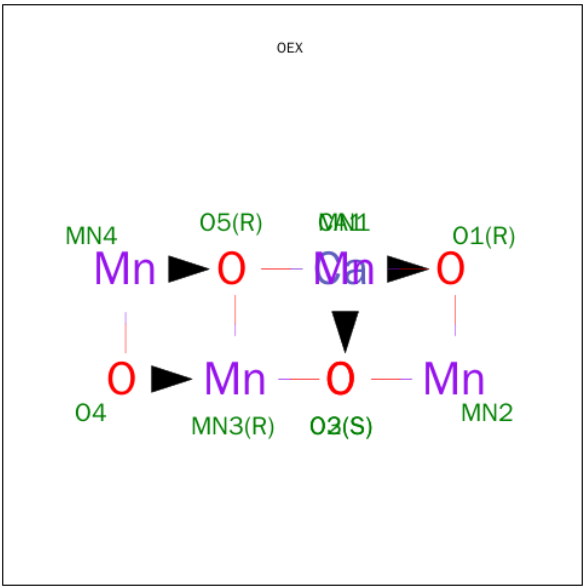
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

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



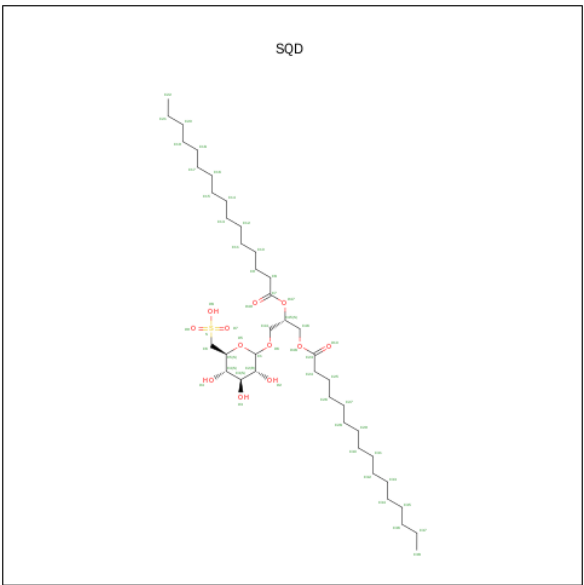
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	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	a	1	Total	C	O	0	0
			51	41	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		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



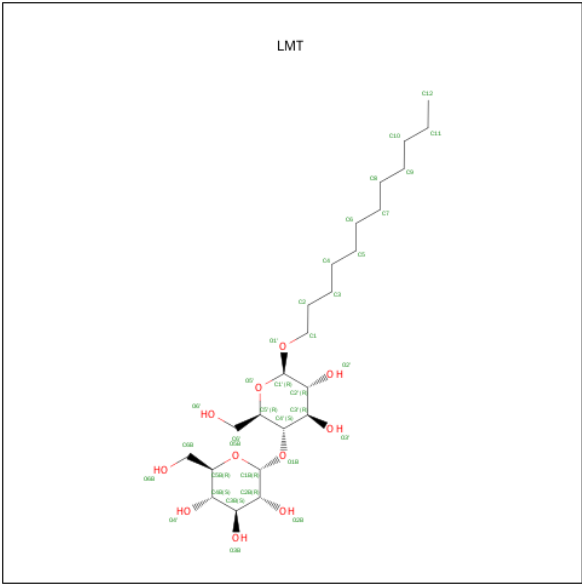
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 29 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
29	A	1	Total	C	O	S	0	0
			51	38	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			43	30	12	1		
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	F	1	Total	C	O	S	0	0
			45	32	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O	S	0	0
			51	38	12	1		
29	b	1	Total	C	O	S	0	0
			47	34	12	1		
29	d	1	Total	C	O	S	0	0
			43	30	12	1		
29	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



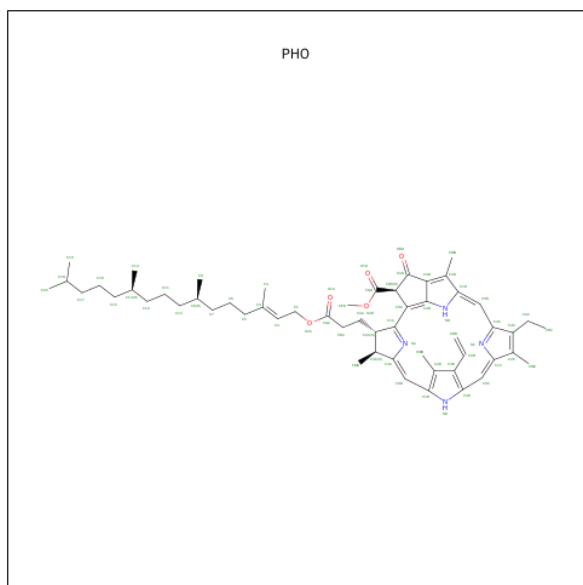
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).

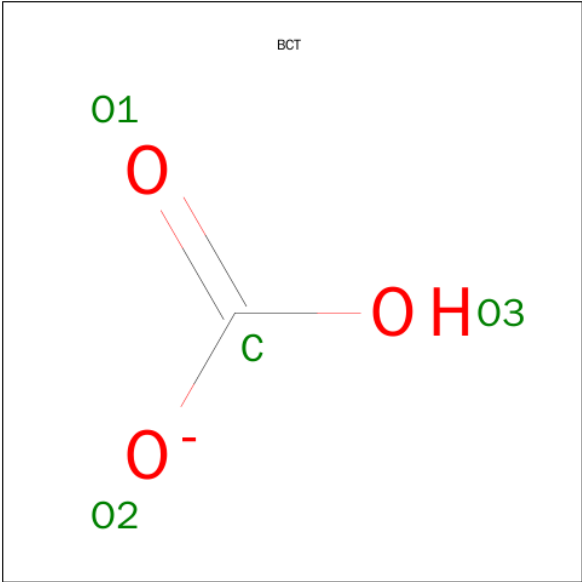


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		

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

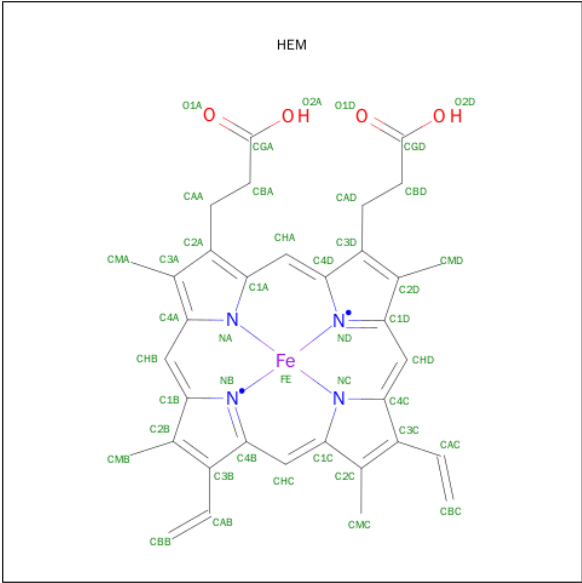
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	a	1	Total	Cl	0	0
			1	1		
32	D	1	Total	Cl	0	0
			1	1		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

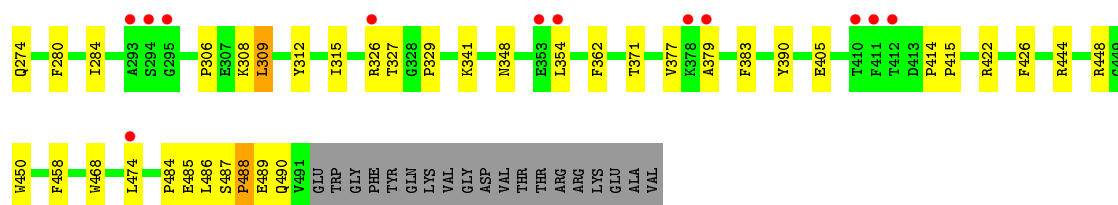
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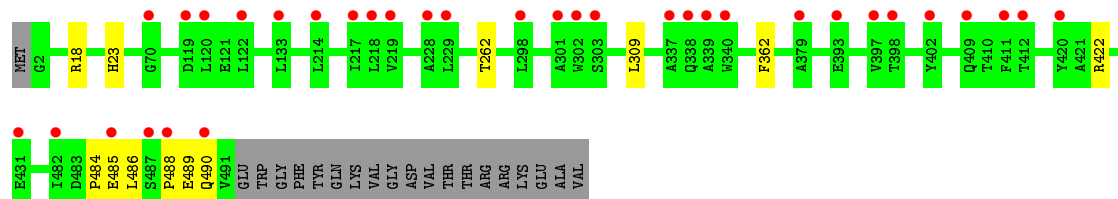
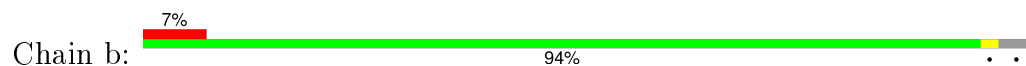
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

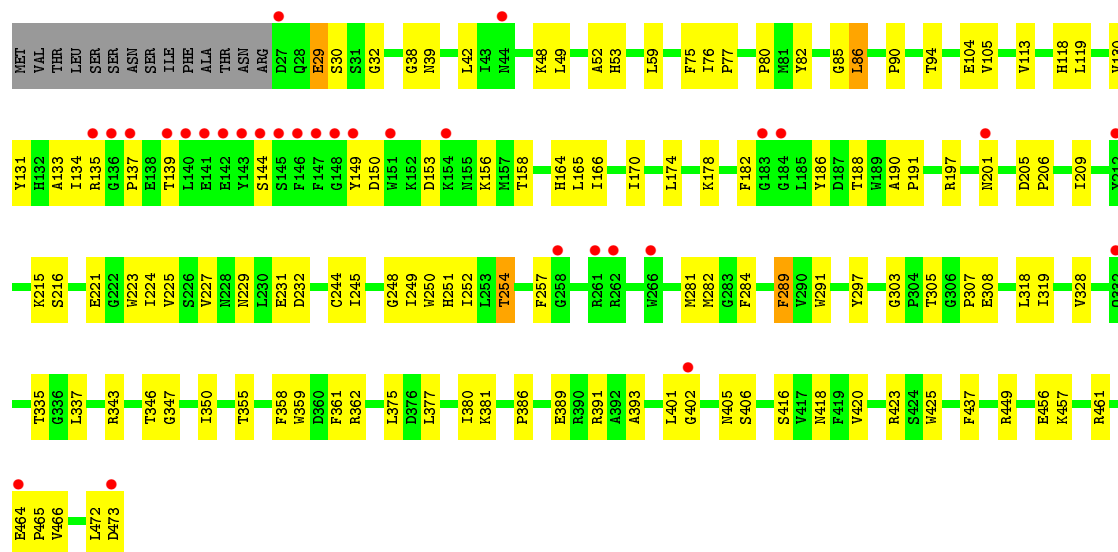
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total 1	Ca 1	0	0
35	O	1	Total 1	Ca 1	0	0
35	K	1	Total 1	Ca 1	0	0
35	k	1	Total 1	Ca 1	0	0



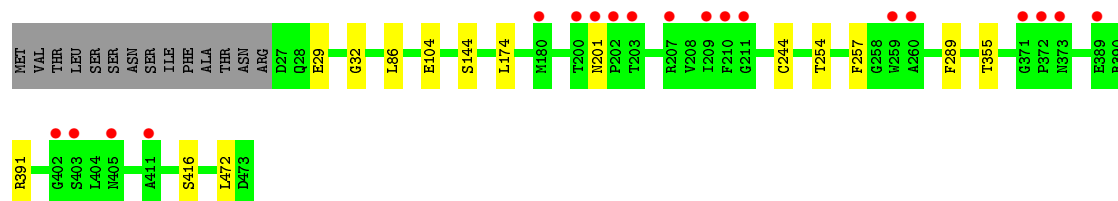
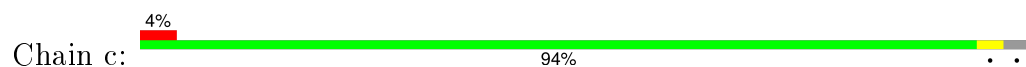
• Molecule 2: Photosystem II core light harvesting protein



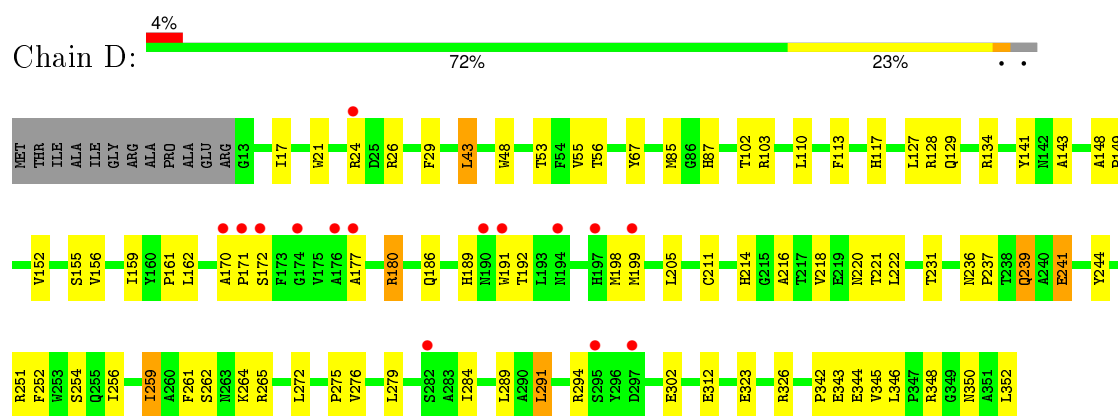
• Molecule 3: Photosystem II CP43 protein



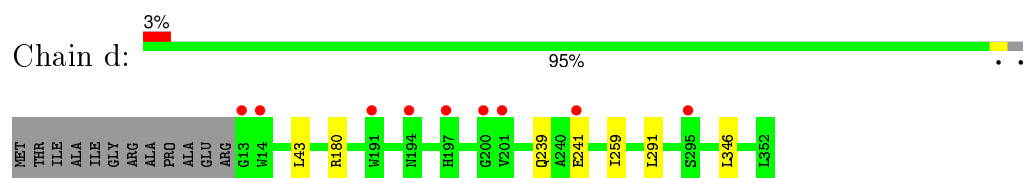
• Molecule 3: Photosystem II CP43 protein



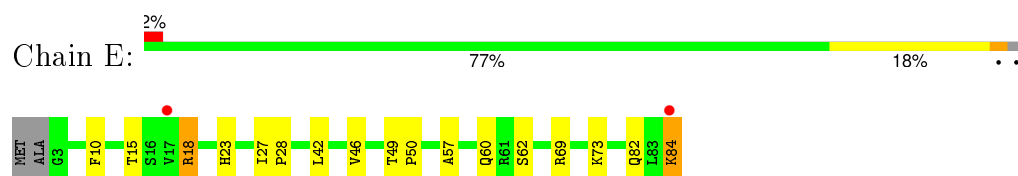
• Molecule 4: Photosystem II D2 protein



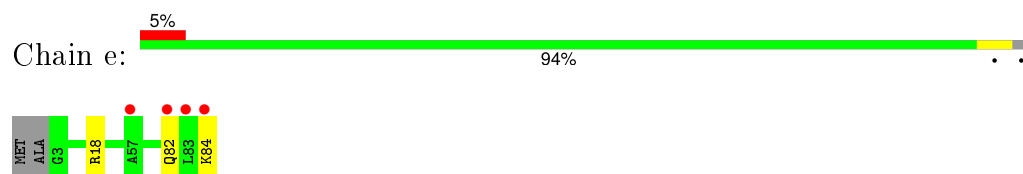
- Molecule 4: Photosystem II D2 protein



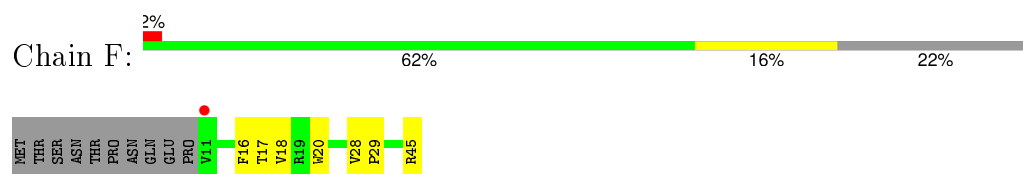
- Molecule 5: Cytochrome b559 subunit alpha



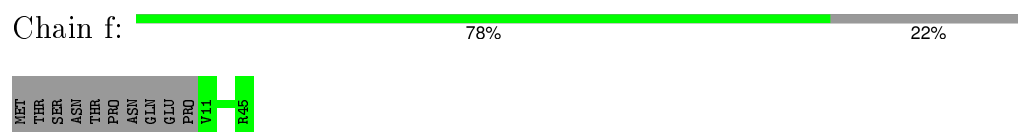
- Molecule 5: Cytochrome b559 subunit alpha



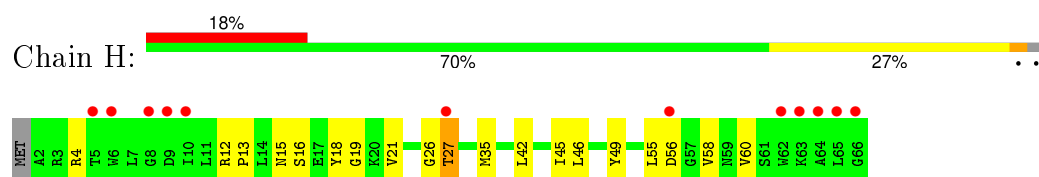
- Molecule 6: Cytochrome b559 subunit beta



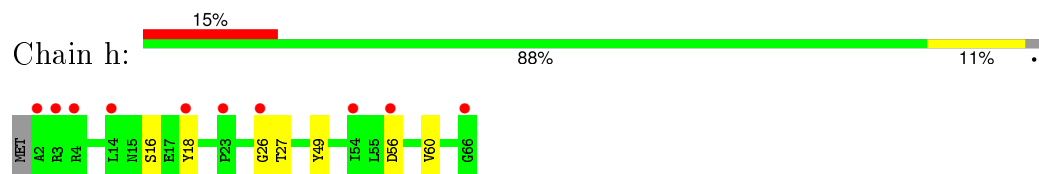
- Molecule 6: Cytochrome b559 subunit beta



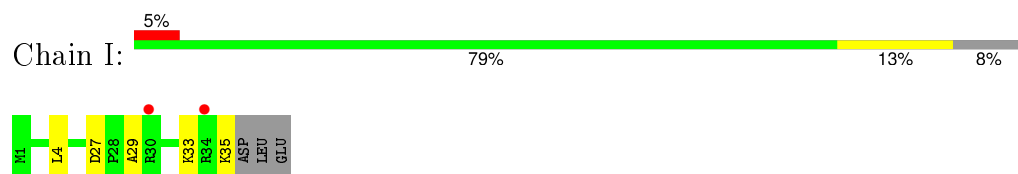
- Molecule 7: Photosystem II reaction center protein H



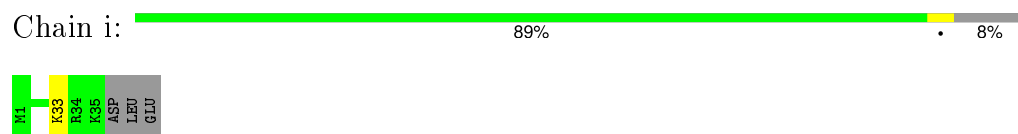
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



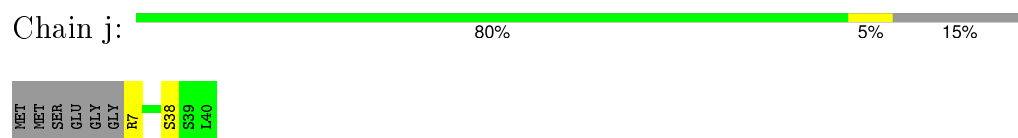
- Molecule 8: Photosystem II reaction center protein I



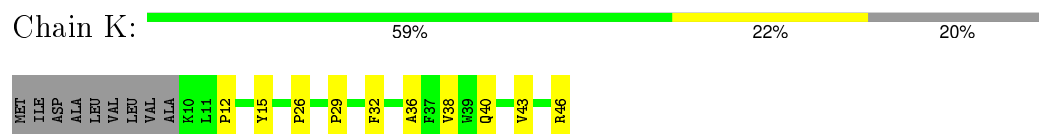
- Molecule 9: Photosystem II reaction center protein J



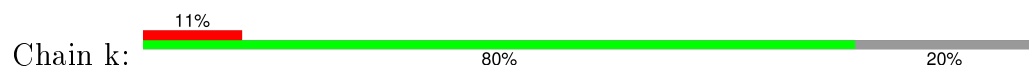
- Molecule 9: Photosystem II reaction center protein J

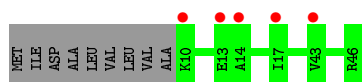


- Molecule 10: Photosystem II reaction center protein K

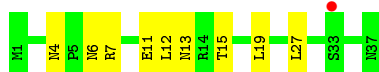
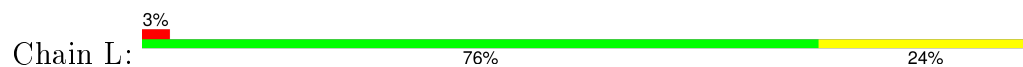


- Molecule 10: Photosystem II reaction center protein K

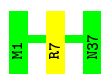




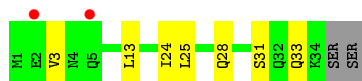
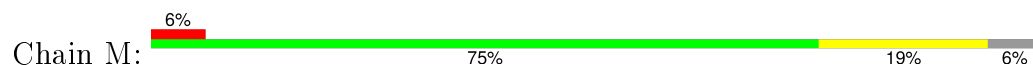
- Molecule 11: Photosystem II reaction center protein L



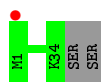
- Molecule 11: Photosystem II reaction center protein L



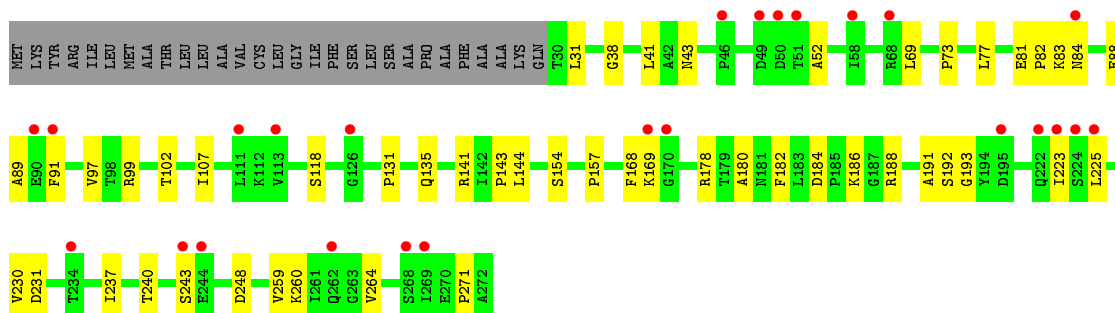
- Molecule 12: Photosystem II reaction center protein M



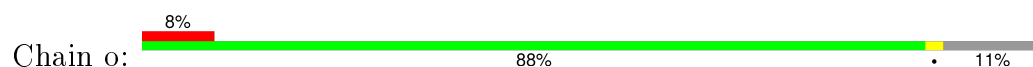
- Molecule 12: Photosystem II reaction center protein M

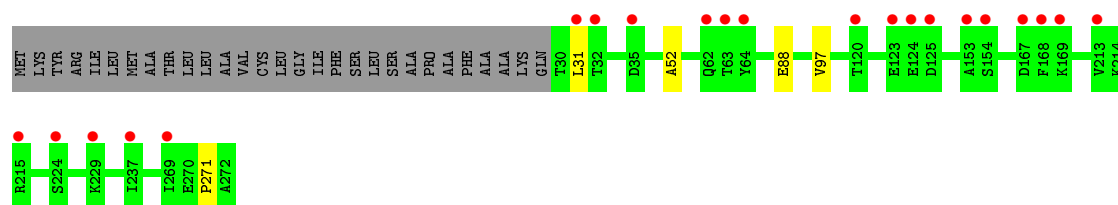


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

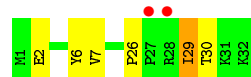
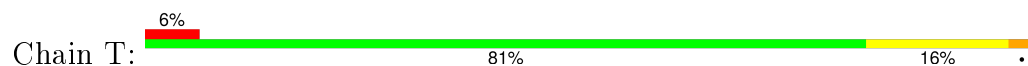


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

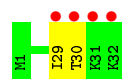




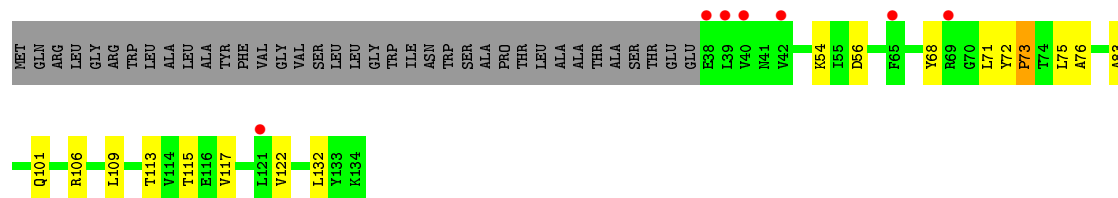
- Molecule 14: Photosystem II reaction center protein T



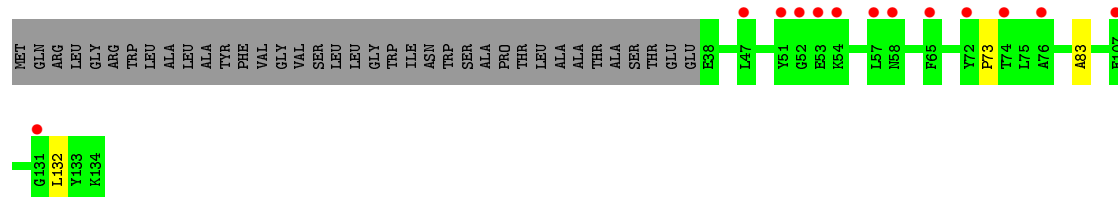
- Molecule 14: Photosystem II reaction center protein T



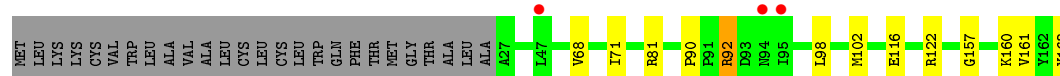
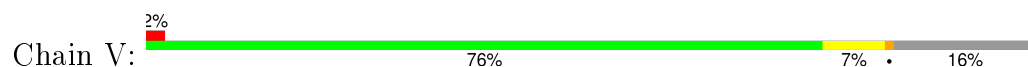
- Molecule 15: Photosystem II 12 kDa extrinsic protein



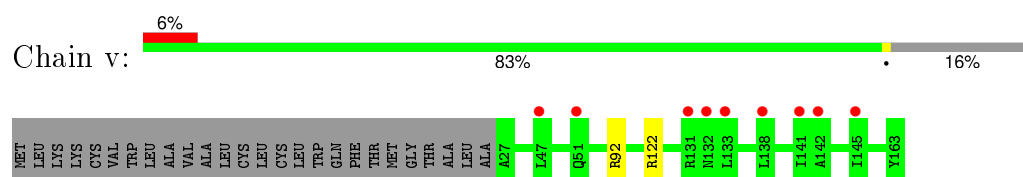
- Molecule 15: Photosystem II 12 kDa extrinsic protein



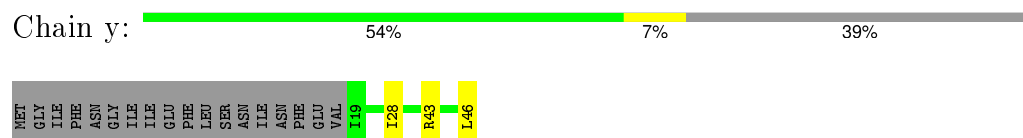
- Molecule 16: Cytochrome c-550



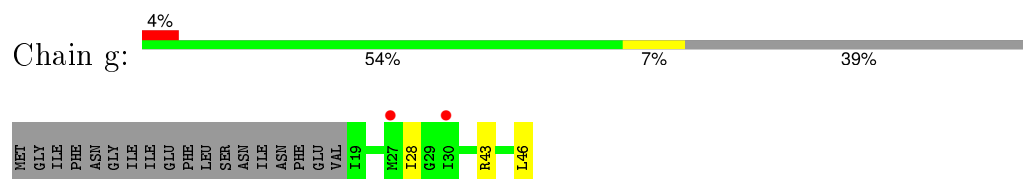
- Molecule 16: Cytochrome c-550



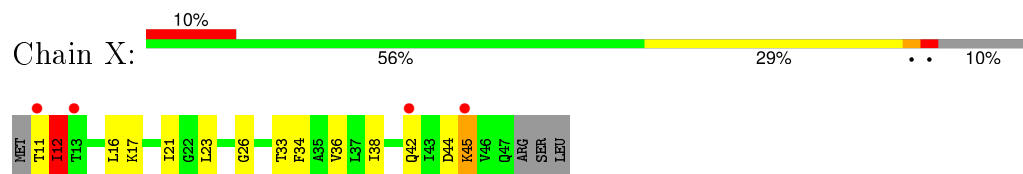
- Molecule 17: Photosystem II reaction center protein Ycf12



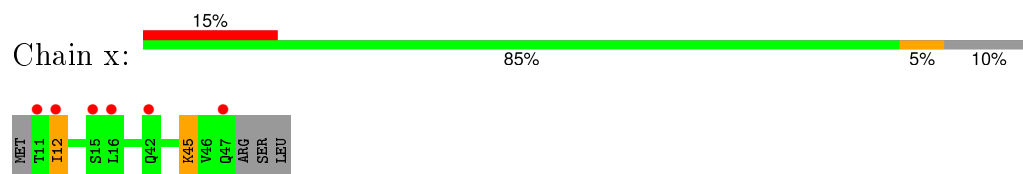
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



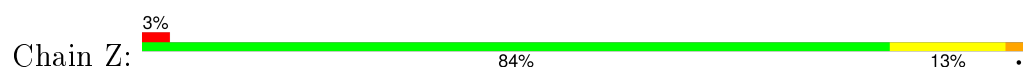
There are no outlier residues recorded for this chain.

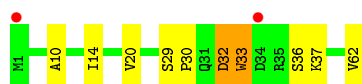
- Molecule 19: Photosystem II reaction center protein Y



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	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.7 (72.96-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.278 , 0.284 0.295 , 0.286	Depositor DCC
R_{free} test set	2522 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 126.1	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 51515 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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	0.22	0/3556	0.41	0/4842
3	c	0.22	0/3556	0.41	0/4842
4	D	0.23	0/2801	0.40	0/3818
4	d	0.24	0/2801	0.40	0/3818
5	E	0.23	0/685	0.42	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	0.45	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.21	0/255	0.39	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.48	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	0.43	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	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.42	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	0.40	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.21	0/202	0.45	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.25	0/273	0.43	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 ⓘ

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	78	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	83	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	74	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	17	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	8	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	7	0
11	l	304	0	316	0	0
12	M	267	0	289	7	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	5	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	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	8	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	44	0
22	B	975	0	1080	90	0
22	C	845	0	936	47	0
22	D	130	0	144	11	0
22	H	65	0	72	9	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	4	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	3	0
24	B	160	0	224	10	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	4	0
24	H	40	0	56	2	0
24	J	40	0	56	1	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	11	0
25	D	63	0	87	2	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	4	0
27	D	143	0	196	11	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	93	0	126	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	m	42	0	54	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	105	0	147	6	0
29	B	90	0	111	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	45	0	54	3	0
29	a	105	0	147	0	0
29	b	47	0	61	0	0
29	d	43	0	50	0	0
29	f	45	0	54	0	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	1	0
30	M	70	0	91	0	0
30	b	140	0	183	0	0
30	d	31	0	35	0	0
30	i	35	0	46	0	0
31	D	128	0	148	15	0
31	d	128	0	148	0	0
32	D	1	0	0	0	0
32	a	1	0	0	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	51372	579	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 579 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	1.55	0.87
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.51	0.81
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.61	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%)	311 (93%)	18 (5%)	4 (1%)	16	62
1	a	333/344 (97%)	309 (93%)	20 (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%)	36 (8%)	4 (1%)	21	67
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	46	83
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	46	83
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	15	60
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	15	60
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	32
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3	32
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	44
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	44
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	16	62
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	42
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5	42
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9	52
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9	52
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	38
17	y	26/46 (56%)	19 (73%)	6 (23%)	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%)	4675 (91%)	408 (8%)	55 (1%)	17	64

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN

5.3.2 Protein sidechains ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	269 (98%)	6 (2%)	60	84
5	E	72/73 (99%)	70 (97%)	2 (3%)	51	79
5	e	72/73 (99%)	70 (97%)	2 (3%)	51	79
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	17	56
7	h	53/55 (96%)	49 (92%)	4 (8%)	17	56
8	I	32/35 (91%)	31 (97%)	1 (3%)	47	78
8	i	32/35 (91%)	31 (97%)	1 (3%)	47	78
9	J	24/28 (86%)	23 (96%)	1 (4%)	36	72
9	j	24/28 (86%)	23 (96%)	1 (4%)	36	72
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	50	79
11	l	35/35 (100%)	34 (97%)	1 (3%)	50	79
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	82	92
13	o	202/228 (89%)	200 (99%)	2 (1%)	82	92
14	T	29/29 (100%)	28 (97%)	1 (3%)	44	77
14	t	29/29 (100%)	28 (97%)	1 (3%)	44	77
15	U	84/112 (75%)	83 (99%)	1 (1%)	78	90
15	u	84/112 (75%)	83 (99%)	1 (1%)	78	90
16	V	116/138 (84%)	114 (98%)	2 (2%)	68	88
16	v	116/138 (84%)	114 (98%)	2 (2%)	68	88
17	g	20/37 (54%)	18 (90%)	2 (10%)	9	41
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	4142 (98%)	102 (2%)	57	83

5 of 102 residues with a non-rotameric sidechain are listed below:

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	A	402	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	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	1.19	6 (9%)
22	CLA	A	405	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
23	PL9	A	406	-	45,45,55	1.12	3 (6%)	56,57,69	1.59	12 (21%)
24	BCR	A	407	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	6 (10%)
25	DGD	A	408	-	57,57,67	0.91	0	71,71,81	1.44	8 (11%)
26	LHG	A	409	-	38,38,48	0.67	0	39,44,54	1.19	3 (7%)
27	LMG	A	410	-	51,51,55	0.74	1 (1%)	59,59,63	1.36	6 (10%)
28	OEX	A	411	1,3	0,15,15	0.00	-	0,32,32	0.00	-
29	SQD	A	412	-	50,51,54	0.95	3 (6%)	58,62,65	1.96	9 (15%)
29	SQD	A	413	-	53,54,54	0.93	3 (5%)	61,65,65	1.64	9 (14%)
27	LMG	A	414	-	42,42,55	0.82	0	50,50,63	1.25	4 (8%)
22	CLA	B	601	-	55,73,73	0.95	4 (7%)	61,113,113	1.20	9 (14%)
22	CLA	B	602	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	9 (14%)
22	CLA	B	603	-	55,73,73	0.95	3 (5%)	61,113,113	1.25	8 (13%)
22	CLA	B	604	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	B	605	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	B	606	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	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	0.97	3 (5%)	61,113,113	1.19	8 (13%)
22	CLA	B	609	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	B	610	-	55,73,73	1.03	4 (7%)	61,113,113	1.33	7 (11%)
22	CLA	B	611	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	8 (13%)
22	CLA	B	612	-	55,73,73	0.92	3 (5%)	61,113,113	1.22	8 (13%)
22	CLA	B	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	B	614	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	8 (13%)
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	1.08	2 (4%)	56,56,56	1.24	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.34	9 (16%)
24	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	11 (19%)
24	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	8 (14%)
25	DGD	B	620	-	59,59,67	0.89	1 (1%)	73,73,81	1.35	7 (9%)
27	LMG	B	621	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	6 (10%)
29	SQD	B	622	-	42,43,54	1.03	2 (4%)	50,54,65	1.89	10 (20%)
30	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	0.99	2 (4%)
30	LMT	B	624	-	36,36,36	1.07	4 (11%)	47,47,47	1.04	3 (6%)
25	DGD	B	625	-	53,53,67	1.05	3 (5%)	67,67,81	1.35	7 (10%)
29	SQD	B	626	-	46,47,54	1.00	4 (8%)	54,58,65	1.94	9 (16%)
30	LMT	B	627	-	36,36,36	1.09	4 (11%)	47,47,47	0.98	2 (4%)
30	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	1.17	8 (13%)
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	1.22	8 (13%)
22	CLA	C	504	-	55,73,73	0.96	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	C	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	8 (13%)
22	CLA	C	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	C	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.25	7 (11%)
22	CLA	C	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	C	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	6 (9%)
22	CLA	C	510	3	55,73,73	0.94	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	C	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	C	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
24	BCR	C	513	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	10 (17%)
24	BCR	C	514	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	9 (16%)
25	DGD	C	515	-	54,54,67	0.95	2 (3%)	68,68,81	1.27	8 (11%)
25	DGD	C	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.45	14 (18%)
25	DGD	C	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.43	10 (12%)
27	LMG	C	518	-	45,45,55	0.76	0	53,53,63	1.28	4 (7%)
26	LHG	C	519	-	36,36,48	0.70	0	37,42,54	1.28	4 (10%)
22	CLA	C	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	8 (13%)
27	LMG	C	521	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
31	PHO	D	401	-	67,69,69	1.21	9 (13%)	84,99,99	1.02	5 (5%)
31	PHO	D	402	-	67,69,69	1.23	10 (14%)	84,99,99	1.02	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	405	-	55,73,73	0.94	3 (5%)	61,113,113	1.17	8 (13%)
22	CLA	D	406	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	D	407	-	55,55,55	1.16	3 (5%)	68,69,69	1.58	15 (22%)
27	LMG	D	408	-	49,49,55	0.75	1 (2%)	57,57,63	1.31	5 (8%)
27	LMG	D	409	-	48,48,55	0.76	0	56,56,63	1.38	5 (8%)
25	DGD	D	410	-	64,64,67	0.90	0	78,78,81	1.34	10 (12%)
30	LMT	D	411	-	32,32,36	1.15	4 (12%)	43,43,47	1.05	2 (4%)
27	LMG	D	412	-	46,46,55	0.76	1 (2%)	54,54,63	1.31	5 (9%)
27	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.29	5 (9%)
34	HEM	F	101	5,6	30,50,50	2.11	10 (33%)	24,82,82	2.31	9 (37%)
24	BCR	F	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
29	SQD	F	103	-	44,45,54	1.02	4 (9%)	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	1.09	2 (4%)	56,56,56	1.22	3 (5%)
27	LMG	I	101	-	43,43,55	0.79	0	51,51,63	1.27	5 (9%)
30	LMT	I	102	-	36,36,36	1.08	4 (11%)	47,47,47	1.08	2 (4%)
23	PL9	J	101	-	35,35,55	1.15	1 (2%)	44,45,69	1.54	6 (13%)
24	BCR	J	102	-	41,41,41	1.05	3 (7%)	56,56,56	1.61	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	0.84	1 (2%)	50,50,63	1.24	4 (8%)
30	LMT	M	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.03	3 (6%)
30	LMT	M	103	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	3 (6%)
34	HEM	V	201	16	30,50,50	2.23	11 (36%)	24,82,82	2.25	6 (25%)
29	SQD	a	401	-	53,54,54	0.94	3 (5%)	61,65,65	1.64	8 (13%)
27	LMG	a	402	-	42,42,55	0.82	0	50,50,63	1.26	4 (8%)
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	1.20	6 (9%)
22	CLA	a	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	a	407	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
23	PL9	a	408	-	45,45,55	1.18	3 (6%)	56,57,69	1.59	13 (23%)
24	BCR	a	409	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	7 (12%)
25	DGD	a	410	-	57,57,67	0.91	1 (1%)	71,71,81	1.42	8 (11%)
26	LHG	a	411	-	38,38,48	0.67	1 (2%)	39,44,54	1.19	3 (7%)
27	LMG	a	412	-	51,51,55	0.75	1 (1%)	59,59,63	1.34	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	OEX	a	414	1,3	0,15,15	0.00	-	0,32,32	0.00	-
29	SQD	a	415	-	50,51,54	0.95	3 (6%)	58,62,65	1.97	9 (15%)
25	DGD	b	601	-	53,53,67	1.03	4 (7%)	67,67,81	1.35	7 (10%)
29	SQD	b	602	-	46,47,54	1.01	4 (8%)	54,58,65	1.97	9 (16%)
30	LMT	b	603	-	36,36,36	1.10	4 (11%)	47,47,47	0.97	1 (2%)
30	LMT	b	604	-	36,36,36	1.10	4 (11%)	47,47,47	1.07	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	1.20	8 (13%)
22	CLA	b	607	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	8 (13%)
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	1.21	6 (9%)
22	CLA	b	610	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	b	611	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	b	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.17	7 (11%)
22	CLA	b	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	b	614	-	55,73,73	1.03	4 (7%)	61,113,113	1.33	7 (11%)
22	CLA	b	615	-	55,73,73	0.94	4 (7%)	61,113,113	1.21	8 (13%)
22	CLA	b	616	-	55,73,73	0.93	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	617	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	b	618	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	9 (14%)
22	CLA	b	619	-	55,73,73	0.94	4 (7%)	61,113,113	1.17	6 (9%)
24	BCR	b	620	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
24	BCR	b	621	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	9 (16%)
24	BCR	b	622	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	10 (17%)
24	BCR	b	623	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	8 (14%)
25	DGD	b	624	-	59,59,67	0.89	0	73,73,81	1.34	6 (8%)
27	LMG	b	625	-	49,49,55	0.76	1 (2%)	57,57,63	1.32	6 (10%)
30	LMT	b	626	-	36,36,36	1.10	4 (11%)	47,47,47	0.98	2 (4%)
30	LMT	b	627	-	36,36,36	1.07	4 (11%)	47,47,47	1.02	3 (6%)
22	CLA	c	501	-	55,73,73	0.96	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	c	502	-	55,73,73	0.96	4 (7%)	61,113,113	1.21	7 (11%)
22	CLA	c	503	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	7 (11%)
22	CLA	c	504	-	55,73,73	0.96	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	c	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.27	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	0.94	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	c	511	-	55,73,73	0.93	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	c	512	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	7 (11%)
24	BCR	c	513	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	10 (17%)
24	BCR	c	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	8 (14%)
25	DGD	c	515	-	54,54,67	0.94	1 (1%)	68,68,81	1.28	7 (10%)
25	DGD	c	516	-	63,63,67	0.89	1 (1%)	77,77,81	1.45	12 (15%)
25	DGD	c	517	-	67,67,67	0.86	2 (2%)	81,81,81	1.42	9 (11%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.28	5 (9%)
26	LHG	c	519	-	36,36,48	0.71	0	37,42,54	1.27	4 (10%)
22	CLA	c	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	8 (13%)
24	BCR	c	521	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	8 (14%)
27	LMG	c	522	-	48,48,55	0.76	0	56,56,63	1.30	5 (8%)
31	PHO	d	401	-	67,69,69	1.21	10 (14%)	84,99,99	1.02	5 (5%)
31	PHO	d	402	-	67,69,69	1.23	8 (11%)	84,99,99	1.00	4 (4%)
29	SQD	d	403	-	42,43,54	1.04	3 (7%)	50,54,65	1.90	10 (20%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	405	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	d	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
23	PL9	d	407	-	55,55,55	1.18	3 (5%)	68,69,69	1.59	14 (20%)
27	LMG	d	408	-	49,49,55	0.75	0	57,57,63	1.31	5 (8%)
27	LMG	d	409	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
25	DGD	d	410	-	64,64,67	0.90	1 (1%)	78,78,81	1.35	10 (12%)
30	LMT	d	411	-	32,32,36	1.15	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	d	412	-	46,46,55	0.77	1 (2%)	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	2.11	12 (40%)	24,82,82	2.32	10 (41%)
24	BCR	f	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
29	SQD	f	103	-	44,45,54	1.02	4 (9%)	52,56,65	1.77	9 (17%)
24	BCR	g	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	6 (10%)
22	CLA	h	101	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
27	LMG	i	101	-	43,43,55	0.80	0	51,51,63	1.28	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	i	102	-	36,36,36	1.07	4 (11%)	47,47,47	1.06	2 (4%)
23	PL9	j	101	-	35,35,55	1.13	2 (5%)	44,45,69	1.54	6 (13%)
24	BCR	j	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.59	13 (23%)
27	LMG	m	101	-	42,42,55	0.84	1 (2%)	50,50,63	1.23	4 (8%)
34	HEM	v	201	16	30,50,50	2.22	11 (36%)	24,82,82	2.24	6 (25%)
24	BCR	x	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	4 (7%)
24	BCR	y	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.27	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	A	406	-	-	0/41/61/73	0/1/1/1
24	BCR	A	407	-	-	0/29/63/63	0/2/2/2
25	DGD	A	408	-	-	0/45/85/95	0/2/2/2
26	LHG	A	409	-	-	0/43/43/53	0/0/0/0
27	LMG	A	410	-	-	0/46/66/70	0/1/1/1
28	OEX	A	411	1,3	-	0/0/68/68	0/0/6/6
29	SQD	A	412	-	-	0/46/66/69	0/1/1/1
29	SQD	A	413	-	-	0/49/69/69	0/1/1/1
27	LMG	A	414	-	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
29	SQD	B	622	-	-	1/38/58/69	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
30	LMT	B	624	-	-	0/21/61/61	0/2/2/2
25	DGD	B	625	-	-	0/41/81/95	0/2/2/2
29	SQD	B	626	-	-	0/42/62/69	0/1/1/1
30	LMT	B	627	-	-	0/21/61/61	0/2/2/2
30	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PHO	D	401	-	-	0/53/103/103	0/1/6/6
31	PHO	D	402	-	-	0/53/103/103	0/1/6/6
33	BCT	D	404	21	-	0/0/0/0	0/0/0/0
22	CLA	D	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	D	406	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PL9	D	407	-	-	0/53/73/73	0/1/1/1
27	LMG	D	408	-	-	0/44/64/70	0/1/1/1
27	LMG	D	409	-	-	0/43/63/70	0/1/1/1
25	DGD	D	410	-	-	0/52/92/95	0/2/2/2
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
27	LMG	D	412	-	-	0/41/61/70	0/1/1/1
27	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
24	BCR	F	102	-	-	0/29/63/63	0/2/2/2
29	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
30	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	-	-	0/37/57/70	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/10/54/54	0/0/8/8
29	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
22	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	a	408	-	-	0/41/61/73	0/1/1/1
24	BCR	a	409	-	-	0/29/63/63	0/2/2/2
25	DGD	a	410	-	-	0/45/85/95	0/2/2/2
26	LHG	a	411	-	-	0/43/43/53	0/0/0/0
27	LMG	a	412	-	-	0/46/66/70	0/1/1/1
28	OEX	a	414	1,3	-	0/0/68/68	0/0/6/6
29	SQD	a	415	-	-	0/46/66/69	0/1/1/1
25	DGD	b	601	-	-	0/41/81/95	0/2/2/2
29	SQD	b	602	-	-	0/42/62/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	b	603	-	-	0/21/61/61	0/2/2/2
30	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
30	LMT	b	626	-	-	0/21/61/61	0/2/2/2
30	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
31	PHO	d	401	-	-	0/53/103/103	0/1/6/6
31	PHO	d	402	-	-	0/53/103/103	0/1/6/6
29	SQD	d	403	-	-	1/38/58/69	0/1/1/1
33	BCT	d	404	21	-	0/0/0/0	0/0/0/0
22	CLA	d	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	406	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PL9	d	407	-	-	0/53/73/73	0/1/1/1
27	LMG	d	408	-	-	0/44/64/70	0/1/1/1
27	LMG	d	409	-	-	0/43/63/70	0/1/1/1
25	DGD	d	410	-	-	0/52/92/95	0/2/2/2
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
27	LMG	d	412	-	-	0/41/61/70	0/1/1/1
27	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
24	BCR	f	102	-	-	0/29/63/63	0/2/2/2
29	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
30	LMT	i	102	-	-	0/21/61/61	0/2/2/2
23	PL9	j	101	-	-	0/29/49/73	0/1/1/1
24	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/10/54/54	0/0/8/8
24	BCR	x	101	-	-	0/29/63/63	0/2/2/2
24	BCR	y	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 492 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-7.27	1.45	1.51
34	v	201	HEM	C3B-C4B	-7.10	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.17	1.46	1.51
34	f	101	HEM	C3B-C4B	-6.11	1.46	1.51
34	f	101	HEM	C3D-C4D	-5.28	1.44	1.51

The worst 5 of 1184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	101	PL9	C7-C3-C2	-6.10	118.36	123.42
23	J	101	PL9	C7-C3-C2	-6.03	118.42	123.42
23	d	407	PL9	C7-C3-C2	-5.87	118.55	123.42
23	D	407	PL9	C7-C3-C2	-5.74	118.66	123.42
23	A	406	PL9	C7-C3-C2	-5.73	118.66	123.42

5 of 209 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	c	516	DGD	C2G-O2G-C1B-C2B
25	C	516	DGD	C2G-O2G-C1B-C2B
29	d	403	SQD	C45-O47-C7-C8
29	B	622	SQD	C45-O47-C7-C8

There are no ring outliers.

79 monomers are involved in 296 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	10	0
22	A	403	CLA	13	0
22	A	404	CLA	15	0
22	A	405	CLA	9	0
23	A	406	PL9	4	0
24	A	407	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	408	DGD	1	0
26	A	409	LHG	3	0
27	A	410	LMG	2	0
29	A	412	SQD	3	0
29	A	413	SQD	3	0
27	A	414	LMG	1	0
22	B	601	CLA	1	0
22	B	602	CLA	11	0
22	B	603	CLA	3	0
22	B	604	CLA	7	0
22	B	605	CLA	7	0
22	B	606	CLA	16	0
22	B	607	CLA	9	0
22	B	608	CLA	13	0
22	B	609	CLA	3	0
22	B	610	CLA	6	0
22	B	611	CLA	11	0
22	B	612	CLA	10	0
22	B	613	CLA	4	0
22	B	614	CLA	2	0
22	B	615	CLA	6	0
24	B	616	BCR	4	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
29	B	622	SQD	3	0
30	B	623	LMT	2	0
25	B	625	DGD	2	0
29	B	626	SQD	1	0
30	B	627	LMT	2	0
30	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	2	0
22	C	506	CLA	6	0
22	C	507	CLA	4	0
22	C	508	CLA	2	0
22	C	509	CLA	6	0
22	C	510	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	511	CLA	2	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	3	0
25	C	517	DGD	5	0
27	C	518	LMG	4	0
26	C	519	LHG	2	0
22	C	520	CLA	4	0
31	D	401	PHO	10	0
31	D	402	PHO	5	0
22	D	405	CLA	8	0
22	D	406	CLA	3	0
23	D	407	PL9	12	0
27	D	408	LMG	4	0
27	D	409	LMG	6	0
25	D	410	DGD	2	0
27	D	412	LMG	1	0
27	E	101	LMG	1	0
34	F	101	HEM	4	0
24	F	102	BCR	4	0
29	F	103	SQD	3	0
22	H	101	CLA	9	0
24	H	102	BCR	2	0
27	I	101	LMG	1	0
30	I	102	LMT	1	0
24	J	102	BCR	1	0
24	K	102	BCR	3	0
27	M	101	LMG	2	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, 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%)	0.50	31 (9%) 11 9	178, 179, 180, 181	0
1	a	335/344 (97%)	0.45	33 (9%) 9 8	178, 179, 180, 181	0
2	B	490/510 (96%)	0.25	27 (5%) 29 23	178, 179, 180, 181	0
2	b	490/510 (96%)	0.38	34 (6%) 20 15	178, 179, 180, 181	0
3	C	447/461 (96%)	0.32	30 (6%) 21 16	178, 179, 180, 181	0
3	c	447/461 (96%)	0.15	19 (4%) 39 31	178, 180, 180, 181	0
4	D	340/352 (96%)	0.24	15 (4%) 38 30	177, 179, 180, 181	0
4	d	340/352 (96%)	0.21	9 (2%) 59 49	177, 179, 180, 181	0
5	E	82/84 (97%)	0.12	2 (2%) 62 53	178, 180, 180, 181	0
5	e	82/84 (97%)	0.02	4 (4%) 33 26	178, 180, 181, 181	0
6	F	35/45 (77%)	-0.15	1 (2%) 55 45	179, 179, 180, 180	0
6	f	35/45 (77%)	-0.44	0 100 100	179, 180, 181, 181	0
7	H	65/66 (98%)	0.45	12 (18%) 2 3	179, 180, 180, 181	0
7	h	65/66 (98%)	0.57	10 (15%) 3 4	179, 180, 181, 181	0
8	I	35/38 (92%)	0.51	2 (5%) 27 21	178, 179, 180, 181	0
8	i	35/38 (92%)	-0.02	0 100 100	179, 179, 181, 181	0
9	J	34/40 (85%)	0.03	2 (5%) 26 19	178, 179, 180, 180	0
9	j	34/40 (85%)	-0.39	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	-0.02	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.52	5 (13%) 4 5	179, 180, 181, 181	0
11	L	37/37 (100%)	0.56	1 (2%) 58 48	178, 179, 180, 181	0
11	l	37/37 (100%)	0.17	0 100 100	178, 179, 180, 181	0
12	M	34/36 (94%)	0.34	2 (5%) 26 19	178, 179, 180, 181	0
12	m	34/36 (94%)	0.11	1 (2%) 55 45	178, 179, 180, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.62	25 (10%) 9 8	177, 179, 180, 181	0
13	o	243/272 (89%)	0.64	21 (8%) 13 11	177, 179, 181, 181	0
14	T	32/32 (100%)	0.23	2 (6%) 23 17	178, 179, 181, 181	0
14	t	32/32 (100%)	0.38	4 (12%) 5 6	178, 179, 180, 181	0
15	U	97/134 (72%)	0.59	7 (7%) 18 14	178, 179, 180, 181	0
15	u	97/134 (72%)	0.82	13 (13%) 4 6	178, 179, 180, 181	0
16	V	137/163 (84%)	0.17	3 (2%) 65 56	178, 179, 180, 181	0
16	v	137/163 (84%)	0.52	9 (6%) 22 16	178, 180, 181, 181	0
17	g	28/46 (60%)	0.46	2 (7%) 19 14	179, 180, 181, 182	0
17	y	28/46 (60%)	0.21	0 100 100	178, 180, 181, 181	0
18	X	37/41 (90%)	0.52	4 (10%) 8 7	179, 179, 181, 181	0
18	x	37/41 (90%)	0.84	6 (16%) 3 4	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.35	2 (3%) 51 41	179, 180, 181, 181	0
20	z	62/62 (100%)	0.95	4 (6%) 22 16	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.35	342 (6%) 22 16	177, 179, 180, 182	0

The worst 5 of 342 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	84	LYS	7.2
15	U	38	GLU	6.7
13	o	169	LYS	6.4
7	H	66	GLY	5.8
1	A	10	SER	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
30	LMT	i	102	35/35	0.51	1.11	7.54	178,181,183,183	0
30	LMT	I	102	35/35	0.48	1.09	7.13	178,180,182,183	0
27	LMG	C	518	45/55	0.65	1.11	5.83	178,179,180,181	0
24	BCR	c	521	40/40	0.85	1.25	5.60	178,179,181,181	0
27	LMG	c	518	45/55	0.74	1.01	5.58	178,180,181,181	0
24	BCR	y	101	40/40	0.76	1.00	5.52	177,179,180,180	0
25	DGD	D	410	63/66	0.74	0.87	5.39	178,181,182,183	0
24	BCR	B	619	40/40	0.73	0.82	5.25	178,179,180,180	0
25	DGD	d	410	63/66	0.64	0.84	5.06	178,180,183,183	0
24	BCR	b	623	40/40	0.73	0.73	4.61	177,178,180,180	0
22	CLA	A	405	65/65	0.80	0.70	4.44	177,179,180,181	0
30	LMT	b	627	35/35	0.67	1.10	4.35	178,180,182,182	0
24	BCR	C	513	40/40	0.88	0.74	4.14	177,179,180,180	0
23	PL9	J	101	35/55	0.25	0.59	4.10	177,180,181,181	0
22	CLA	b	605	65/65	0.59	1.12	3.73	179,180,182,183	0
30	LMT	D	411	31/35	0.66	0.87	3.33	179,180,182,182	0
22	CLA	c	512	65/65	0.76	0.80	3.26	178,180,181,182	0
22	CLA	B	603	65/65	0.78	0.53	3.16	176,179,180,180	0
24	BCR	H	102	40/40	0.67	1.01	3.15	178,180,181,182	0
22	CLA	D	406	65/65	0.89	0.67	2.96	177,179,180,181	0
23	PL9	j	101	35/55	0.52	0.35	2.92	179,180,181,181	0
24	BCR	a	409	40/40	0.69	0.69	2.84	177,178,180,180	0
22	CLA	a	407	65/65	0.77	0.71	2.71	178,179,180,181	0
24	BCR	c	513	40/40	0.76	0.89	2.71	178,179,180,180	0
22	CLA	B	601	65/65	0.61	0.95	2.70	177,180,181,182	0
24	BCR	g	101	40/40	0.57	0.89	2.67	178,179,180,180	0
25	DGD	b	601	52/66	0.71	0.55	2.57	178,180,181,182	0
22	CLA	c	511	65/65	0.87	0.68	2.52	178,180,181,182	0
30	LMT	d	411	31/35	0.49	0.79	2.46	178,181,182,183	0
25	DGD	B	625	52/66	0.76	0.59	2.43	177,180,182,182	0
27	LMG	M	101	42/55	0.69	0.55	2.36	178,180,181,182	0
30	LMT	B	624	35/35	0.80	0.50	2.32	178,180,182,183	0
24	BCR	B	617	40/40	0.67	0.50	2.31	177,179,180,180	0
24	BCR	K	102	40/40	0.71	0.89	2.27	178,180,181,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	BCR	J	102	40/40	0.53	0.37	2.26	178,180,181,181	0
30	LMT	B	627	35/35	0.64	0.64	2.25	178,180,182,182	0
29	SQD	f	103	45/54	0.86	0.57	2.12	177,179,181,182	0
24	BCR	C	514	40/40	0.81	0.77	2.10	178,179,180,181	0
24	BCR	F	102	40/40	0.61	0.53	2.09	177,179,180,180	0
22	CLA	b	606	65/65	0.88	0.59	2.07	177,179,180,181	0
22	CLA	c	503	65/65	0.82	0.56	2.04	177,179,180,181	0
30	LMT	b	604	35/35	0.71	0.57	2.04	177,179,181,182	0
24	BCR	f	102	40/40	0.78	0.33	2.02	177,179,181,181	0
27	LMG	e	101	44/55	0.77	0.37	1.97	177,179,181,181	0
22	CLA	B	611	65/65	0.92	0.41	1.95	177,179,180,180	0
29	SQD	B	626	47/54	0.74	0.56	1.95	175,179,181,183	0
22	CLA	b	613	65/65	0.86	0.76	1.94	178,179,180,181	0
24	BCR	A	407	40/40	0.76	0.53	1.92	177,179,180,180	0
27	LMG	a	402	42/55	0.64	0.49	1.82	177,180,181,182	0
22	CLA	c	508	65/65	0.86	0.46	1.80	177,179,180,181	0
22	CLA	c	501	65/65	0.86	0.49	1.79	177,179,180,181	0
22	CLA	C	506	65/65	0.81	0.75	1.75	177,179,180,180	0
22	CLA	C	502	65/65	0.68	0.54	1.70	178,179,180,180	0
22	CLA	B	604	65/65	0.89	0.72	1.70	177,179,180,180	0
22	CLA	d	406	65/65	0.83	0.56	1.68	177,179,180,181	0
24	BCR	c	514	40/40	0.73	0.78	1.65	177,179,180,180	0
22	CLA	b	609	65/65	0.85	0.64	1.65	178,179,180,181	0
29	SQD	a	401	54/54	0.84	0.65	1.64	178,180,181,183	0
29	SQD	d	403	43/54	0.67	0.86	1.59	178,180,182,186	0
22	CLA	c	502	65/65	0.55	0.64	1.59	178,179,180,181	0
22	CLA	C	508	65/65	0.83	0.85	1.58	177,179,180,180	0
22	CLA	c	506	65/65	0.88	0.58	1.58	178,179,180,181	0
22	CLA	b	607	65/65	0.82	0.43	1.48	177,179,180,181	0
30	LMT	b	603	35/35	0.68	0.50	1.47	178,179,181,182	0
25	DGD	b	624	58/66	0.72	0.43	1.47	177,178,180,180	0
22	CLA	B	608	65/65	0.86	0.58	1.44	177,179,180,180	0
22	CLA	b	608	65/65	0.88	0.52	1.41	178,179,180,181	0
24	BCR	B	618	40/40	0.87	0.32	1.41	177,178,179,179	0
27	LMG	A	414	42/55	0.62	0.52	1.39	177,179,182,182	0
22	CLA	c	510	65/65	0.80	0.56	1.38	178,179,181,181	0
24	BCR	B	616	40/40	0.68	0.47	1.36	176,178,180,180	0
22	CLA	B	614	65/65	0.85	0.67	1.32	177,179,180,181	0
22	CLA	B	609	65/65	0.90	0.51	1.29	178,179,180,181	0
27	LMG	E	101	44/55	0.63	0.61	1.24	176,179,181,182	0
22	CLA	C	501	65/65	0.86	0.47	1.22	178,179,180,180	0
22	CLA	h	101	65/65	0.84	0.46	1.19	176,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	BCR	x	101	40/40	0.74	0.86	1.16	178,179,180,181	0
22	CLA	b	619	65/65	0.67	0.76	1.16	177,179,180,181	0
22	CLA	C	512	65/65	0.81	0.91	1.12	177,180,181,182	0
22	CLA	b	615	65/65	0.88	0.40	1.12	177,179,180,180	0
29	SQD	b	602	47/54	0.80	0.42	1.08	176,179,182,185	0
22	CLA	C	511	65/65	0.90	0.88	1.05	178,179,180,181	0
24	BCR	b	622	40/40	0.75	0.37	1.03	176,178,179,179	0
25	DGD	a	410	56/66	0.71	0.41	0.97	178,180,181,182	0
22	CLA	B	605	65/65	0.87	0.69	0.93	178,179,180,180	0
22	CLA	B	615	65/65	0.83	0.73	0.93	176,179,180,181	0
29	SQD	A	413	54/54	0.87	0.38	0.91	178,180,182,184	0
29	SQD	F	103	45/54	0.82	0.64	0.90	178,180,182,182	0
22	CLA	C	510	65/65	0.77	0.54	0.88	177,179,180,181	0
25	DGD	A	408	56/66	0.73	0.42	0.88	178,179,181,182	0
22	CLA	b	612	65/65	0.84	0.63	0.85	176,179,181,181	0
27	LMG	m	101	42/55	0.79	0.42	0.83	175,179,181,181	0
27	LMG	a	412	51/55	0.78	0.36	0.81	177,179,180,180	0
34	HEM	f	101	43/43	0.89	0.35	0.80	178,180,180,181	0
24	BCR	b	621	40/40	0.79	0.38	0.79	178,178,179,179	0
22	CLA	C	505	65/65	0.81	0.47	0.74	177,179,180,181	0
30	LMT	B	628	35/35	0.57	0.49	0.74	177,180,182,183	0
22	CLA	b	618	65/65	0.81	0.68	0.72	177,179,180,180	0
34	HEM	F	101	43/43	0.94	0.42	0.70	178,180,181,182	0
22	CLA	C	503	65/65	0.86	0.40	0.69	177,179,180,180	0
23	PL9	a	408	45/55	0.81	0.30	0.67	176,179,180,180	0
34	HEM	V	201	43/43	0.91	0.39	0.61	176,178,180,180	0
23	PL9	A	406	45/55	0.72	0.41	0.59	177,179,180,180	0
22	CLA	B	602	65/65	0.92	0.50	0.59	176,178,180,180	0
22	CLA	c	505	65/65	0.81	0.51	0.59	177,179,180,181	0
25	DGD	c	515	53/66	0.83	0.40	0.56	176,179,181,182	0
22	CLA	C	504	65/65	0.87	0.39	0.46	177,179,180,180	0
34	HEM	v	201	43/43	0.91	0.53	0.45	177,179,180,180	0
24	BCR	b	620	40/40	0.85	0.37	0.44	177,179,179,180	0
22	CLA	c	504	65/65	0.89	0.31	0.42	177,179,180,180	0
22	CLA	b	616	65/65	0.94	0.30	0.41	177,179,180,180	0
22	CLA	a	404	65/65	0.76	0.61	0.41	177,178,180,180	0
22	CLA	b	617	65/65	0.83	0.42	0.41	178,179,180,182	0
27	LMG	C	521	48/55	0.77	0.31	0.33	177,179,180,181	0
29	SQD	B	622	43/54	0.85	0.43	0.31	177,180,182,185	0
22	CLA	a	405	65/65	0.80	0.58	0.29	174,178,179,180	0
22	CLA	B	607	65/65	0.89	0.38	0.27	178,179,180,181	0
22	CLA	C	509	65/65	0.85	0.36	0.27	177,179,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	B	613	65/65	0.74	0.44	0.24	177,179,180,180	0
27	LMG	d	412	46/55	0.92	0.24	0.24	177,178,180,180	0
27	LMG	D	412	46/55	0.80	0.32	0.19	178,179,180,181	0
22	CLA	b	611	65/65	0.86	0.35	0.18	177,179,180,180	0
22	CLA	C	507	65/65	0.84	0.36	0.14	178,179,180,181	0
23	PL9	d	407	55/55	0.60	0.41	0.11	177,179,180,181	0
31	PHO	d	401	64/64	0.73	0.42	0.08	178,179,180,180	0
23	PL9	D	407	55/55	0.71	0.40	0.08	177,178,179,180	0
31	PHO	D	402	64/64	0.79	0.36	0.06	177,179,180,181	0
29	SQD	a	415	51/54	0.79	0.31	0.04	178,179,181,182	0
27	LMG	A	410	51/55	0.81	0.32	0.03	177,178,180,181	0
22	CLA	H	101	65/65	0.87	0.32	0.02	177,179,180,181	0
25	DGD	B	620	58/66	0.83	0.33	0.02	176,179,181,182	0
24	BCR	j	102	40/40	0.69	0.30	0.00	179,180,182,183	0
27	LMG	D	409	48/55	0.88	0.28	-0.03	175,178,180,181	0
26	LHG	A	409	39/49	0.86	0.30	-0.04	178,179,181,181	0
22	CLA	b	614	65/65	0.91	0.28	-0.08	178,179,180,180	0
32	CL	a	413	1/1	0.94	0.54	-0.09	177,177,177,177	0
22	CLA	A	403	65/65	0.92	0.50	-0.09	177,179,179,180	0
25	DGD	C	517	66/66	0.74	0.41	-0.13	177,179,180,181	0
22	CLA	C	520	65/65	0.85	0.33	-0.16	178,179,180,181	0
27	LMG	d	409	48/55	0.84	0.30	-0.17	177,179,180,180	0
29	SQD	A	412	51/54	0.80	0.31	-0.18	178,179,180,181	0
31	PHO	D	401	64/64	0.87	0.35	-0.20	177,179,180,180	0
26	LHG	c	519	37/49	0.73	0.31	-0.21	178,180,183,187	0
22	CLA	B	610	65/65	0.87	0.36	-0.22	177,179,180,180	0
27	LMG	c	522	48/55	0.85	0.28	-0.25	178,180,180,181	0
22	CLA	A	402	65/65	0.92	0.41	-0.26	178,179,180,181	0
22	CLA	d	405	65/65	0.88	0.44	-0.30	177,178,179,180	0
25	DGD	C	515	53/66	0.87	0.31	-0.31	177,178,179,180	0
22	CLA	D	405	65/65	0.91	0.39	-0.32	177,179,180,180	0
22	CLA	c	509	65/65	0.86	0.32	-0.38	177,179,180,180	0
22	CLA	c	507	65/65	0.90	0.27	-0.44	177,179,180,181	0
27	LMG	D	408	49/55	0.78	0.32	-0.44	177,178,180,180	0
30	LMT	M	103	35/35	0.80	0.46	-0.44	177,179,180,180	0
22	CLA	B	606	65/65	0.86	0.34	-0.45	177,179,180,180	0
22	CLA	A	404	65/65	0.81	0.36	-0.52	176,178,180,181	0
26	LHG	C	519	37/49	0.77	0.34	-0.55	176,180,184,188	0
25	DGD	c	517	66/66	0.78	0.32	-0.58	177,179,181,181	0
22	CLA	c	520	65/65	0.90	0.30	-0.60	177,179,180,181	0
28	OEX	A	411	10/10	0.92	0.42	-0.60	172,175,178,178	0
26	LHG	a	411	39/49	0.85	0.26	-0.62	177,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	BCT	D	404	4/4	0.90	0.26	-0.64	178,179,179,179	0
22	CLA	b	610	65/65	0.89	0.28	-0.67	177,179,180,180	0
22	CLA	B	612	65/65	0.92	0.26	-0.76	176,178,180,181	0
27	LMG	b	625	49/55	0.86	0.29	-0.80	178,179,180,180	0
22	CLA	a	406	65/65	0.84	0.30	-0.88	177,179,180,181	0
31	PHO	d	402	64/64	0.86	0.24	-0.94	178,179,180,181	0
25	DGD	C	516	62/66	0.86	0.25	-1.02	177,179,180,181	0
27	LMG	d	408	49/55	0.94	0.20	-1.16	178,179,180,180	0
27	LMG	B	621	49/55	0.91	0.26	-1.22	177,179,180,180	0
30	LMT	M	102	35/35	0.73	0.36	-1.27	178,179,181,182	0
28	OEX	a	414	10/10	0.94	0.41	-1.36	174,177,179,182	0
32	CL	D	403	1/1	0.79	0.28	-1.56	180,180,180,180	0
25	DGD	c	516	62/66	0.88	0.27	-1.57	178,179,180,181	0
33	BCT	d	404	4/4	0.95	0.18	-1.88	178,180,180,180	0
21	FE2	A	401	1/1	0.92	0.20	-2.13	176,176,176,176	0
21	FE2	a	403	1/1	0.88	0.07	-3.50	182,182,182,182	0
30	LMT	b	626	35/35	0.65	0.67	-	178,180,182,183	0
30	LMT	B	623	35/35	0.69	0.86	-	177,181,182,183	0
27	LMG	I	101	43/55	0.59	1.02	-	178,180,181,182	0
35	CA	O	301	1/1	0.62	0.42	-	182,182,182,182	0
35	CA	k	101	1/1	0.87	0.27	-	180,180,180,180	0
35	CA	K	101	1/1	0.67	0.52	-	184,184,184,184	0
35	CA	o	301	1/1	0.77	0.56	-	184,184,184,184	0
27	LMG	i	101	43/55	0.77	0.79	-	177,180,182,184	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.