



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:37 PM GMT

PDB ID : 4V62  
Title : Crystal Structure of cyanobacterial Photosystem II  
Authors : Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.  
Deposited on : 2008-01-17  
Resolution : 2.90 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

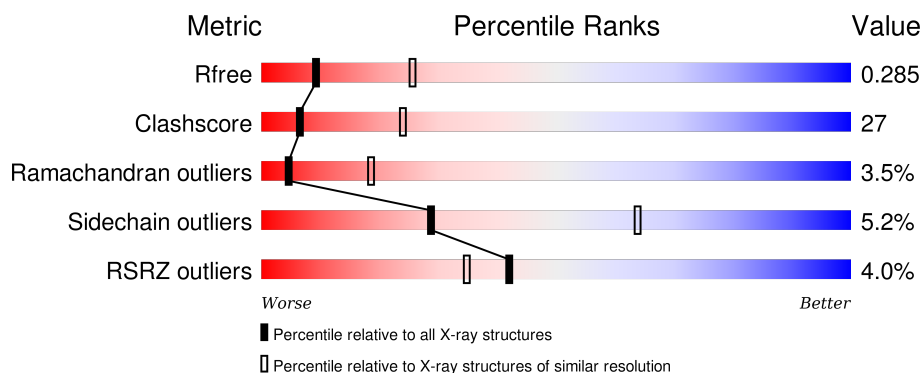
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	AA	344	<div> <div>2%</div> <div>51%42% . .</div> </div>
1	BA	344	<div> <div>%</div> <div>50%43%5% .</div> </div>
2	AB	510	<div> <div>2%</div> <div>56%35% . . .</div> </div>
2	BB	510	<div> <div>2%</div> <div>55%36% . . .</div> </div>
3	AC	473	<div> <div>3%</div> <div>45%43%6%5%</div> </div>

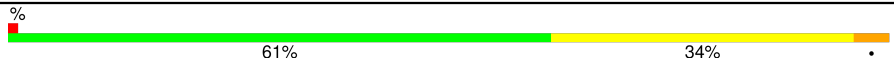


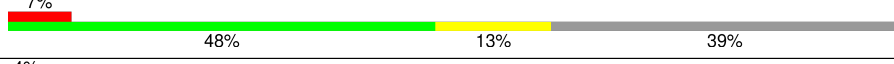
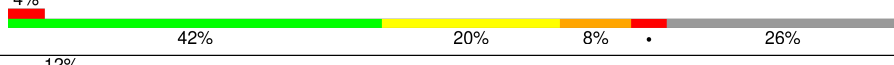
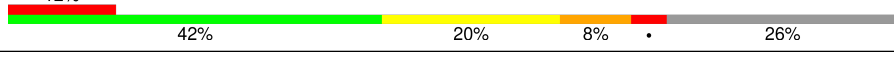
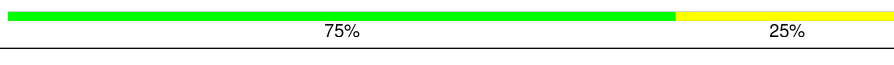

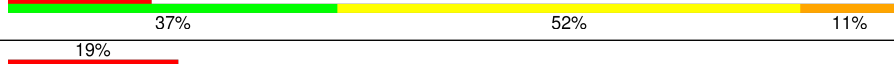
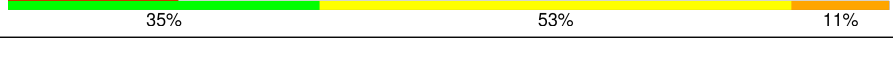
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Mol	Chain	Length	Quality of chain
3	BC	473	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	

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Mol	Chain	Length	Quality of chain
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	50	
18	BX	50	
19	AY	28	
19	BY	28	
20	AZ	62	
20	BZ	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	AA	402	X	-	-	-
22	CLA	AA	403	X	-	-	-
22	CLA	AA	404	X	-	-	-
22	CLA	AA	406	X	-	-	X
22	CLA	AB	601	X	-	-	X
22	CLA	AB	602	X	-	-	-
22	CLA	AB	603	X	-	-	-
22	CLA	AB	604	X	-	-	X
22	CLA	AB	605	X	-	-	-
22	CLA	AB	606	X	-	-	-
22	CLA	AB	607	X	-	-	-
22	CLA	AB	608	X	-	-	-
22	CLA	AB	609	X	-	-	X
22	CLA	AB	610	X	-	-	-
22	CLA	AB	611	X	-	-	-
22	CLA	AB	612	X	-	-	-
22	CLA	AB	613	X	-	-	-
22	CLA	AB	614	X	-	-	-
22	CLA	AB	615	X	-	-	-
22	CLA	AB	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	AC	501	X	-	-	-
22	CLA	AC	502	X	-	-	-
22	CLA	AC	503	X	-	-	X
22	CLA	AC	504	X	-	-	X
22	CLA	AC	505	X	-	-	-
22	CLA	AC	506	X	-	-	-
22	CLA	AC	507	X	-	-	X
22	CLA	AC	508	X	-	-	-
22	CLA	AC	509	X	-	-	-
22	CLA	AC	510	X	-	-	-
22	CLA	AC	511	X	-	-	-
22	CLA	AC	512	X	-	-	X
22	CLA	AC	513	X	-	-	-
22	CLA	AD	402	X	-	-	X
22	CLA	AD	404	X	-	-	X
22	CLA	BA	403	X	-	-	-
22	CLA	BA	404	X	-	-	-
22	CLA	BA	405	X	-	-	X
22	CLA	BA	407	X	-	-	X
22	CLA	BB	604	X	-	-	-
22	CLA	BB	605	X	-	-	-
22	CLA	BB	606	X	-	-	-
22	CLA	BB	607	X	-	-	-
22	CLA	BB	608	X	-	-	-
22	CLA	BB	609	X	-	-	-
22	CLA	BB	610	X	-	-	-
22	CLA	BB	611	X	-	-	-
22	CLA	BB	612	X	-	-	X
22	CLA	BB	613	X	-	-	-
22	CLA	BB	614	X	-	-	-
22	CLA	BB	615	X	-	-	-
22	CLA	BB	616	X	-	-	-
22	CLA	BB	617	X	-	-	-
22	CLA	BB	618	X	-	-	-
22	CLA	BB	619	X	-	-	-
22	CLA	BC	501	X	-	-	-
22	CLA	BC	502	X	-	-	-
22	CLA	BC	503	X	-	-	-
22	CLA	BC	504	X	-	-	-
22	CLA	BC	505	X	-	-	-
22	CLA	BC	506	X	-	-	-
22	CLA	BC	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	BC	508	X	-	-	-
22	CLA	BC	509	X	-	-	-
22	CLA	BC	510	X	-	-	-
22	CLA	BC	511	X	-	-	-
22	CLA	BC	512	X	-	-	-
22	CLA	BC	513	X	-	-	X
22	CLA	BD	402	X	-	-	-
22	CLA	BD	404	X	-	-	-
23	PHO	BD	403	-	-	-	X
24	PL9	AA	407	-	-	-	X
24	PL9	AJ	101	-	-	-	X
24	PL9	BA	408	-	-	-	X
24	PL9	BJ	101	-	-	-	X
26	BCR	AH	101	-	-	-	X
26	BCR	AJ	102	-	-	-	X
26	BCR	AK	102	-	-	-	X
26	BCR	AZ	101	-	-	-	X
26	BCR	BJ	102	-	-	-	X
26	BCR	BK	102	-	-	-	X
27	DGD	AA	410	X	-	-	-
27	DGD	AB	626	X	-	-	X
27	DGD	AC	516	X	-	-	-
27	DGD	AC	517	X	-	-	X
27	DGD	AC	518	X	-	-	-
27	DGD	AD	410	X	-	-	X
27	DGD	AH	102	X	-	-	-
27	DGD	BA	411	X	-	-	X
27	DGD	BB	602	X	-	-	X
27	DGD	BC	516	X	-	-	-
27	DGD	BC	517	X	-	-	-
27	DGD	BC	518	X	-	-	-
27	DGD	BD	410	X	-	-	X
27	DGD	BH	101	X	-	-	-
28	LHG	AC	521	-	-	-	X
28	LHG	BC	521	-	-	-	X
29	SQD	AA	415	-	-	-	X
29	SQD	AF	101	-	-	-	X
29	SQD	BA	401	-	-	-	X
29	SQD	BF	101	-	-	-	X
30	LMG	AA	413	X	-	-	-
30	LMG	AA	416	X	-	-	X
30	LMG	AB	621	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	LMG	AB	622	X	-	-	-
30	LMG	AB	623	X	-	-	X
30	LMG	AC	519	X	-	-	-
30	LMG	AC	520	X	-	-	X
30	LMG	AD	407	X	-	-	-
30	LMG	AD	408	X	-	-	X
30	LMG	AE	102	X	-	-	-
30	LMG	AI	101	X	-	-	-
30	LMG	AM	101	X	-	-	-
30	LMG	BA	414	X	-	-	-
30	LMG	BB	623	X	-	-	-
30	LMG	BB	624	X	-	-	-
30	LMG	BC	519	X	-	-	-
30	LMG	BC	520	X	-	-	X
30	LMG	BD	407	X	-	-	X
30	LMG	BD	408	X	-	-	X
30	LMG	BE	102	X	-	-	X
30	LMG	BI	101	X	-	-	-
30	LMG	BM	102	X	-	-	-
31	CL	AA	414	-	-	-	X
31	CL	BA	415	-	-	-	X
32	LMT	AB	625	-	-	-	X
32	LMT	AB	627	-	-	-	X
32	LMT	AD	411	-	-	-	X
32	LMT	AI	102	-	-	-	X
32	LMT	AT	101	-	-	-	X
32	LMT	BD	411	-	-	-	X
32	LMT	BI	102	-	-	-	X
32	LMT	BT	101	-	-	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50234 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	BA	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	AB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	BB	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	AC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	BC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
AC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
AC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
AC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
AC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
AC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8
BC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
BC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
BC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
BC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8
BC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
BC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
BC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	BD	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	AE	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	BE	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	AF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	BF	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	AH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	BH	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	AI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	BI	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	AJ	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	BJ	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	AK	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	BK	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	AL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	BL	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	AM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	BM	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	AO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	BO	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	AT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	BT	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	AU	97	Total	C	N	O		0	0	0
			774	491	129	154				
15	BU	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	AV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	BV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Ay	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	By	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

- Molecule 18 is a protein called Photosystem II PsbX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AX	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	BX	37	Total	C	N	O	0	0	0
			270	182	41	47			

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

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

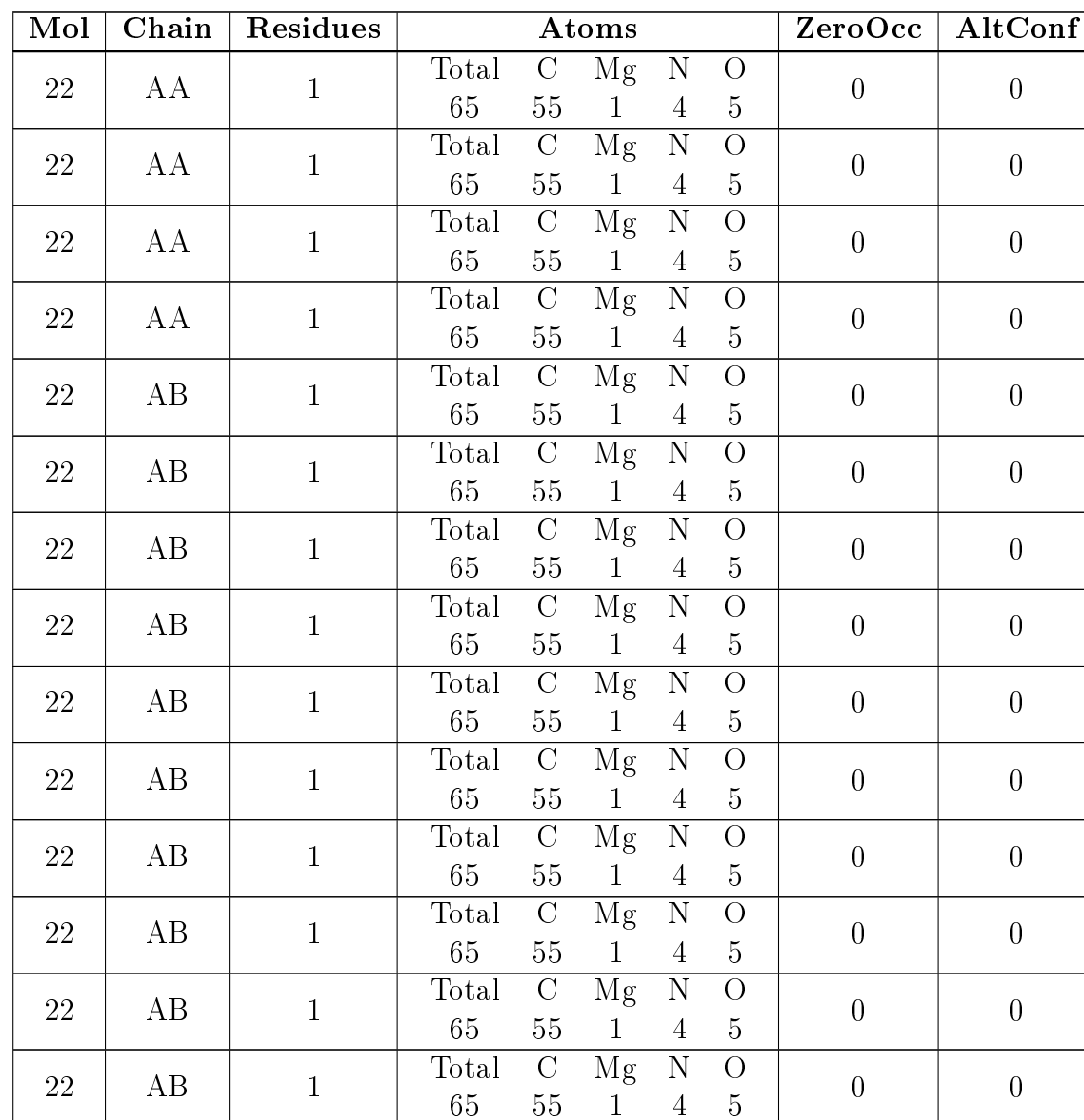
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	BZ	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	AA	1	Total	Fe	0	0
			1	1		
21	BA	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

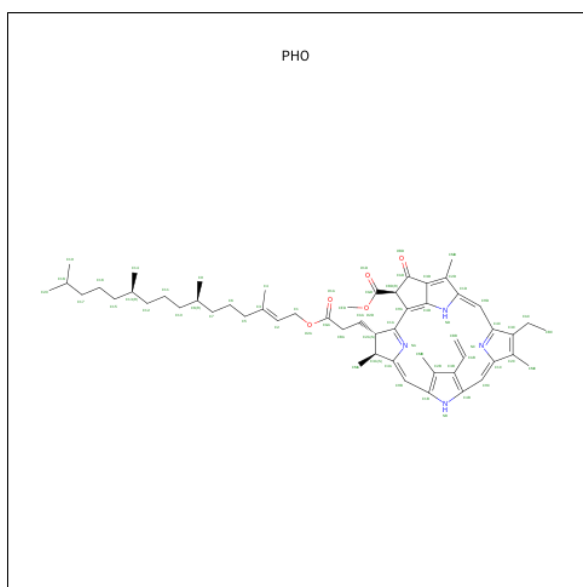
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0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

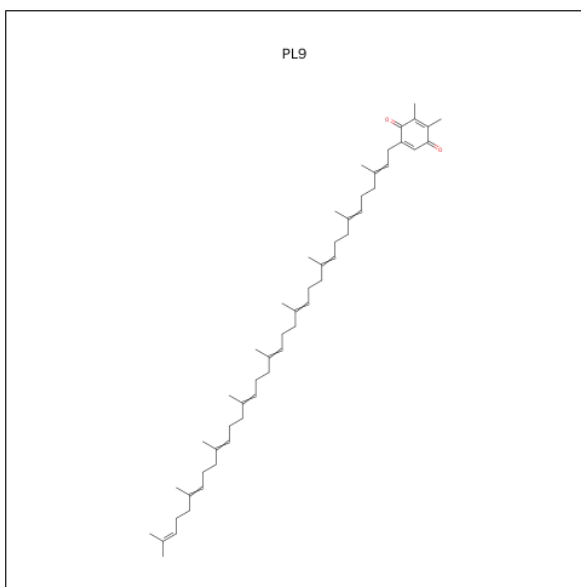
- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).





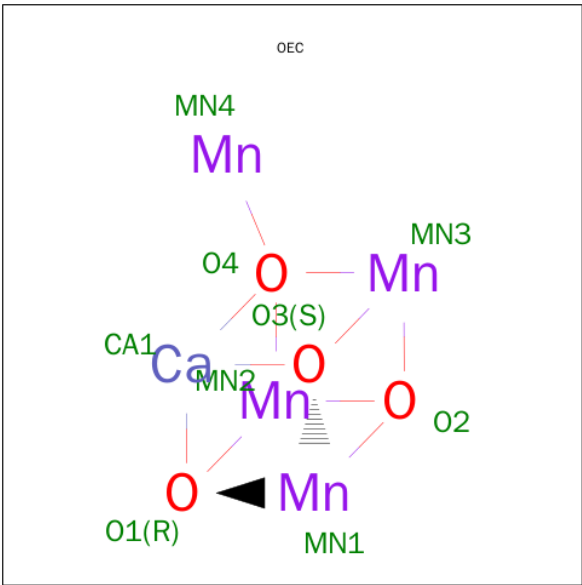
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	AA	1	Total	C	N	O	0	0
			64	55	4	5		
23	AD	1	Total	C	N	O	0	0
			64	55	4	5		
23	BA	1	Total	C	N	O	0	0
			64	55	4	5		
23	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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:  $C_{53}H_{80}O_2$ ).



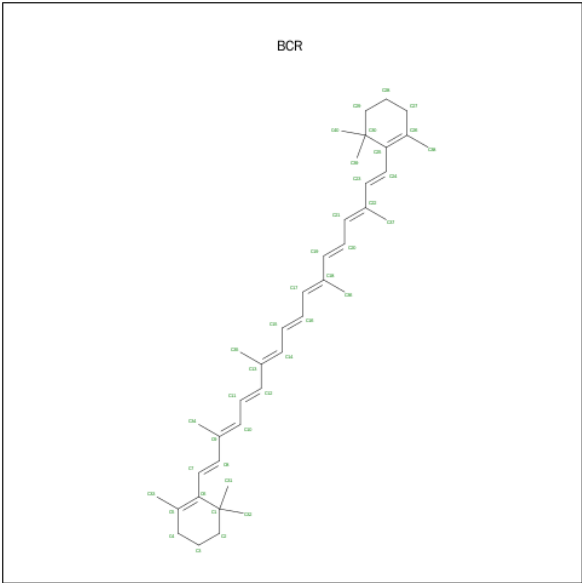
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	AA	1	Total	C	O	0	0
			45	43	2		
24	AD	1	Total	C	O	0	0
			55	53	2		
24	AJ	1	Total	C	O	0	0
			35	33	2		
24	BA	1	Total	C	O	0	0
			45	43	2		
24	BD	1	Total	C	O	0	0
			55	53	2		
24	BJ	1	Total	C	O	0	0
			35	33	2		

- Molecule 25 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula:  $\text{CaMn}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	AA	1	Total	Ca	Mn	0	0
			5	1	4		
25	BA	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	AA	1	Total	C	0	0
			40	40		
26	AB	1	Total	C	0	0
			40	40		

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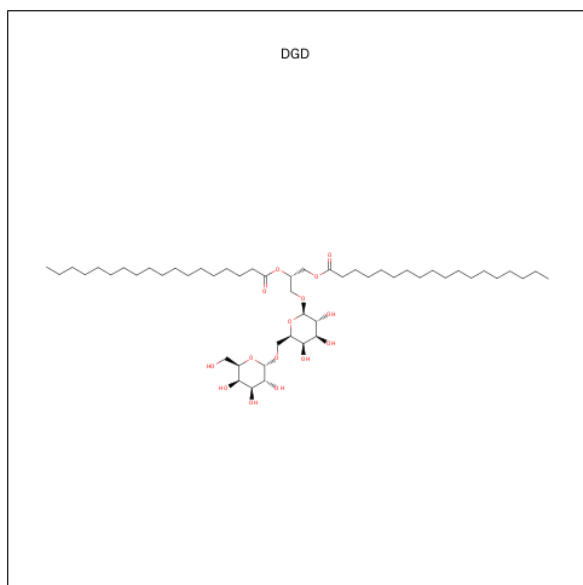
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AD	1	Total C 40 40	0	0
26	AH	1	Total C 40 40	0	0
26	AJ	1	Total C 40 40	0	0
26	AK	1	Total C 40 40	0	0
26	AT	1	Total C 40 40	0	0
26	AZ	1	Total C 40 40	0	0
26	BA	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BD	1	Total C 40 40	0	0
26	BJ	1	Total C 40 40	0	0
26	BK	1	Total C 40 40	0	0
26	BX	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	BZ	1	Total C 40 40	0	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



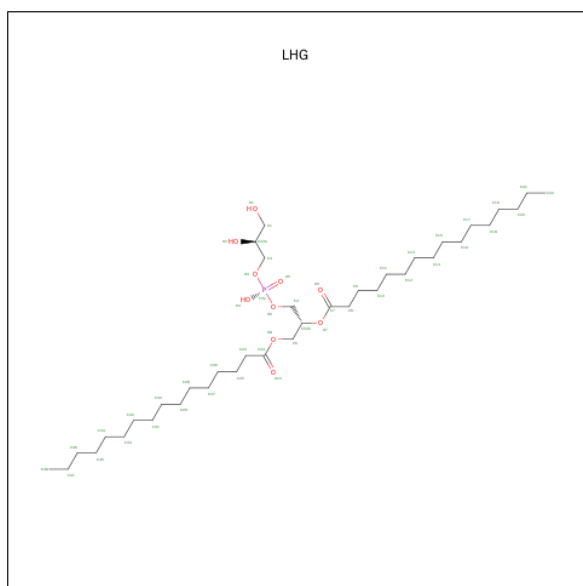
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C O 56 41 15	0	0
27	AB	1	Total C O 52 37 15	0	0
27	AC	1	Total C O 53 38 15	0	0
27	AC	1	Total C O 62 47 15	0	0
27	AC	1	Total C O 66 51 15	0	0
27	AD	1	Total C O 63 48 15	0	0
27	AH	1	Total C O 58 43 15	0	0
27	BA	1	Total C O 56 41 15	0	0
27	BB	1	Total C O 52 37 15	0	0
27	BC	1	Total C O 53 38 15	0	0

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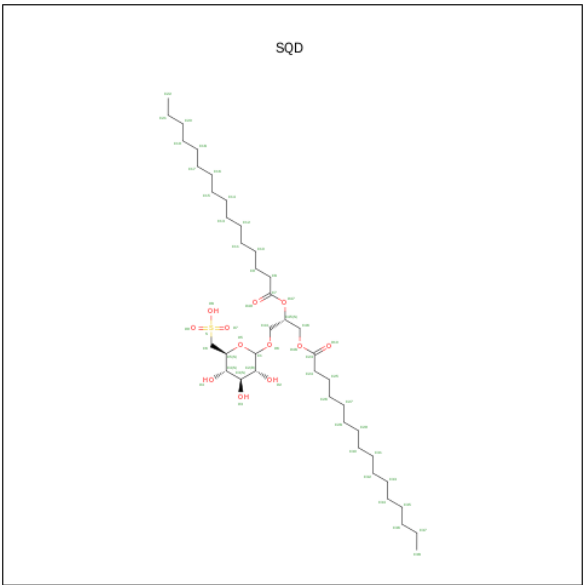
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	BC	1	Total	C	O	0	0
			62	47	15		
27	BC	1	Total	C	O	0	0
			66	51	15		
27	BD	1	Total	C	O	0	0
			63	48	15		
27	BH	1	Total	C	O	0	0
			58	43	15		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



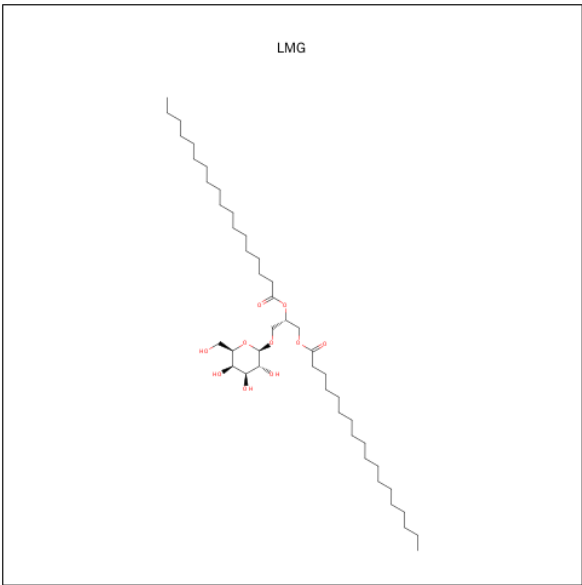
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	AA	1	Total	C	O	P	0	0
			39	28	10	1		
28	AC	1	Total	C	O	P	0	0
			37	26	10	1		
28	BA	1	Total	C	O	P	0	0
			39	28	10	1		
28	BC	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 29 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
29	AA	1	Total	C	O	S	0	0
			51	38	12	1		
29	AA	1	Total	C	O	S	0	0
			54	41	12	1		
29	AD	1	Total	C	O	S	0	0
			43	30	12	1		
29	AF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BA	1	Total	C	O	S	0	0
			54	41	12	1		
29	BA	1	Total	C	O	S	0	0
			51	38	12	1		
29	BB	1	Total	C	O	S	0	0
			47	34	12	1		
29	BD	1	Total	C	O	S	0	0
			43	30	12	1		
29	BF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BL	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 30 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
30	AA	1	Total	C	O	0	0
			51	41	10		
30	AA	1	Total	C	O	0	0
			42	32	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			42	32	10		
30	AC	1	Total	C	O	0	0
			48	38	10		
30	AC	1	Total	C	O	0	0
			45	35	10		
30	AD	1	Total	C	O	0	0
			46	36	10		
30	AD	1	Total	C	O	0	0
			48	38	10		
30	AE	1	Total	C	O	0	0
			44	34	10		
30	AI	1	Total	C	O	0	0
			43	33	10		
30	AM	1	Total	C	O	0	0
			42	32	10		
30	BA	1	Total	C	O	0	0
			51	41	10		
30	BB	1	Total	C	O	0	0
			49	39	10		

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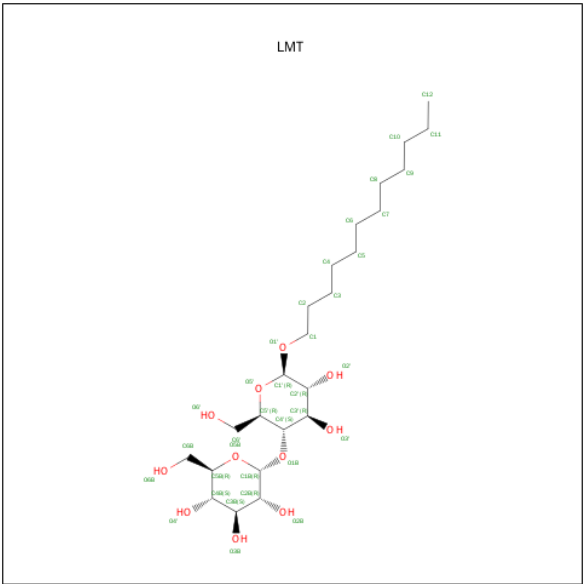
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	BB	1	Total	C	O	0	0
			49	39	10		
30	BC	1	Total	C	O	0	0
			48	38	10		
30	BC	1	Total	C	O	0	0
			45	35	10		
30	BD	1	Total	C	O	0	0
			46	36	10		
30	BD	1	Total	C	O	0	0
			48	38	10		
30	BE	1	Total	C	O	0	0
			44	34	10		
30	BI	1	Total	C	O	0	0
			43	33	10		
30	BM	1	Total	C	O	0	0
			42	32	10		

- Molecule 31 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

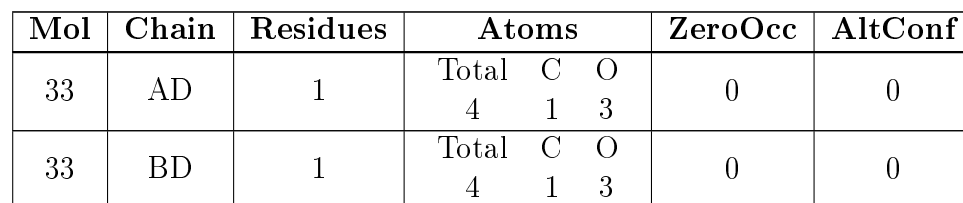
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	AA	1	Total	Cl	0	0
			1	1		
31	BA	1	Total	Cl	0	0
			1	1		

- Molecule 32 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
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM	1	Total	C	O	0	0
			35	24	11		
32	AT	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BD	1	Total	C	O	0	0
			31	20	11		
32	BI	1	Total	C	O	0	0
			35	24	11		
32	BM	1	Total	C	O	0	0
			35	24	11		
32	BT	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



- 
- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

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



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

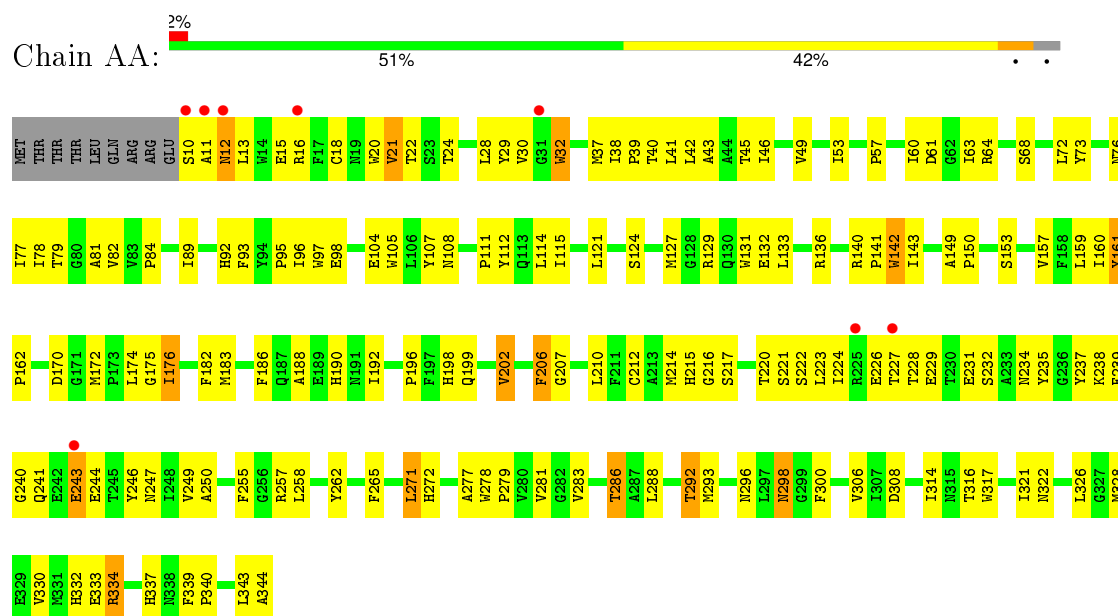
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	AO	1	Total 1	Ca 1	0	0
35	BO	1	Total 1	Ca 1	0	0
35	AK	1	Total 1	Ca 1	0	0
35	BK	1	Total 1	Ca 1	0	0

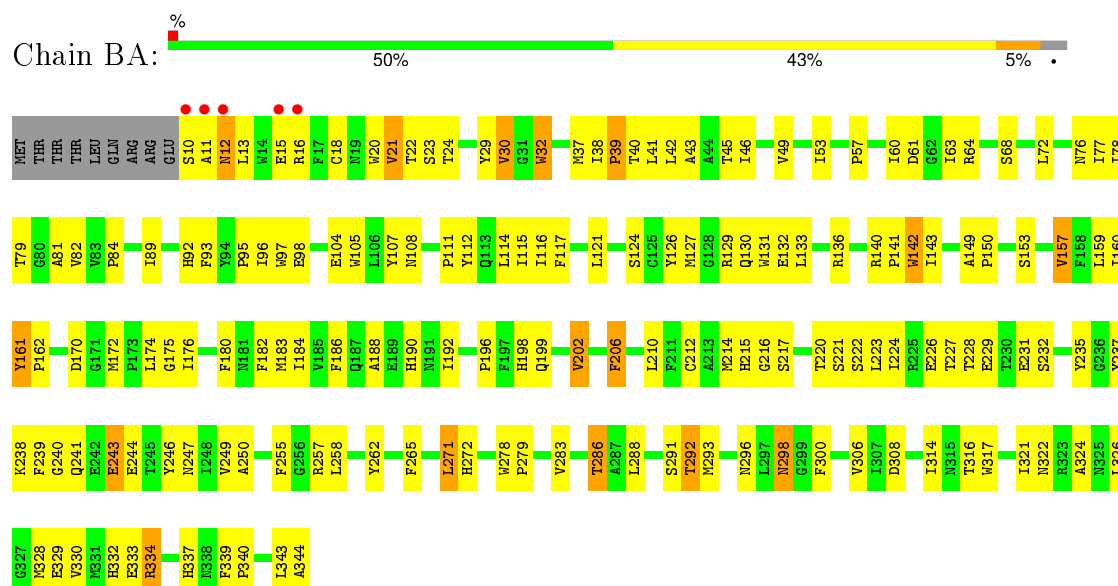
### 3 Residue-property plots

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

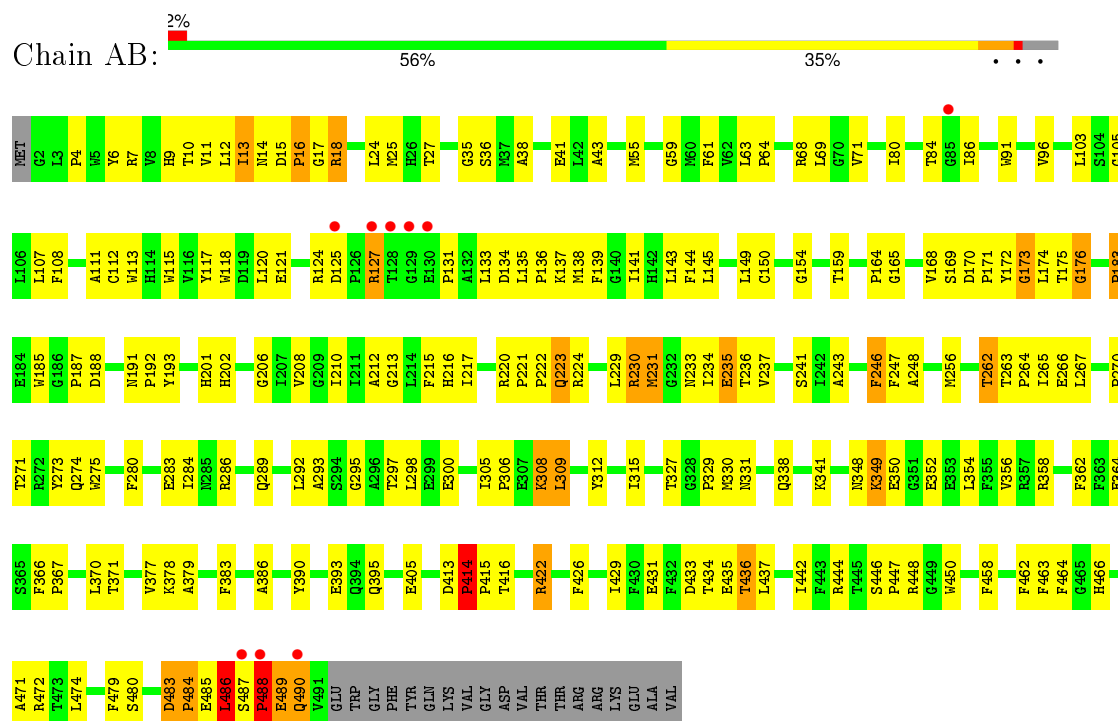
#### • Molecule 1: Photosystem Q(B) protein



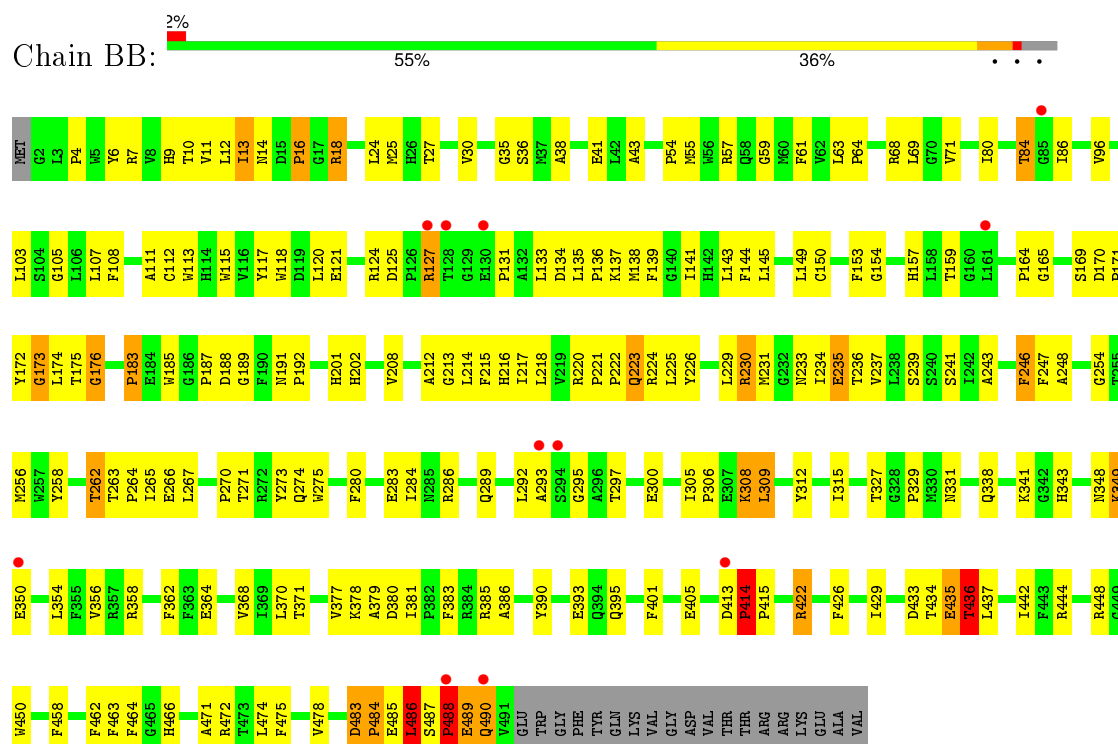
#### • Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II core light harvesting protein

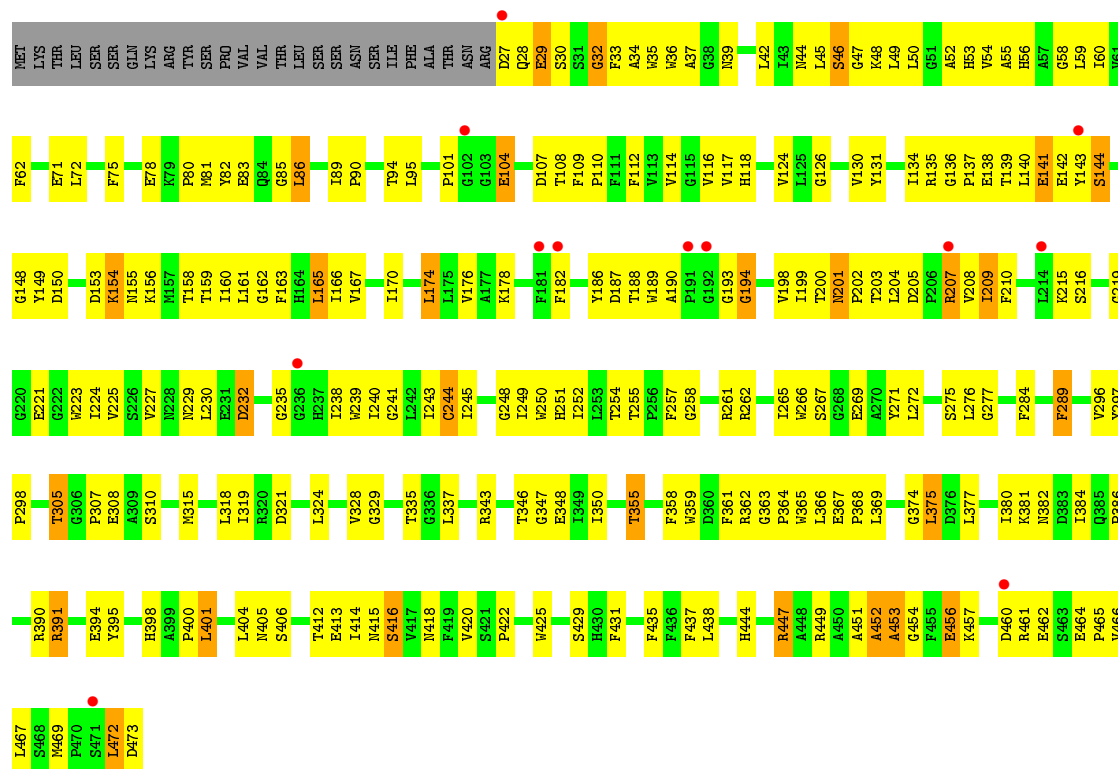


- Molecule 2: Photosystem II core light harvesting protein



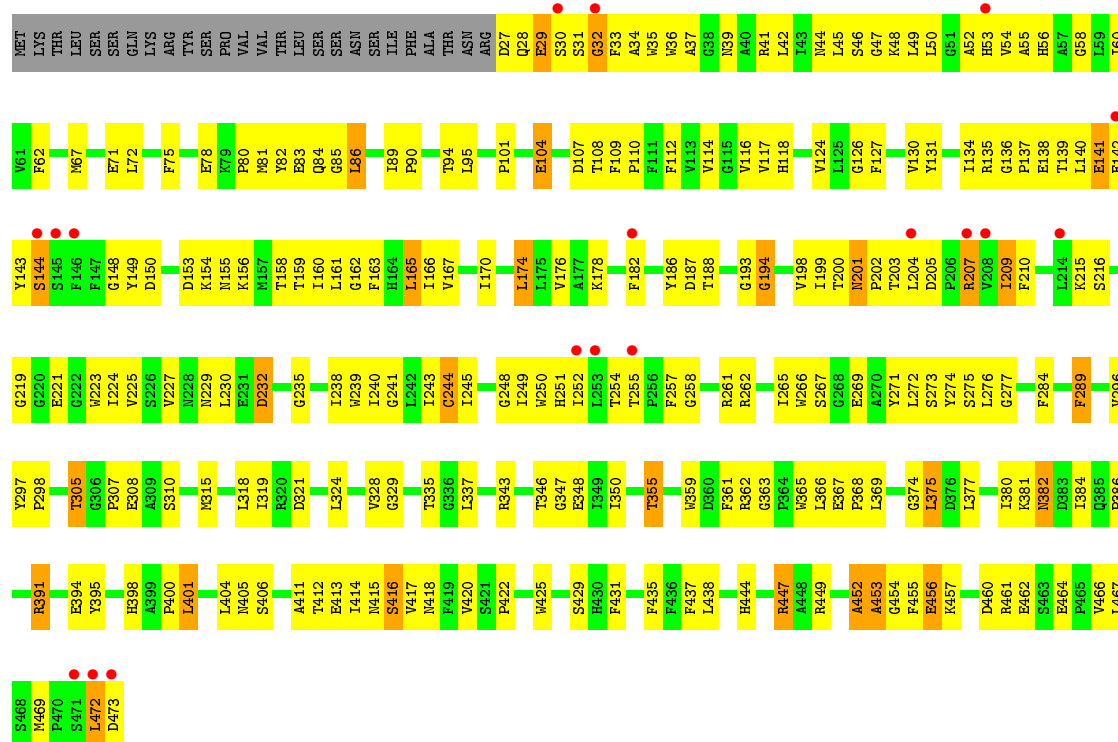
- Molecule 3: Photosystem II CP43 protein



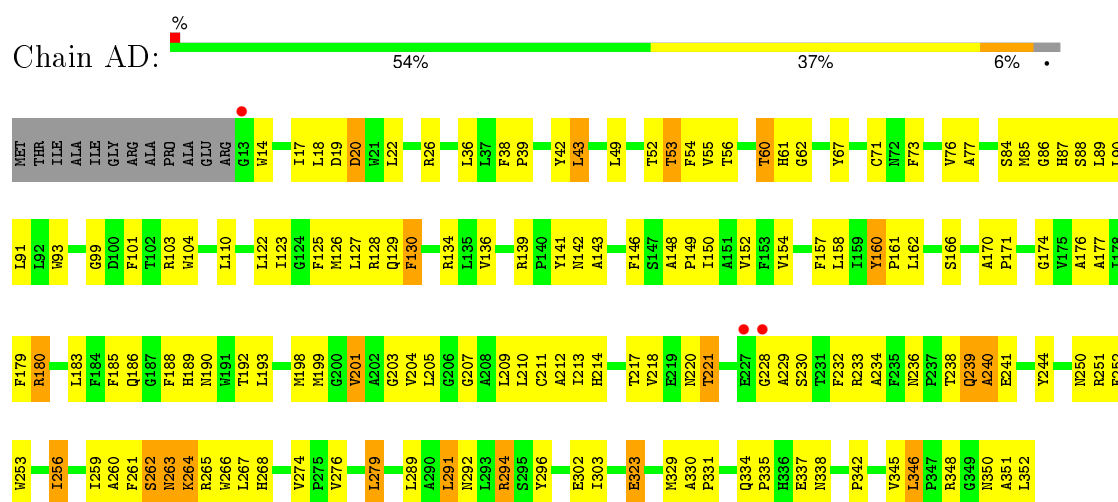


• Molecule 3: Photosystem II CP43 protein

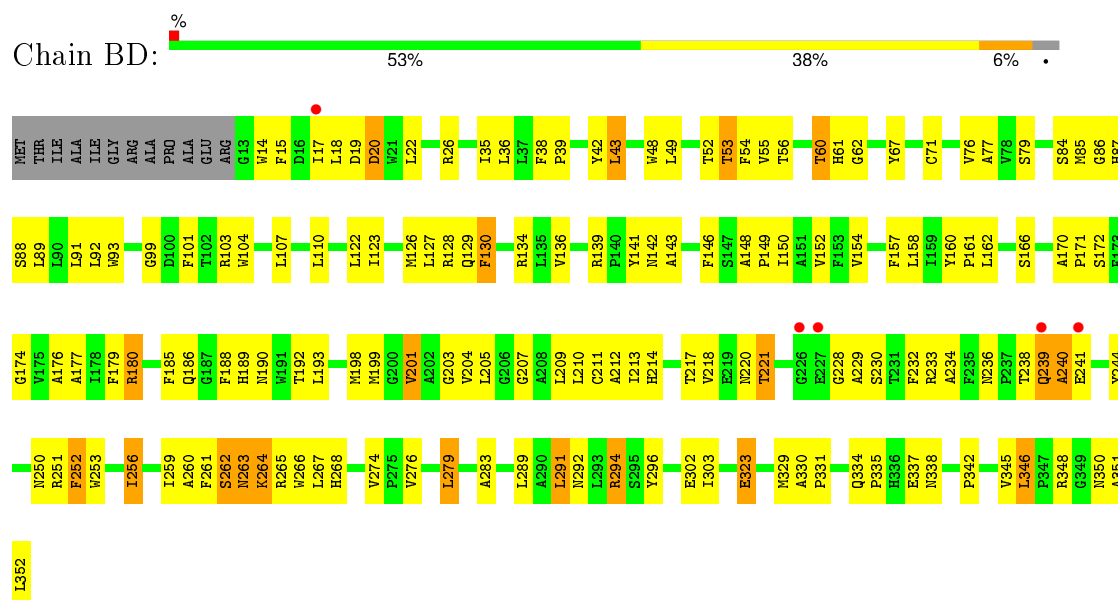
Chain BC: 4% 45% 44% 6% 5%



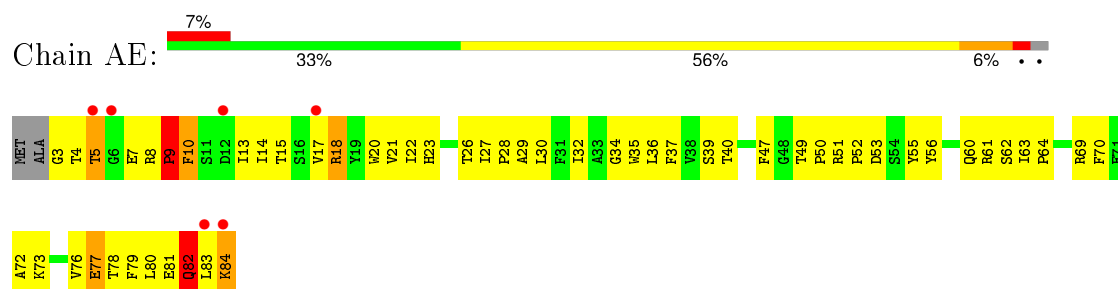
• Molecule 4: Photosystem II reaction center D2 protein



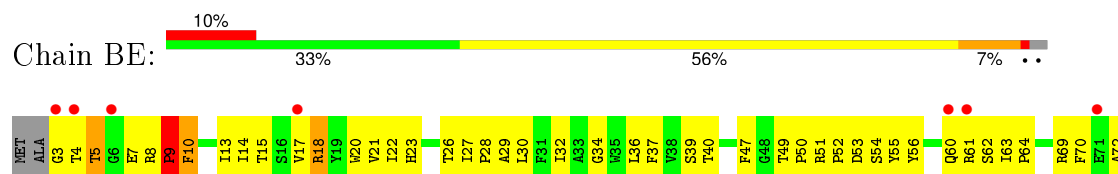
• Molecule 4: Photosystem II reaction center D2 protein



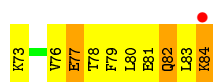
• Molecule 5: Cytochrome b559 subunit alpha



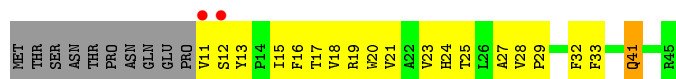
• Molecule 5: Cytochrome b559 subunit alpha



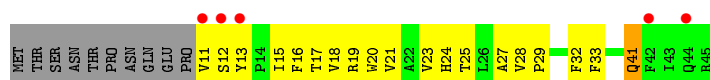




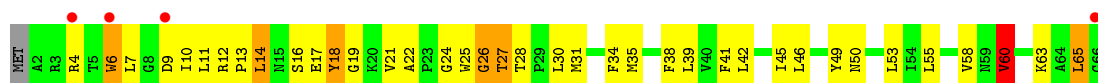
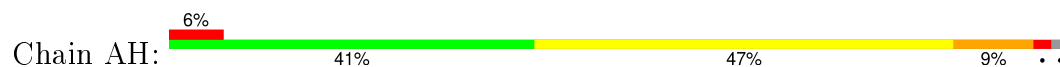
- Molecule 6: Cytochrome b559 subunit beta



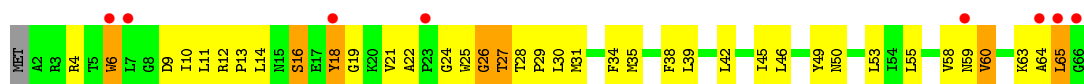
- Molecule 6: Cytochrome b559 subunit beta



- 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

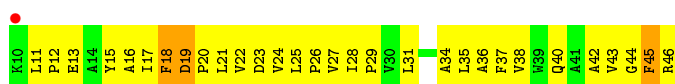




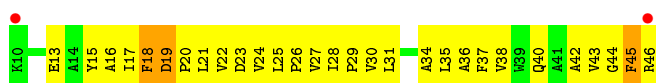
- Molecule 9: Photosystem II reaction center protein J



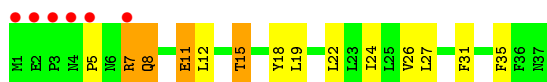
- Molecule 10: Photosystem II reaction center protein K



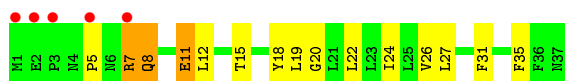
- Molecule 10: Photosystem II reaction center protein K



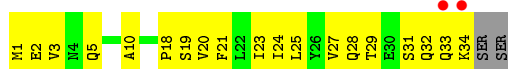
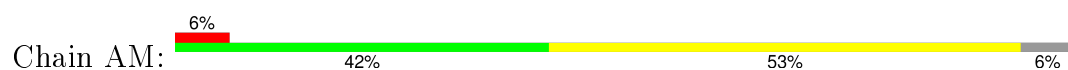
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



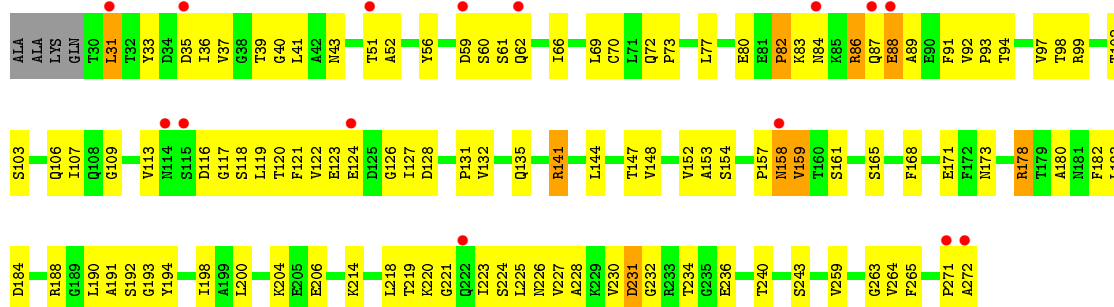
- Molecule 12: Photosystem II reaction center protein M





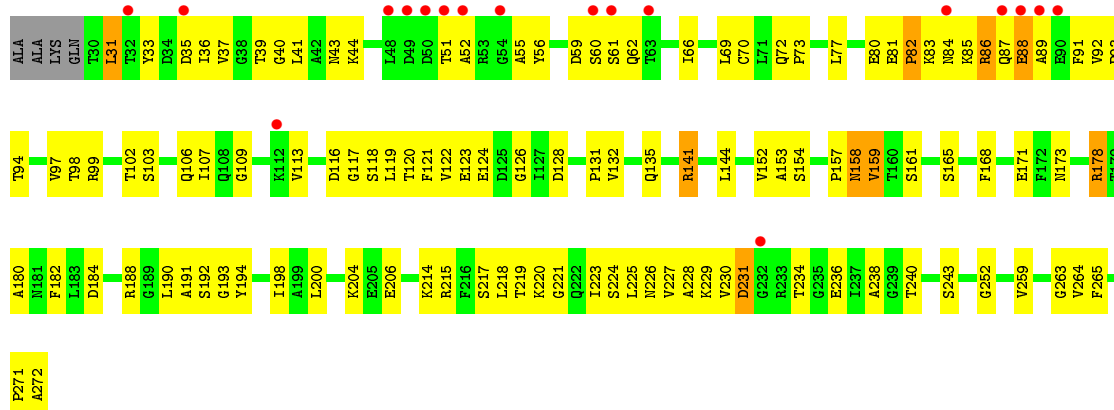
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain AO:



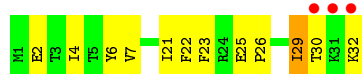
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain BO:



- Molecule 14: Photosystem II reaction center protein T

Chain AT:

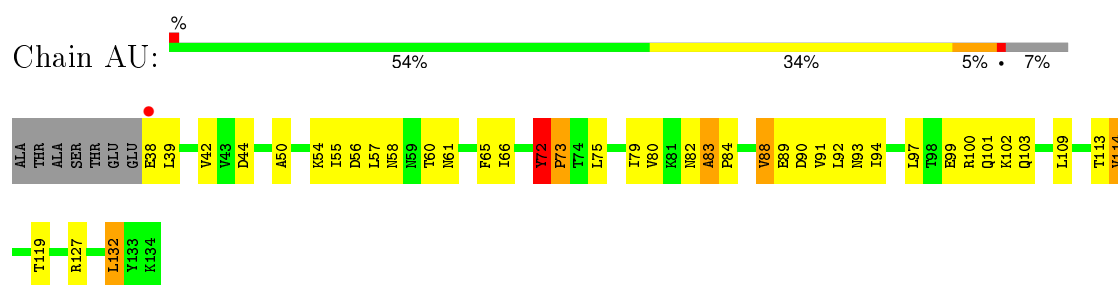


- Molecule 14: Photosystem II reaction center protein T

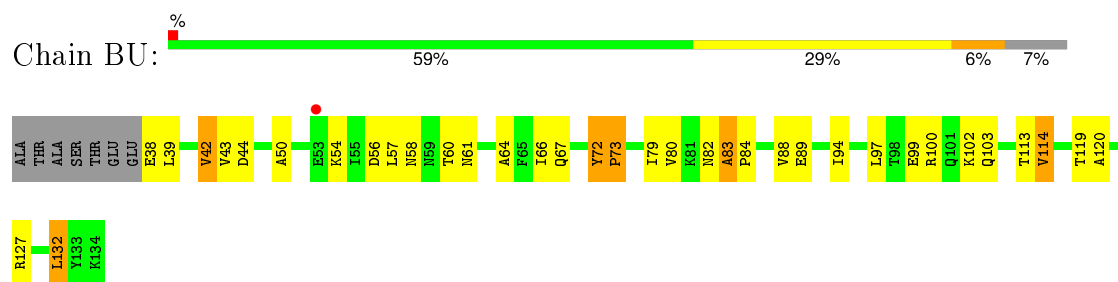
Chain BT:



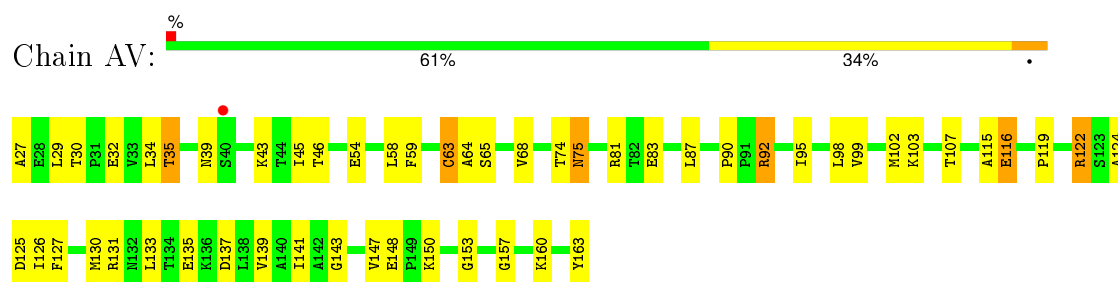
- Molecule 15: Photosystem II 12 kDa extrinsic protein



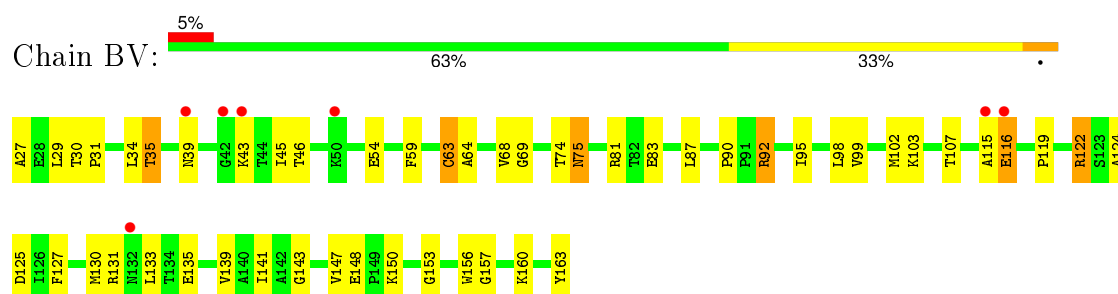
- Molecule 15: Photosystem II 12 kDa extrinsic protein



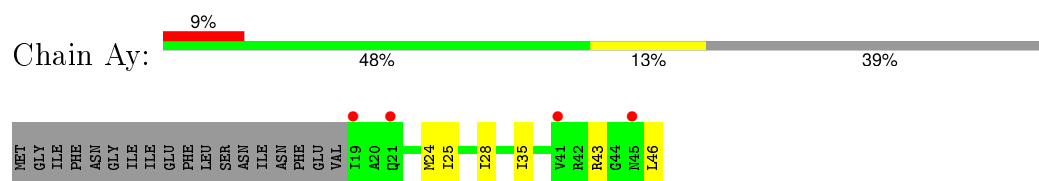
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

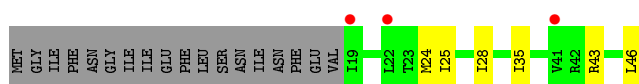


- Molecule 17: Protein ycf12



- Molecule 17: Protein ycf12

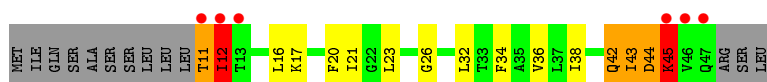
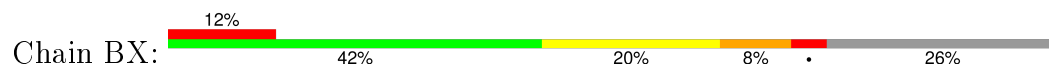




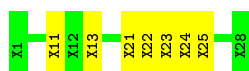
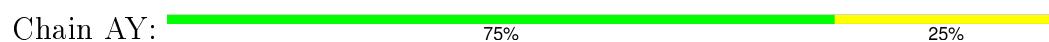
- Molecule 18: Photosystem II PsbX protein



- Molecule 18: Photosystem II PsbX protein



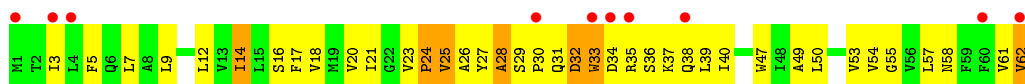
- Molecule 19: Photosystem II protein Y



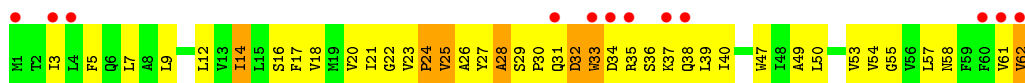
- Molecule 19: Photosystem II protein Y



- 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, $\alpha$ , $\beta$ , $\gamma$	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.90) 99.3 (20.00-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.292 0.246 , 0.285	Depositor DCC
$R_{free}$ test set	3784 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 71.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 193457 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	50234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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	AA	0.44	0/2713	0.66	0/3700
1	BA	0.43	0/2713	0.65	0/3700
2	AB	0.44	0/3986	0.67	3/5433 (0.1%)
2	BB	0.43	0/3986	0.66	3/5433 (0.1%)
3	AC	0.41	0/3556	0.64	1/4842 (0.0%)
3	BC	0.39	0/3556	0.63	1/4842 (0.0%)
4	AD	0.47	0/2801	0.65	0/3818
4	BD	0.45	0/2801	0.65	0/3818
5	AE	0.45	0/685	0.71	0/933
5	BE	0.45	0/685	0.70	0/933
6	AF	0.45	0/291	0.59	0/397
6	BF	0.47	0/291	0.57	0/397
7	AH	0.42	0/520	0.73	1/709 (0.1%)
7	BH	0.40	0/520	0.72	1/709 (0.1%)
8	AI	0.51	0/293	0.68	0/395
8	BI	0.50	0/293	0.67	0/395
9	AJ	0.43	0/255	0.69	0/346
9	BJ	0.45	0/255	0.66	0/346
10	AK	0.43	0/303	0.63	0/416
10	BK	0.44	0/303	0.61	0/416
11	AL	0.39	0/311	0.65	0/422
11	BL	0.41	0/311	0.65	0/422
12	AM	0.44	0/270	0.70	0/367
12	BM	0.45	0/270	0.67	0/367
13	AO	0.44	0/1876	0.70	0/2548
13	BO	0.43	0/1876	0.70	0/2548
14	AT	0.50	0/284	0.62	0/381
14	BT	0.48	0/284	0.62	0/381
15	AU	0.42	0/785	0.73	1/1064 (0.1%)
15	BU	0.40	0/785	0.73	0/1064
16	AV	0.38	0/1081	0.65	0/1468
16	BV	0.37	0/1081	0.64	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	Ay	0.46	0/202	0.73	0/272
17	By	0.41	0/202	0.74	0/272
18	AX	0.43	0/273	0.63	0/370
18	BX	0.41	0/273	0.63	0/370
20	AZ	0.45	0/490	0.69	0/669
20	BZ	0.47	0/490	0.70	0/669
All	All	0.43	0/41950	0.66	11/57100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
1	BA	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	486	LEU	CA-CB-CG	7.12	131.67	115.30
2	AB	486	LEU	CA-CB-CG	6.99	131.39	115.30
2	AB	488	PRO	N-CA-C	5.86	127.33	112.10
2	AB	489	GLU	N-CA-C	5.76	126.56	111.00
7	AH	65	LEU	CA-CB-CG	5.72	128.45	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	161	TYR	Sidechain
1	BA	161	TYR	Sidechain

## 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	AA	2628	0	2524	179	0
1	BA	2628	0	2524	179	0
2	AB	3850	0	3718	224	0
2	BB	3850	0	3718	227	0
3	AC	3444	0	3365	258	0
3	BC	3444	0	3365	263	0
4	AD	2706	0	2608	177	0
4	BD	2706	0	2608	184	0
5	AE	666	0	651	71	0
5	BE	666	0	651	74	0
6	AF	282	0	291	28	0
6	BF	282	0	291	29	0
7	AH	507	0	521	52	0
7	BH	507	0	521	50	0
8	AI	286	0	308	15	0
8	BI	286	0	308	18	0
9	AJ	249	0	262	28	0
9	BJ	249	0	262	26	0
10	AK	293	0	305	42	0
10	BK	293	0	305	44	0
11	AL	304	0	316	15	0
11	BL	304	0	316	17	0
12	AM	267	0	289	27	0
12	BM	267	0	289	26	0
13	AO	1845	0	1801	115	0
13	BO	1845	0	1801	118	0
14	AT	275	0	288	21	0
14	BT	275	0	288	20	0
15	AU	774	0	773	46	0
15	BU	774	0	773	42	0
16	AV	1060	0	1068	42	0
16	BV	1060	0	1068	39	0
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	27	0
18	BX	270	0	299	25	0
19	AY	140	0	32	4	0
19	BY	140	0	32	6	0
20	AZ	479	0	516	54	0
20	BZ	479	0	516	55	0
21	AA	1	0	0	0	0
21	BA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AA	260	0	288	18	0
22	AB	1040	0	1152	77	0
22	AC	845	0	936	61	0
22	AD	130	0	144	11	0
22	BA	260	0	288	18	0
22	BB	1040	0	1152	83	0
22	BC	845	0	936	62	0
22	BD	130	0	144	12	0
23	AA	64	0	74	5	0
23	AD	64	0	74	2	0
23	BA	64	0	74	5	0
23	BD	64	0	74	5	0
24	AA	45	0	61	5	0
24	AD	55	0	80	9	0
24	AJ	35	0	45	0	0
24	BA	45	0	61	6	0
24	BD	55	0	80	8	0
24	BJ	35	0	45	0	0
25	AA	5	0	0	0	0
25	BA	5	0	0	0	0
26	AA	40	0	56	6	0
26	AB	160	0	224	10	0
26	AC	80	0	112	15	0
26	AD	40	0	56	3	0
26	AH	40	0	56	5	0
26	AJ	40	0	56	5	0
26	AK	40	0	56	13	0
26	AT	40	0	56	8	0
26	AZ	40	0	56	5	0
26	BA	40	0	56	3	0
26	BB	120	0	168	5	0
26	BC	80	0	112	17	0
26	BD	40	0	56	3	0
26	BJ	40	0	56	5	0
26	BK	40	0	56	13	0
26	BX	40	0	56	6	0
26	BZ	40	0	56	5	0
27	AA	56	0	70	0	0
27	AB	52	0	62	3	0
27	AC	181	0	245	19	0
27	AD	63	0	87	0	0
27	AH	58	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BA	56	0	70	0	0
27	BB	52	0	62	3	0
27	BC	181	0	245	21	0
27	BD	63	0	87	0	0
27	BH	58	0	74	1	0
28	AA	39	0	51	3	0
28	AC	37	0	44	5	0
28	BA	39	0	51	4	0
28	BC	37	0	44	4	0
29	AA	105	0	145	10	0
29	AD	43	0	49	2	0
29	AF	45	0	53	2	0
29	BA	105	0	145	6	0
29	BB	47	0	60	2	0
29	BD	43	0	49	2	0
29	BF	45	0	53	1	0
29	BL	47	0	60	2	0
30	AA	93	0	126	5	0
30	AB	140	0	190	4	0
30	AC	93	0	126	6	0
30	AD	94	0	128	9	0
30	AE	44	0	58	4	0
30	AI	43	0	56	3	0
30	AM	42	0	54	4	0
30	BA	51	0	72	2	0
30	BB	98	0	136	2	0
30	BC	93	0	126	8	0
30	BD	94	0	128	10	0
30	BE	44	0	58	4	0
30	BI	43	0	56	3	0
30	BM	42	0	54	4	0
31	AA	1	0	0	0	0
31	BA	1	0	0	0	0
32	AB	105	0	138	6	0
32	AD	31	0	35	2	0
32	AI	35	0	46	4	0
32	AM	35	0	46	1	0
32	AT	35	0	46	3	0
32	BB	105	0	138	5	0
32	BD	31	0	35	1	0
32	BI	35	0	46	3	0
32	BM	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BT	35	0	46	3	0
33	AD	4	0	0	1	0
33	BD	4	0	0	1	0
34	AE	43	0	30	5	0
34	AV	43	0	30	3	0
34	BE	43	0	30	6	0
34	BV	43	0	30	3	0
35	AK	1	0	0	0	0
35	AO	1	0	0	0	0
35	BK	1	0	0	0	0
35	BO	1	0	0	0	0
All	All	50234	0	51364	2715	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 27.

The worst 5 of 2715 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)
16:AV:63:CYS:SG	34:AV:201:HEM:HAB	1.85	1.16
15:BU:83:ALA:HB1	15:BU:84:PRO:HD2	1.23	1.16
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.23	1.16
16:BV:63:CYS:SG	34:BV:201:HEM:HAB	1.85	1.15
9:BJ:15:THR:HG21	10:BK:38:VAL:HG13	1.24	1.13

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	<b>9</b> <b>32</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	9	32
2	AB	488/510 (96%)	417 (86%)	57 (12%)	14 (3%)	6	23
2	BB	488/510 (96%)	422 (86%)	52 (11%)	14 (3%)	6	23
3	AC	445/473 (94%)	371 (83%)	58 (13%)	16 (4%)	4	18
3	BC	445/473 (94%)	372 (84%)	56 (13%)	17 (4%)	4	16
4	AD	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	6	25
4	BD	338/352 (96%)	288 (85%)	42 (12%)	8 (2%)	7	29
5	AE	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	3	9
5	BE	80/84 (95%)	70 (88%)	6 (8%)	4 (5%)	3	9
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	22
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	22
7	AH	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	1	2
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	2	5
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	5
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	5
9	AJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	5
9	BJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	5
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	6
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	6
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	AM	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	199 (83%)	30 (12%)	12 (5%)	3	9
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	3	11
14	AT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	20
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	20
15	AU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	13
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	13
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	26	63
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	26	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Ay	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
17	By	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
18	AX	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	0	1
18	BX	35/50 (70%)	27 (77%)	4 (11%)	4 (11%)	0	1
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	9
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	9
All	All	5138/5480 (94%)	4278 (83%)	679 (13%)	181 (4%)	4	18

5 of 181 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG

### 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	AA	271/280 (97%)	258 (95%)	13 (5%)	31	67
1	BA	271/280 (97%)	259 (96%)	12 (4%)	35	70
2	AB	390/407 (96%)	374 (96%)	16 (4%)	37	73
2	BB	390/407 (96%)	373 (96%)	17 (4%)	35	70
3	AC	347/374 (93%)	329 (95%)	18 (5%)	29	64
3	BC	347/374 (93%)	329 (95%)	18 (5%)	29	64
4	AD	275/283 (97%)	256 (93%)	19 (7%)	19	48
4	BD	275/283 (97%)	256 (93%)	19 (7%)	19	48
5	AE	72/73 (99%)	66 (92%)	6 (8%)	14	38
5	BE	72/73 (99%)	66 (92%)	6 (8%)	14	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	29/39 (74%)	29 (100%)	0	100	100
6	BF	29/39 (74%)	29 (100%)	0	100	100
7	AH	53/55 (96%)	50 (94%)	3 (6%)	25	59
7	BH	53/55 (96%)	50 (94%)	3 (6%)	25	59
8	AI	32/35 (91%)	31 (97%)	1 (3%)	47	82
8	BI	32/35 (91%)	31 (97%)	1 (3%)	47	82
9	AJ	24/28 (86%)	23 (96%)	1 (4%)	36	73
9	BJ	24/28 (86%)	23 (96%)	1 (4%)	36	73
10	AK	30/30 (100%)	28 (93%)	2 (7%)	20	50
10	BK	30/30 (100%)	28 (93%)	2 (7%)	20	50
11	AL	35/35 (100%)	31 (89%)	4 (11%)	7	21
11	BL	35/35 (100%)	32 (91%)	3 (9%)	13	36
12	AM	31/33 (94%)	31 (100%)	0	100	100
12	BM	31/33 (94%)	31 (100%)	0	100	100
13	AO	202/208 (97%)	195 (96%)	7 (4%)	43	78
13	BO	202/208 (97%)	194 (96%)	8 (4%)	38	74
14	AT	29/29 (100%)	28 (97%)	1 (3%)	44	79
14	BT	29/29 (100%)	28 (97%)	1 (3%)	44	79
15	AU	84/89 (94%)	80 (95%)	4 (5%)	31	67
15	BU	84/89 (94%)	80 (95%)	4 (5%)	31	67
16	AV	116/117 (99%)	111 (96%)	5 (4%)	35	71
16	BV	116/117 (99%)	111 (96%)	5 (4%)	35	71
17	Ay	20/37 (54%)	18 (90%)	2 (10%)	9	28
17	By	20/37 (54%)	18 (90%)	2 (10%)	9	28
18	AX	30/42 (71%)	26 (87%)	4 (13%)	5	14
18	BX	30/42 (71%)	26 (87%)	4 (13%)	5	14
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	10	31
20	BZ	52/52 (100%)	47 (90%)	5 (10%)	10	31
All	All	4244/4492 (94%)	4022 (95%)	222 (5%)	29	64

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Ay	28	ILE
2	BB	18	ARG
15	BU	132	LEU
18	AX	12	ILE
1	BA	32	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
15	AU	93	ASN
1	BA	241	GLN
13	BO	222	GLN
17	Ay	21	GLN
1	BA	12	ASN

### 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	AA	402	1	55,73,73	0.97	4 (7%)	61,113,113	1.46	11 (18%)
22	CLA	AA	403	-	55,73,73	1.06	4 (7%)	61,113,113	1.65	11 (18%)
22	CLA	AA	404	-	55,73,73	0.95	4 (7%)	61,113,113	1.43	11 (18%)
23	PHO	AA	405	-	67,69,69	0.99	2 (2%)	84,99,99	1.33	11 (13%)
22	CLA	AA	406	1	55,73,73	0.98	3 (5%)	61,113,113	1.46	9 (14%)
24	PL9	AA	407	-	45,45,55	0.98	1 (2%)	56,57,69	1.86	16 (28%)
25	OEC	AA	408	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	BCR	AA	409	-	41,41,41	1.63	7 (17%)	56,56,56	2.13	19 (33%)
27	DGD	AA	410	-	57,57,67	1.47	12 (21%)	71,71,81	1.45	8 (11%)
28	LHG	AA	411	-	38,38,48	1.89	5 (13%)	39,44,54	1.31	3 (7%)
29	SQD	AA	412	-	50,51,54	2.38	24 (48%)	58,62,65	3.00	17 (29%)
30	LMG	AA	413	-	51,51,55	0.89	2 (3%)	59,59,63	1.00	4 (6%)
29	SQD	AA	415	-	53,54,54	2.49	28 (52%)	61,65,65	2.85	18 (29%)
30	LMG	AA	416	-	42,42,55	1.50	8 (19%)	50,50,63	1.01	3 (6%)
22	CLA	AB	601	-	55,73,73	1.05	3 (5%)	61,113,113	1.43	11 (18%)
22	CLA	AB	602	2	55,73,73	0.99	3 (5%)	61,113,113	1.42	10 (16%)
22	CLA	AB	603	2	55,73,73	1.05	5 (9%)	61,113,113	1.51	11 (18%)
22	CLA	AB	604	2	55,73,73	1.01	3 (5%)	61,113,113	1.38	9 (14%)
22	CLA	AB	605	-	55,73,73	0.95	3 (5%)	61,113,113	1.42	9 (14%)
22	CLA	AB	606	2	55,73,73	0.93	3 (5%)	61,113,113	1.38	10 (16%)
22	CLA	AB	607	-	55,73,73	1.12	5 (9%)	61,113,113	1.43	7 (11%)
22	CLA	AB	608	2	55,73,73	1.08	5 (9%)	61,113,113	1.52	12 (19%)
22	CLA	AB	609	2	55,73,73	0.99	3 (5%)	61,113,113	1.42	11 (18%)
22	CLA	AB	610	-	55,73,73	0.99	4 (7%)	61,113,113	1.51	12 (19%)
22	CLA	AB	611	2	55,73,73	1.03	4 (7%)	61,113,113	1.48	10 (16%)
22	CLA	AB	612	-	55,73,73	0.95	2 (3%)	61,113,113	1.49	10 (16%)
22	CLA	AB	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.42	11 (18%)
22	CLA	AB	614	2	55,73,73	1.09	4 (7%)	61,113,113	1.57	13 (21%)
22	CLA	AB	615	-	55,73,73	0.90	4 (7%)	61,113,113	1.49	10 (16%)
22	CLA	AB	616	-	55,73,73	1.07	5 (9%)	61,113,113	1.50	11 (18%)
26	BCR	AB	617	-	41,41,41	1.70	7 (17%)	56,56,56	2.04	14 (25%)
26	BCR	AB	618	-	41,41,41	1.70	6 (14%)	56,56,56	2.25	27 (48%)
26	BCR	AB	619	-	41,41,41	1.93	8 (19%)	56,56,56	2.14	15 (26%)
26	BCR	AB	620	-	41,41,41	1.84	7 (17%)	56,56,56	2.12	17 (30%)
30	LMG	AB	621	-	49,49,55	1.01	5 (10%)	57,57,63	1.03	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	LMG	AB	622	-	49,49,55	1.06	5 (10%)	57,57,63	1.06	6 (10%)
30	LMG	AB	623	-	42,42,55	1.46	7 (16%)	50,50,63	1.02	3 (6%)
32	LMT	AB	624	-	36,36,36	1.43	6 (16%)	47,47,47	1.20	3 (6%)
32	LMT	AB	625	-	36,36,36	1.37	7 (19%)	47,47,47	0.95	3 (6%)
27	DGD	AB	626	-	53,53,67	1.83	16 (30%)	67,67,81	1.65	8 (11%)
32	LMT	AB	627	-	36,36,36	1.44	5 (13%)	47,47,47	1.03	3 (6%)
22	CLA	AC	501	3	55,73,73	0.98	2 (3%)	61,113,113	1.48	11 (18%)
22	CLA	AC	502	3	55,73,73	0.98	3 (5%)	61,113,113	1.43	10 (16%)
22	CLA	AC	503	3	55,73,73	1.01	3 (5%)	61,113,113	1.40	8 (13%)
22	CLA	AC	504	-	55,73,73	1.04	4 (7%)	61,113,113	1.35	8 (13%)
22	CLA	AC	505	3	55,73,73	1.04	4 (7%)	61,113,113	1.54	12 (19%)
22	CLA	AC	506	3	55,73,73	0.97	4 (7%)	61,113,113	1.45	11 (18%)
22	CLA	AC	507	-	55,73,73	0.96	3 (5%)	61,113,113	1.49	10 (16%)
22	CLA	AC	508	3	55,73,73	0.95	4 (7%)	61,113,113	1.50	10 (16%)
22	CLA	AC	509	-	55,73,73	1.01	4 (7%)	61,113,113	1.51	10 (16%)
22	CLA	AC	510	-	55,73,73	0.98	4 (7%)	61,113,113	1.42	8 (13%)
22	CLA	AC	511	3	55,73,73	0.94	3 (5%)	61,113,113	1.43	9 (14%)
22	CLA	AC	512	-	55,73,73	1.00	3 (5%)	61,113,113	1.52	11 (18%)
22	CLA	AC	513	3	55,73,73	1.10	4 (7%)	61,113,113	1.46	10 (16%)
26	BCR	AC	514	-	41,41,41	1.75	7 (17%)	56,56,56	2.18	21 (37%)
26	BCR	AC	515	-	41,41,41	1.68	6 (14%)	56,56,56	2.21	20 (35%)
27	DGD	AC	516	-	54,54,67	1.21	8 (14%)	68,68,81	1.59	8 (11%)
27	DGD	AC	517	-	63,63,67	1.05	5 (7%)	77,77,81	1.61	8 (10%)
27	DGD	AC	518	-	67,67,67	1.02	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	AC	519	-	48,48,55	1.23	5 (10%)	56,56,63	0.87	3 (5%)
30	LMG	AC	520	-	45,45,55	1.52	8 (17%)	53,53,63	1.04	4 (7%)
28	LHG	AC	521	-	36,36,48	1.05	2 (5%)	37,42,54	1.15	3 (8%)
33	BCT	AD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	AD	402	4	55,73,73	1.05	4 (7%)	61,113,113	1.54	12 (19%)
23	PHO	AD	403	-	67,69,69	1.05	4 (5%)	84,99,99	1.35	12 (14%)
22	CLA	AD	404	-	55,73,73	1.06	3 (5%)	61,113,113	1.46	8 (13%)
24	PL9	AD	405	-	55,55,55	0.55	0	68,69,69	1.82	18 (26%)
26	BCR	AD	406	-	41,41,41	1.83	7 (17%)	56,56,56	2.36	20 (35%)
30	LMG	AD	407	-	46,46,55	0.95	4 (8%)	54,54,63	0.92	2 (3%)
30	LMG	AD	408	-	48,48,55	1.04	3 (6%)	56,56,63	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	SQD	AD	409	-	42,43,54	2.71	20 (47%)	50,54,65	3.26	14 (28%)
27	DGD	AD	410	-	64,64,67	1.79	16 (25%)	78,78,81	1.43	7 (8%)
32	LMT	AD	411	-	32,32,36	1.49	4 (12%)	43,43,47	0.99	2 (4%)
34	HEM	AE	101	5,6	30,50,50	2.37	13 (43%)	24,82,82	3.37	9 (37%)
30	LMG	AE	102	-	44,44,55	1.32	6 (13%)	52,52,63	1.12	5 (9%)
29	SQD	AF	101	-	44,45,54	2.46	21 (47%)	52,56,65	3.05	17 (32%)
26	BCR	AH	101	-	41,41,41	1.86	8 (19%)	56,56,56	2.30	21 (37%)
27	DGD	AH	102	-	59,59,67	1.24	8 (13%)	73,73,81	1.47	7 (9%)
30	LMG	AI	101	-	43,43,55	1.47	8 (18%)	51,51,63	1.08	4 (7%)
32	LMT	AI	102	-	36,36,36	1.40	4 (11%)	47,47,47	0.96	1 (2%)
24	PL9	AJ	101	-	35,35,55	1.39	4 (11%)	44,45,69	1.82	13 (29%)
26	BCR	AJ	102	-	41,41,41	2.05	8 (19%)	56,56,56	3.42	22 (39%)
26	BCR	AK	102	-	41,41,41	1.84	7 (17%)	56,56,56	2.56	25 (44%)
30	LMG	AM	101	-	42,42,55	1.59	6 (14%)	50,50,63	1.21	5 (10%)
32	LMT	AM	102	-	36,36,36	1.18	2 (5%)	47,47,47	0.94	2 (4%)
32	LMT	AT	101	-	36,36,36	1.35	5 (13%)	47,47,47	1.09	4 (8%)
26	BCR	AT	102	-	41,41,41	1.62	6 (14%)	56,56,56	2.25	25 (44%)
34	HEM	AV	201	16	30,50,50	2.31	13 (43%)	24,82,82	3.24	8 (33%)
26	BCR	AZ	101	-	41,41,41	1.83	7 (17%)	56,56,56	2.14	18 (32%)
29	SQD	BA	401	-	53,54,54	2.55	29 (54%)	61,65,65	2.91	20 (32%)
22	CLA	BA	403	1	55,73,73	1.07	5 (9%)	61,113,113	1.44	10 (16%)
22	CLA	BA	404	-	55,73,73	1.04	2 (3%)	61,113,113	1.66	11 (18%)
22	CLA	BA	405	-	55,73,73	0.90	3 (5%)	61,113,113	1.44	10 (16%)
23	PHO	BA	406	-	67,69,69	1.01	4 (5%)	84,99,99	1.31	11 (13%)
22	CLA	BA	407	1	55,73,73	0.97	3 (5%)	61,113,113	1.46	10 (16%)
24	PL9	BA	408	-	45,45,55	1.04	2 (4%)	56,57,69	1.80	14 (25%)
25	OEC	BA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	BCR	BA	410	-	41,41,41	1.69	7 (17%)	56,56,56	2.12	23 (41%)
27	DGD	BA	411	-	57,57,67	1.59	13 (22%)	71,71,81	1.45	7 (9%)
28	LHG	BA	412	-	38,38,48	1.85	6 (15%)	39,44,54	1.30	3 (7%)
29	SQD	BA	413	-	50,51,54	2.40	23 (46%)	58,62,65	2.96	18 (31%)
30	LMG	BA	414	-	51,51,55	0.91	4 (7%)	59,59,63	1.02	4 (6%)
29	SQD	BB	601	-	46,47,54	2.61	23 (50%)	54,58,65	2.94	15 (27%)
27	DGD	BB	602	-	53,53,67	1.83	16 (30%)	67,67,81	1.63	9 (13%)
32	LMT	BB	603	-	36,36,36	1.42	7 (19%)	47,47,47	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	BB	604	-	55,73,73	1.09	3 (5%)	61,113,113	1.43	11 (18%)
22	CLA	BB	605	2	55,73,73	1.01	3 (5%)	61,113,113	1.44	10 (16%)
22	CLA	BB	606	2	55,73,73	1.00	3 (5%)	61,113,113	1.50	10 (16%)
22	CLA	BB	607	2	55,73,73	1.01	3 (5%)	61,113,113	1.36	9 (14%)
22	CLA	BB	608	2	55,73,73	0.92	3 (5%)	61,113,113	1.41	9 (14%)
22	CLA	BB	609	2	55,73,73	0.96	2 (3%)	61,113,113	1.41	10 (16%)
22	CLA	BB	610	-	55,73,73	1.15	6 (10%)	61,113,113	1.44	8 (13%)
22	CLA	BB	611	2	55,73,73	1.05	6 (10%)	61,113,113	1.53	12 (19%)
22	CLA	BB	612	2	55,73,73	0.98	2 (3%)	61,113,113	1.42	9 (14%)
22	CLA	BB	613	-	55,73,73	1.02	5 (9%)	61,113,113	1.50	12 (19%)
22	CLA	BB	614	2	55,73,73	0.95	3 (5%)	61,113,113	1.46	10 (16%)
22	CLA	BB	615	-	55,73,73	0.95	4 (7%)	61,113,113	1.50	11 (18%)
22	CLA	BB	616	-	55,73,73	0.96	3 (5%)	61,113,113	1.44	11 (18%)
22	CLA	BB	617	2	55,73,73	1.05	3 (5%)	61,113,113	1.55	13 (21%)
22	CLA	BB	618	-	55,73,73	0.90	3 (5%)	61,113,113	1.45	10 (16%)
22	CLA	BB	619	-	55,73,73	1.11	5 (9%)	61,113,113	1.50	12 (19%)
26	BCR	BB	620	-	41,41,41	1.56	8 (19%)	56,56,56	2.05	14 (25%)
26	BCR	BB	621	-	41,41,41	1.85	7 (17%)	56,56,56	2.18	17 (30%)
26	BCR	BB	622	-	41,41,41	1.81	7 (17%)	56,56,56	2.10	18 (32%)
30	LMG	BB	623	-	49,49,55	1.07	5 (10%)	57,57,63	1.05	4 (7%)
30	LMG	BB	624	-	49,49,55	1.04	5 (10%)	57,57,63	1.04	3 (5%)
32	LMT	BB	625	-	36,36,36	1.53	8 (22%)	47,47,47	1.23	3 (6%)
32	LMT	BB	626	-	36,36,36	1.35	5 (13%)	47,47,47	0.93	2 (4%)
22	CLA	BC	501	3	55,73,73	0.95	3 (5%)	61,113,113	1.49	10 (16%)
22	CLA	BC	502	3	55,73,73	0.96	3 (5%)	61,113,113	1.42	10 (16%)
22	CLA	BC	503	3	55,73,73	0.99	2 (3%)	61,113,113	1.40	8 (13%)
22	CLA	BC	504	-	55,73,73	1.05	4 (7%)	61,113,113	1.38	8 (13%)
22	CLA	BC	505	3	55,73,73	1.00	4 (7%)	61,113,113	1.54	12 (19%)
22	CLA	BC	506	3	55,73,73	1.04	4 (7%)	61,113,113	1.41	10 (16%)
22	CLA	BC	507	-	55,73,73	0.96	3 (5%)	61,113,113	1.49	11 (18%)
22	CLA	BC	508	3	55,73,73	0.98	4 (7%)	61,113,113	1.47	10 (16%)
22	CLA	BC	509	-	55,73,73	1.05	6 (10%)	61,113,113	1.50	11 (18%)
22	CLA	BC	510	-	55,73,73	0.92	3 (5%)	61,113,113	1.45	9 (14%)
22	CLA	BC	511	3	55,73,73	0.98	4 (7%)	61,113,113	1.43	8 (13%)
22	CLA	BC	512	-	55,73,73	0.99	2 (3%)	61,113,113	1.52	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	BC	513	3	55,73,73	1.07	4 (7%)	61,113,113	1.45	9 (14%)
26	BCR	BC	514	-	41,41,41	1.89	7 (17%)	56,56,56	2.17	21 (37%)
26	BCR	BC	515	-	41,41,41	1.81	7 (17%)	56,56,56	2.20	20 (35%)
27	DGD	BC	516	-	54,54,67	1.32	9 (16%)	68,68,81	1.55	8 (11%)
27	DGD	BC	517	-	63,63,67	1.08	6 (9%)	77,77,81	1.61	8 (10%)
27	DGD	BC	518	-	67,67,67	1.14	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	BC	519	-	48,48,55	1.26	6 (12%)	56,56,63	0.87	3 (5%)
30	LMG	BC	520	-	45,45,55	1.54	10 (22%)	53,53,63	1.06	4 (7%)
28	LHG	BC	521	-	36,36,48	1.04	2 (5%)	37,42,54	1.15	3 (8%)
33	BCT	BD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	BD	402	4	55,73,73	1.04	3 (5%)	61,113,113	1.53	12 (19%)
23	PHO	BD	403	-	67,69,69	1.03	5 (7%)	84,99,99	1.36	11 (13%)
22	CLA	BD	404	-	55,73,73	1.08	5 (9%)	61,113,113	1.40	8 (13%)
24	PL9	BD	405	-	55,55,55	0.53	0	68,69,69	1.83	18 (26%)
26	BCR	BD	406	-	41,41,41	1.92	8 (19%)	56,56,56	2.35	19 (33%)
30	LMG	BD	407	-	46,46,55	1.02	4 (8%)	54,54,63	0.93	2 (3%)
30	LMG	BD	408	-	48,48,55	1.12	3 (6%)	56,56,63	1.02	3 (5%)
29	SQD	BD	409	-	42,43,54	2.68	20 (47%)	50,54,65	3.26	14 (28%)
27	DGD	BD	410	-	64,64,67	1.73	17 (26%)	78,78,81	1.43	7 (8%)
32	LMT	BD	411	-	32,32,36	1.39	4 (12%)	43,43,47	0.94	2 (4%)
34	HEM	BE	101	5,6	30,50,50	2.37	14 (46%)	24,82,82	3.36	9 (37%)
30	LMG	BE	102	-	44,44,55	1.33	6 (13%)	52,52,63	1.12	5 (9%)
29	SQD	BF	101	-	44,45,54	2.56	20 (45%)	52,56,65	3.03	16 (30%)
27	DGD	BH	101	-	59,59,67	1.20	9 (15%)	73,73,81	1.47	7 (9%)
30	LMG	BI	101	-	43,43,55	1.54	8 (18%)	51,51,63	1.10	5 (9%)
32	LMT	BI	102	-	36,36,36	1.50	4 (11%)	47,47,47	0.97	1 (2%)
24	PL9	BJ	101	-	35,35,55	1.43	5 (14%)	44,45,69	1.76	13 (29%)
26	BCR	BJ	102	-	41,41,41	2.16	8 (19%)	56,56,56	3.42	24 (42%)
26	BCR	BK	102	-	41,41,41	1.85	7 (17%)	56,56,56	2.56	27 (48%)
29	SQD	BL	101	-	46,47,54	2.72	22 (47%)	54,58,65	2.97	15 (27%)
32	LMT	BM	101	-	36,36,36	1.18	3 (8%)	47,47,47	0.96	2 (4%)
30	LMG	BM	102	-	42,42,55	1.62	8 (19%)	50,50,63	1.15	4 (8%)
32	LMT	BT	101	-	36,36,36	1.29	4 (11%)	47,47,47	1.06	3 (6%)
34	HEM	BV	201	16	30,50,50	2.34	10 (33%)	24,82,82	3.28	7 (29%)
26	BCR	BX	101	-	41,41,41	1.85	8 (19%)	56,56,56	2.31	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	BZ	101	-	41,41,41	1.94	9 (21%)	56,56,56	2.12	20 (35%)

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	AA	402	1	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AA	403	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AA	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PHO	AA	405	-	-	1/53/103/103	0/1/6/6
22	CLA	AA	406	1	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	AA	407	-	-	0/41/61/73	0/1/1/1
25	OEC	AA	408	1,3	-	0/0/0/54	0/0/0/5
26	BCR	AA	409	-	-	0/29/63/63	0/2/2/2
27	DGD	AA	410	-	3/3/13/13	0/45/85/95	0/2/2/2
28	LHG	AA	411	-	-	0/43/43/53	0/0/0/0
29	SQD	AA	412	-	-	0/46/66/69	0/1/1/1
30	LMG	AA	413	-	2/2/8/8	0/46/66/70	0/1/1/1
29	SQD	AA	415	-	-	0/49/69/69	0/1/1/1
30	LMG	AA	416	-	2/2/8/8	0/37/57/70	0/1/1/1
22	CLA	AB	601	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	602	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AB	603	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	604	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	606	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AB	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	608	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	609	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	611	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AB	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	614	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	615	-	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	AB	616	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	AB	617	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	618	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	620	-	-	0/29/63/63	0/2/2/2
30	LMG	AB	621	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	AB	622	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	AB	623	-	2/2/8/8	0/37/57/70	0/1/1/1
32	LMT	AB	624	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	625	-	-	0/21/61/61	0/2/2/2
27	DGD	AB	626	-	3/3/13/13	0/41/81/95	0/2/2/2
32	LMT	AB	627	-	-	0/21/61/61	0/2/2/2
22	CLA	AC	501	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	502	3	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AC	503	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	505	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	506	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	508	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	509	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AC	510	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AC	511	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	513	3	3/3/20/25	1/37/135/135	0/0/9/9
26	BCR	AC	514	-	-	0/29/63/63	0/2/2/2
26	BCR	AC	515	-	-	0/29/63/63	0/2/2/2
27	DGD	AC	516	-	3/3/13/13	0/42/82/95	0/2/2/2
27	DGD	AC	517	-	3/3/13/13	0/51/91/95	0/2/2/2
27	DGD	AC	518	-	3/3/13/13	0/55/95/95	0/2/2/2
30	LMG	AC	519	-	2/2/8/8	0/43/63/70	0/1/1/1
30	LMG	AC	520	-	2/2/8/8	0/40/60/70	0/1/1/1
28	LHG	AC	521	-	-	0/41/41/53	0/0/0/0
33	BCT	AD	401	21	-	0/0/0/0	0/0/0/0
22	CLA	AD	402	4	2/2/20/25	0/37/135/135	0/0/9/9
23	PHO	AD	403	-	-	0/53/103/103	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	AD	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	AD	405	-	-	0/53/73/73	0/1/1/1
26	BCR	AD	406	-	-	0/29/63/63	0/2/2/2
30	LMG	AD	407	-	2/2/8/8	0/41/61/70	0/1/1/1
30	LMG	AD	408	-	2/2/8/8	1/43/63/70	0/1/1/1
29	SQD	AD	409	-	-	2/38/58/69	0/1/1/1
27	DGD	AD	410	-	3/3/13/13	0/52/92/95	0/2/2/2
32	LMT	AD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	AE	101	5,6	-	0/10/54/54	0/0/8/8
30	LMG	AE	102	-	2/2/8/8	0/39/59/70	0/1/1/1
29	SQD	AF	101	-	-	0/40/60/69	0/1/1/1
26	BCR	AH	101	-	-	0/29/63/63	0/2/2/2
27	DGD	AH	102	-	3/3/13/13	0/47/87/95	0/2/2/2
30	LMG	AI	101	-	2/2/8/8	0/38/58/70	0/1/1/1
32	LMT	AI	102	-	-	0/21/61/61	0/2/2/2
24	PL9	AJ	101	-	-	0/29/49/73	0/1/1/1
26	BCR	AJ	102	-	-	0/29/63/63	0/2/2/2
26	BCR	AK	102	-	-	0/29/63/63	0/2/2/2
30	LMG	AM	101	-	2/2/8/8	1/37/57/70	0/1/1/1
32	LMT	AM	102	-	-	0/21/61/61	0/2/2/2
32	LMT	AT	101	-	-	0/21/61/61	0/2/2/2
26	BCR	AT	102	-	-	0/29/63/63	0/2/2/2
34	HEM	AV	201	16	-	0/10/54/54	0/0/8/8
26	BCR	AZ	101	-	-	0/29/63/63	0/2/2/2
29	SQD	BA	401	-	-	0/49/69/69	0/1/1/1
22	CLA	BA	403	1	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BA	404	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BA	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PHO	BA	406	-	-	1/53/103/103	0/1/6/6
22	CLA	BA	407	1	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	BA	408	-	-	0/41/61/73	0/1/1/1
25	OEC	BA	409	1,3	-	0/0/0/54	0/0/0/5
26	BCR	BA	410	-	-	0/29/63/63	0/2/2/2
27	DGD	BA	411	-	3/3/13/13	0/45/85/95	0/2/2/2
28	LHG	BA	412	-	-	0/43/43/53	0/0/0/0
29	SQD	BA	413	-	-	0/46/66/69	0/1/1/1
30	LMG	BA	414	-	2/2/8/8	0/46/66/70	0/1/1/1
29	SQD	BB	601	-	-	0/42/62/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	BB	602	-	3/3/13/13	0/41/81/95	0/2/2/2
32	LMT	BB	603	-	-	0/21/61/61	0/2/2/2
22	CLA	BB	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	605	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BB	606	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	607	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	608	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	609	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BB	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	611	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	612	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	614	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BB	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	617	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	619	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	BB	620	-	-	0/29/63/63	0/2/2/2
26	BCR	BB	621	-	-	0/29/63/63	0/2/2/2
26	BCR	BB	622	-	-	0/29/63/63	0/2/2/2
30	LMG	BB	623	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	BB	624	-	2/2/8/8	0/44/64/70	0/1/1/1
32	LMT	BB	625	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	626	-	-	0/21/61/61	0/2/2/2
22	CLA	BC	501	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	502	3	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BC	503	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	505	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	506	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	508	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	509	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BC	510	-	3/3/20/25	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BC	511	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	513	3	3/3/20/25	1/37/135/135	0/0/9/9
26	BCR	BC	514	-	-	0/29/63/63	0/2/2/2
26	BCR	BC	515	-	-	0/29/63/63	0/2/2/2
27	DGD	BC	516	-	3/3/13/13	0/42/82/95	0/2/2/2
27	DGD	BC	517	-	3/3/13/13	0/51/91/95	0/2/2/2
27	DGD	BC	518	-	3/3/13/13	0/55/95/95	0/2/2/2
30	LMG	BC	519	-	2/2/8/8	0/43/63/70	0/1/1/1
30	LMG	BC	520	-	2/2/8/8	0/40/60/70	0/1/1/1
28	LHG	BC	521	-	-	0/41/41/53	0/0/0/0
33	BCT	BD	401	21	-	0/0/0/0	0/0/0/0
22	CLA	BD	402	4	2/2/20/25	0/37/135/135	0/0/9/9
23	PHO	BD	403	-	-	0/53/103/103	0/1/6/6
22	CLA	BD	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	BD	405	-	-	0/53/73/73	0/1/1/1
26	BCR	BD	406	-	-	0/29/63/63	0/2/2/2
30	LMG	BD	407	-	2/2/8/8	0/41/61/70	0/1/1/1
30	LMG	BD	408	-	2/2/8/8	1/43/63/70	0/1/1/1
29	SQD	BD	409	-	-	2/38/58/69	0/1/1/1
27	DGD	BD	410	-	3/3/13/13	0/52/92/95	0/2/2/2
32	LMT	BD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	BE	101	5,6	-	0/10/54/54	0/0/8/8
30	LMG	BE	102	-	2/2/8/8	0/39/59/70	0/1/1/1
29	SQD	BF	101	-	-	0/40/60/69	0/1/1/1
27	DGD	BH	101	-	3/3/13/13	0/47/87/95	0/2/2/2
30	LMG	BI	101	-	2/2/8/8	0/38/58/70	0/1/1/1
32	LMT	BI	102	-	-	0/21/61/61	0/2/2/2
24	PL9	BJ	101	-	-	0/29/49/73	0/1/1/1
26	BCR	BJ	102	-	-	0/29/63/63	0/2/2/2
26	BCR	BK	102	-	-	0/29/63/63	0/2/2/2
29	SQD	BL	101	-	-	0/42/62/69	0/1/1/1
32	LMT	BM	101	-	-	0/21/61/61	0/2/2/2
30	LMG	BM	102	-	2/2/8/8	1/37/57/70	0/1/1/1
32	LMT	BT	101	-	-	0/21/61/61	0/2/2/2
34	HEM	BV	201	16	-	0/10/54/54	0/0/8/8
26	BCR	BX	101	-	-	0/29/63/63	0/2/2/2
26	BCR	BZ	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1087 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BV	201	HEM	C2D-C3D	-4.77	1.40	1.54
34	AE	101	HEM	C2D-C3D	-4.71	1.40	1.54
34	BE	101	HEM	C2D-C3D	-4.69	1.40	1.54
34	AV	201	HEM	C2D-C3D	-4.52	1.41	1.54
34	AV	201	HEM	C3B-C4B	-4.28	1.48	1.51

The worst 5 of 1765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AJ	102	BCR	C32-C1-C6	-10.35	94.07	110.30
26	BJ	102	BCR	C32-C1-C6	-10.19	94.32	110.30
26	BJ	102	BCR	C32-C1-C31	-9.18	78.96	108.37
26	AJ	102	BCR	C32-C1-C31	-8.87	79.94	108.37
34	BV	201	HEM	C3C-CAC-CBC	-8.33	111.69	124.46

5 of 294 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AB	614	CLA	NC
22	AB	614	CLA	ND
22	AB	614	CLA	NA
22	BB	617	CLA	NC
22	BB	617	CLA	ND

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AB	611	CLA	C1-C2-C3-C4
22	BB	614	CLA	C1-C2-C3-C4
22	AC	513	CLA	C1-C2-C3-C4
22	BC	513	CLA	C1-C2-C3-C4
22	BC	510	CLA	C1-C2-C3-C4

There are no ring outliers.

165 monomers are involved in 627 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AA	402	CLA	7	0
22	AA	403	CLA	7	0
22	AA	404	CLA	2	0
23	AA	405	PHO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AA	406	CLA	3	0
24	AA	407	PL9	5	0
26	AA	409	BCR	6	0
28	AA	411	LHG	3	0
29	AA	412	SQD	5	0
30	AA	413	LMG	1	0
29	AA	415	SQD	5	0
30	AA	416	LMG	4	0
22	AB	601	CLA	2	0
22	AB	602	CLA	5	0
22	AB	603	CLA	7	0
22	AB	604	CLA	5	0
22	AB	605	CLA	5	0
22	AB	606	CLA	5	0
22	AB	607	CLA	15	0
22	AB	608	CLA	9	0
22	AB	609	CLA	6	0
22	AB	610	CLA	3	0
22	AB	611	CLA	4	0
22	AB	612	CLA	5	0
22	AB	613	CLA	3	0
22	AB	614	CLA	1	0
22	AB	615	CLA	7	0
22	AB	616	CLA	4	0
26	AB	617	BCR	3	0
26	AB	618	BCR	5	0
26	AB	620	BCR	2	0
30	AB	621	LMG	1	0
30	AB	622	LMG	1	0
30	AB	623	LMG	2	0
32	AB	624	LMT	1	0
32	AB	625	LMT	2	0
27	AB	626	DGD	3	0
32	AB	627	LMT	3	0
22	AC	501	CLA	3	0
22	AC	502	CLA	4	0
22	AC	503	CLA	4	0
22	AC	504	CLA	5	0
22	AC	505	CLA	10	0
22	AC	506	CLA	3	0
22	AC	507	CLA	4	0
22	AC	508	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AC	509	CLA	2	0
22	AC	510	CLA	4	0
22	AC	511	CLA	9	0
22	AC	512	CLA	9	0
22	AC	513	CLA	3	0
26	AC	514	BCR	9	0
26	AC	515	BCR	6	0
27	AC	516	DGD	3	0
27	AC	517	DGD	8	0
27	AC	518	DGD	8	0
30	AC	519	LMG	2	0
30	AC	520	LMG	4	0
28	AC	521	LHG	5	0
33	AD	401	BCT	1	0
22	AD	402	CLA	7	0
23	AD	403	PHO	2	0
22	AD	404	CLA	4	0
24	AD	405	PL9	9	0
26	AD	406	BCR	3	0
30	AD	407	LMG	2	0
30	AD	408	LMG	7	0
29	AD	409	SQD	2	0
32	AD	411	LMT	2	0
34	AE	101	HEM	5	0
30	AE	102	LMG	4	0
29	AF	101	SQD	2	0
26	AH	101	BCR	5	0
27	AH	102	DGD	1	0
30	AI	101	LMG	3	0
32	AI	102	LMT	4	0
26	AJ	102	BCR	5	0
26	AK	102	BCR	13	0
30	AM	101	LMG	4	0
32	AM	102	LMT	1	0
32	AT	101	LMT	3	0
26	AT	102	BCR	8	0
34	AV	201	HEM	3	0
26	AZ	101	BCR	5	0
29	BA	401	SQD	2	0
22	BA	403	CLA	7	0
22	BA	404	CLA	6	0
22	BA	405	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	BA	406	PHO	5	0
22	BA	407	CLA	3	0
24	BA	408	PL9	6	0
26	BA	410	BCR	3	0
28	BA	412	LHG	4	0
29	BA	413	SQD	4	0
30	BA	414	LMG	2	0
29	BB	601	SQD	2	0
27	BB	602	DGD	3	0
32	BB	603	LMT	3	0
22	BB	604	CLA	1	0
22	BB	605	CLA	6	0
22	BB	606	CLA	7	0
22	BB	607	CLA	5	0
22	BB	608	CLA	5	0
22	BB	609	CLA	6	0
22	BB	610	CLA	14	0
22	BB	611	CLA	9	0
22	BB	612	CLA	7	0
22	BB	613	CLA	3	0
22	BB	614	CLA	7	0
22	BB	615	CLA	5	0
22	BB	616	CLA	3	0
22	BB	617	CLA	2	0
22	BB	618	CLA	6	0
22	BB	619	CLA	6	0
26	BB	620	BCR	3	0
26	BB	622	BCR	2	0
30	BB	623	LMG	1	0
30	BB	624	LMG	1	0
32	BB	626	LMT	2	0
22	BC	501	CLA	3	0
22	BC	502	CLA	4	0
22	BC	503	CLA	5	0
22	BC	504	CLA	6	0
22	BC	505	CLA	10	0
22	BC	506	CLA	3	0
22	BC	507	CLA	4	0
22	BC	508	CLA	7	0
22	BC	509	CLA	2	0
22	BC	510	CLA	3	0
22	BC	511	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	BC	512	CLA	7	0
22	BC	513	CLA	4	0
26	BC	514	BCR	10	0
26	BC	515	BCR	7	0
27	BC	516	DGD	3	0
27	BC	517	DGD	10	0
27	BC	518	DGD	8	0
30	BC	519	LMG	3	0
30	BC	520	LMG	5	0
28	BC	521	LHG	4	0
33	BD	401	BCT	1	0
22	BD	402	CLA	8	0
23	BD	403	PHO	5	0
22	BD	404	CLA	4	0
24	BD	405	PL9	8	0
26	BD	406	BCR	3	0
30	BD	407	LMG	2	0
30	BD	408	LMG	8	0
29	BD	409	SQD	2	0
32	BD	411	LMT	1	0
34	BE	101	HEM	6	0
30	BE	102	LMG	4	0
29	BF	101	SQD	1	0
27	BH	101	DGD	1	0
30	BI	101	LMG	3	0
32	BI	102	LMT	3	0
26	BJ	102	BCR	5	0
26	BK	102	BCR	13	0
29	BL	101	SQD	2	0
32	BM	101	LMT	1	0
30	BM	102	LMG	4	0
32	BT	101	LMT	3	0
34	BV	201	HEM	3	0
26	BX	101	BCR	6	0
26	BZ	101	BCR	5	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	AA	335/344 (97%)	-0.44	8 (2%) 62 57	23, 59, 88, 103	0
1	BA	335/344 (97%)	-0.24	5 (1%) 76 74	47, 70, 89, 103	0
2	AB	490/510 (96%)	-0.23	9 (1%) 71 68	37, 63, 86, 99	0
2	BB	490/510 (96%)	-0.24	11 (2%) 65 60	41, 64, 87, 103	0
3	AC	447/473 (94%)	-0.19	12 (2%) 58 52	43, 72, 87, 102	0
3	BC	447/473 (94%)	0.06	18 (4%) 42 35	54, 83, 95, 101	0
4	AD	340/352 (96%)	-0.43	3 (0%) 85 84	29, 59, 84, 95	0
4	BD	340/352 (96%)	-0.32	5 (1%) 76 74	40, 69, 91, 101	0
5	AE	82/84 (97%)	0.10	6 (7%) 18 12	54, 75, 93, 99	0
5	BE	82/84 (97%)	0.51	8 (9%) 10 6	71, 85, 98, 104	0
6	AF	35/45 (77%)	-0.13	2 (5%) 27 21	56, 73, 94, 97	0
6	BF	35/45 (77%)	0.39	5 (14%) 4 2	75, 82, 97, 99	0
7	AH	65/66 (98%)	0.16	4 (6%) 24 17	57, 76, 92, 97	0
7	BH	65/66 (98%)	0.30	8 (12%) 5 3	62, 80, 91, 103	0
8	AI	35/38 (92%)	-0.07	3 (8%) 13 8	57, 70, 87, 94	0
8	BI	35/38 (92%)	-0.03	0 100 100	69, 80, 92, 95	0
9	AJ	34/40 (85%)	-0.41	0 100 100	65, 74, 83, 89	0
9	BJ	34/40 (85%)	-0.20	1 (2%) 55 49	73, 81, 93, 98	0
10	AK	37/37 (100%)	-0.35	1 (2%) 58 52	67, 75, 87, 93	0
10	BK	37/37 (100%)	0.01	2 (5%) 29 23	84, 90, 96, 101	0
11	AL	37/37 (100%)	0.19	6 (16%) 3 1	45, 60, 98, 107	0
11	BL	37/37 (100%)	0.26	5 (13%) 4 2	46, 62, 94, 102	0
12	AM	34/36 (94%)	-0.05	2 (5%) 26 19	51, 65, 94, 100	0
12	BM	34/36 (94%)	-0.16	2 (5%) 26 19	55, 61, 76, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AO	243/247 (98%)	0.11	15 (6%) 24 17	39, 70, 93, 107	0
13	BO	243/247 (98%)	0.24	18 (7%) 17 11	48, 76, 97, 107	0
14	AT	32/32 (100%)	0.10	3 (9%) 11 6	53, 63, 102, 104	0
14	BT	32/32 (100%)	-0.12	2 (6%) 23 17	57, 67, 93, 103	0
15	AU	97/104 (93%)	-0.05	1 (1%) 84 82	43, 63, 78, 86	0
15	BU	97/104 (93%)	-0.20	1 (1%) 84 82	55, 67, 77, 87	0
16	AV	137/137 (100%)	-0.19	1 (0%) 89 88	49, 66, 76, 79	0
16	BV	137/137 (100%)	0.15	7 (5%) 32 25	64, 79, 95, 102	0
17	Ay	28/46 (60%)	0.40	4 (14%) 4 2	79, 91, 97, 99	0
17	By	28/46 (60%)	0.43	3 (10%) 8 4	89, 98, 102, 106	0
18	AX	37/50 (74%)	-0.17	2 (5%) 29 23	70, 79, 93, 95	0
18	BX	37/50 (74%)	0.35	6 (16%) 3 1	75, 82, 91, 94	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.33	10 (16%) 3 1	76, 85, 103, 110	0
20	BZ	62/62 (100%)	0.69	12 (19%) 1 1	86, 96, 105, 110	0
All	All	5214/5536 (94%)	-0.11	211 (4%) 42 35	23, 71, 94, 110	0

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BH	65	LEU	8.7
12	AM	33	GLN	6.9
3	BC	473	ASP	6.3
11	BL	1	MET	6.3
14	AT	30	THR	6.3

## 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
31	CL	AA	414	1/1	0.94	0.62	21.13	73,73,73,73	0
27	DGD	AD	410	63/66	0.63	0.53	10.64	91,97,107,108	0
26	BCR	BJ	102	40/40	0.68	0.49	9.03	93,98,101,102	0
24	PL9	AJ	101	35/55	0.60	0.56	8.38	93,101,107,109	0
27	DGD	BD	410	63/66	0.64	0.51	7.79	84,100,105,105	0
24	PL9	BJ	101	35/55	0.71	0.44	7.20	78,99,111,112	0
30	LMG	AA	416	42/55	0.72	0.37	6.04	67,92,96,99	0
32	LMT	BI	102	35/35	0.62	0.57	6.03	90,104,106,106	0
32	LMT	AI	102	35/35	0.78	0.49	5.79	74,92,95,95	0
22	CLA	AD	404	65/65	0.83	0.32	5.62	80,83,102,103	0
26	BCR	AJ	102	40/40	0.71	0.41	5.54	85,91,101,102	0
22	CLA	BA	407	65/65	0.75	0.35	5.50	72,76,103,104	0
30	LMG	AB	623	42/55	0.71	0.36	5.29	70,89,92,93	0
27	DGD	AB	626	52/66	0.79	0.29	4.84	79,94,105,107	0
24	PL9	AA	407	45/55	0.85	0.32	4.81	83,87,94,95	0
22	CLA	AB	601	65/65	0.74	0.39	4.80	88,97,102,105	0
32	LMT	AD	411	31/35	0.74	0.46	4.77	52,96,104,104	0
30	LMG	BC	520	45/55	0.71	0.48	4.69	86,93,101,102	0
30	LMG	AC	520	45/55	0.65	0.42	4.48	75,92,97,98	0
22	CLA	AA	406	65/65	0.79	0.31	4.39	54,60,89,90	0
24	PL9	BA	408	45/55	0.86	0.30	4.26	82,88,90,92	0
32	LMT	AT	101	35/35	0.70	0.34	4.21	72,91,97,98	0
29	SQD	BA	401	54/54	0.75	0.34	4.13	82,91,107,108	0
28	LHG	AC	521	37/49	0.68	0.44	3.88	78,99,109,109	0
32	LMT	AB	625	35/35	0.74	0.43	3.76	82,98,100,101	0
27	DGD	BB	602	52/66	0.72	0.31	3.73	71,85,104,105	0
28	LHG	BC	521	37/49	0.68	0.49	3.59	90,100,113,114	0
26	BCR	AK	102	40/40	0.85	0.31	3.54	73,77,81,81	0
32	LMT	BD	411	31/35	0.65	0.50	3.46	67,91,99,100	0
22	CLA	AB	604	65/65	0.89	0.25	3.43	67,73,91,91	0
30	LMG	BD	408	48/55	0.85	0.26	3.40	68,75,85,87	0
29	SQD	AA	415	54/54	0.83	0.27	3.39	71,87,105,105	0
26	BCR	AZ	101	40/40	0.79	0.32	3.16	75,82,90,91	0
26	BCR	BK	102	40/40	0.84	0.35	3.14	76,81,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	LMG	BD	407	46/55	0.88	0.24	3.05	70,80,92,94	0
22	CLA	AC	512	65/65	0.81	0.32	2.98	91,95,106,106	0
32	LMT	AB	627	35/35	0.47	0.54	2.92	73,103,106,107	0
31	CL	BA	415	1/1	0.93	0.29	2.87	81,81,81,81	0
30	LMG	BE	102	44/55	0.81	0.37	2.84	75,92,98,99	0
22	CLA	BB	612	65/65	0.88	0.28	2.77	82,89,92,95	0
22	CLA	AC	504	65/65	0.90	0.23	2.66	78,86,107,107	0
29	SQD	AF	101	45/54	0.72	0.35	2.63	82,97,102,103	0
23	PHO	BD	403	64/64	0.93	0.23	2.61	77,88,92,93	0
30	LMG	AD	408	48/55	0.90	0.23	2.46	63,68,74,80	0
29	SQD	BF	101	45/54	0.66	0.38	2.40	95,98,103,104	0
22	CLA	AC	507	65/65	0.87	0.27	2.33	83,90,95,97	0
22	CLA	AD	402	65/65	0.94	0.21	2.24	47,58,69,71	0
22	CLA	BA	405	65/65	0.94	0.20	2.23	72,76,104,105	0
26	BCR	AH	101	40/40	0.78	0.32	2.19	76,88,95,95	0
27	DGD	AC	517	62/66	0.89	0.22	2.17	70,78,91,92	0
22	CLA	AC	503	65/65	0.94	0.21	2.14	78,86,92,95	0
22	CLA	AB	609	65/65	0.88	0.26	2.12	76,87,91,92	0
22	CLA	BC	513	65/65	0.82	0.34	2.08	96,99,106,107	0
27	DGD	BA	411	56/66	0.76	0.35	2.07	76,85,103,104	0
32	LMT	BT	101	35/35	0.78	0.34	2.02	77,91,94,95	0
33	BCT	BD	401	4/4	0.95	0.20	1.96	84,86,87,88	0
26	BCR	BC	514	40/40	0.90	0.24	1.94	81,83,87,87	0
26	BCR	AC	514	40/40	0.90	0.23	1.93	56,66,73,74	0
32	LMT	BB	626	35/35	0.77	0.31	1.93	76,93,101,102	0
30	LMG	AC	519	48/55	0.79	0.31	1.92	75,84,89,90	0
26	BCR	BZ	101	40/40	0.81	0.27	1.91	81,90,93,94	0
32	LMT	BM	101	35/35	0.79	0.31	1.89	70,88,97,101	0
22	CLA	AC	513	65/65	0.77	0.35	1.86	92,98,104,106	0
22	CLA	AB	614	65/65	0.91	0.23	1.83	78,85,98,99	0
26	BCR	AT	102	40/40	0.92	0.21	1.83	72,79,91,91	0
26	BCR	AB	618	40/40	0.90	0.20	1.79	75,78,82,83	0
24	PL9	BD	405	55/55	0.93	0.21	1.78	63,70,76,78	0
30	LMG	AE	102	44/55	0.77	0.34	1.76	81,91,96,96	0
26	BCR	BB	622	40/40	0.92	0.25	1.72	67,71,79,80	0
22	CLA	BC	510	65/65	0.92	0.22	1.68	79,83,92,92	0
22	CLA	BD	404	65/65	0.83	0.26	1.68	89,92,101,102	0
26	BCR	AB	620	40/40	0.87	0.24	1.67	75,77,83,84	0
30	LMG	BB	623	49/55	0.88	0.23	1.66	70,78,88,91	0
34	HEM	AE	101	43/43	0.93	0.29	1.65	85,92,103,106	0
22	CLA	AA	404	65/65	0.93	0.20	1.63	63,72,97,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	LMG	BC	519	48/55	0.86	0.31	1.61	83,90,94,95	0
24	PL9	AD	405	55/55	0.93	0.20	1.61	52,67,71,73	0
22	CLA	AC	505	65/65	0.93	0.20	1.60	69,73,77,79	0
26	BCR	BC	515	40/40	0.79	0.30	1.60	74,80,91,92	0
27	DGD	AC	516	53/66	0.89	0.23	1.59	57,72,91,92	0
22	CLA	BB	609	65/65	0.83	0.26	1.58	72,80,96,96	0
26	BCR	BD	406	40/40	0.88	0.23	1.56	66,78,92,92	0
26	BCR	BB	620	40/40	0.92	0.20	1.56	66,69,72,73	0
27	DGD	BC	517	62/66	0.86	0.22	1.52	78,82,100,101	0
27	DGD	AA	410	56/66	0.76	0.32	1.48	78,86,91,92	0
27	DGD	BC	516	53/66	0.90	0.23	1.48	69,77,96,97	0
28	LHG	AA	411	39/49	0.90	0.22	1.43	63,68,76,78	0
22	CLA	AB	602	65/65	0.94	0.22	1.42	81,85,88,90	0
26	BCR	AB	619	40/40	0.91	0.19	1.38	62,70,82,83	0
30	LMG	AA	413	51/55	0.88	0.24	1.33	70,74,77,79	0
22	CLA	AB	606	65/65	0.85	0.25	1.31	73,87,96,96	0
34	HEM	BE	101	43/43	0.92	0.28	1.30	93,95,104,107	0
22	CLA	BB	617	65/65	0.92	0.22	1.29	75,79,99,100	0
27	DGD	BC	518	66/66	0.86	0.24	1.29	71,78,89,90	0
30	LMG	AD	407	46/55	0.92	0.20	1.27	63,71,90,92	0
22	CLA	BB	613	65/65	0.92	0.22	1.26	69,77,82,84	0
30	LMG	AB	621	49/55	0.87	0.23	1.26	62,75,80,83	0
22	CLA	BC	507	65/65	0.89	0.24	1.24	84,92,96,97	0
27	DGD	AC	518	66/66	0.89	0.22	1.23	62,68,84,86	0
32	LMT	AM	102	35/35	0.83	0.30	1.20	67,89,93,96	0
26	BCR	AA	409	40/40	0.92	0.21	1.20	59,67,70,71	0
22	CLA	AB	605	65/65	0.94	0.20	1.19	68,76,84,85	0
22	CLA	AA	402	65/65	0.96	0.17	1.16	51,58,66,69	0
23	PHO	AD	403	64/64	0.93	0.18	1.16	39,56,70,72	0
22	CLA	BB	605	65/65	0.94	0.20	1.16	77,82,86,89	0
29	SQD	AD	409	43/54	0.82	0.24	1.14	68,92,108,111	0
22	CLA	BC	512	65/65	0.81	0.31	1.13	95,99,109,110	0
22	CLA	AB	608	65/65	0.93	0.19	1.10	72,79,87,91	0
22	CLA	AB	616	65/65	0.80	0.27	1.10	73,85,105,106	0
27	DGD	BH	101	58/66	0.91	0.19	1.10	66,73,80,81	0
29	SQD	BA	413	51/54	0.81	0.25	1.07	73,90,103,104	0
30	LMG	BM	102	42/55	0.79	0.31	1.06	72,90,95,98	0
22	CLA	AA	403	65/65	0.95	0.16	1.06	41,48,56,60	0
22	CLA	BC	505	65/65	0.90	0.22	1.04	88,93,94,95	0
34	HEM	AV	201	43/43	0.96	0.20	1.03	60,63,66,67	0
22	CLA	AC	508	65/65	0.91	0.20	1.02	80,86,99,101	0
26	BCR	BB	621	40/40	0.92	0.19	1.02	57,69,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	BB	604	65/65	0.71	0.34	1.00	86,98,107,109	0
29	SQD	AA	412	51/54	0.83	0.23	0.97	73,83,98,99	0
22	CLA	BB	606	65/65	0.93	0.19	0.97	58,61,74,76	0
32	LMT	BB	603	35/35	0.67	0.35	0.94	68,86,95,96	0
30	LMG	AB	622	49/55	0.89	0.19	0.93	64,73,80,83	0
22	CLA	AB	612	65/65	0.93	0.21	0.91	63,75,81,83	0
22	CLA	AB	610	65/65	0.91	0.21	0.89	60,67,79,80	0
22	CLA	BC	508	65/65	0.89	0.23	0.88	92,97,101,106	0
22	CLA	BD	402	65/65	0.96	0.17	0.88	50,57,79,83	0
22	CLA	BB	607	65/65	0.93	0.19	0.86	53,64,86,87	0
22	CLA	BB	608	65/65	0.95	0.18	0.85	45,53,76,78	0
22	CLA	AC	501	65/65	0.95	0.20	0.80	78,83,85,86	0
22	CLA	BB	619	65/65	0.74	0.29	0.78	75,81,93,95	0
26	BCR	BX	101	40/40	0.80	0.30	0.74	76,79,89,90	0
29	SQD	BD	409	43/54	0.80	0.25	0.71	73,88,110,111	0
30	LMG	BB	624	49/55	0.91	0.18	0.70	68,72,78,79	0
22	CLA	AC	511	65/65	0.89	0.25	0.70	77,85,89,90	0
23	PHO	AA	405	64/64	0.95	0.16	0.70	40,64,67,69	0
26	BCR	BA	410	40/40	0.92	0.20	0.67	61,74,82,83	0
26	BCR	AD	406	40/40	0.94	0.16	0.66	64,72,85,85	0
28	LHG	BA	412	39/49	0.91	0.23	0.65	72,77,80,81	0
22	CLA	BB	615	65/65	0.94	0.18	0.64	60,72,77,81	0
22	CLA	BB	610	65/65	0.95	0.17	0.61	60,70,77,81	0
22	CLA	AC	506	65/65	0.86	0.22	0.61	83,87,101,102	0
30	LMG	BA	414	51/55	0.90	0.20	0.58	62,71,78,80	0
29	SQD	BB	601	47/54	0.88	0.23	0.57	74,87,109,111	0
22	CLA	AB	613	65/65	0.95	0.17	0.53	65,69,84,87	0
34	HEM	BV	201	43/43	0.96	0.19	0.52	58,67,76,79	0
22	CLA	BC	504	65/65	0.92	0.19	0.52	87,92,102,102	0
27	DGD	AH	102	58/66	0.92	0.19	0.51	57,72,85,86	0
22	CLA	AB	611	65/65	0.94	0.19	0.51	62,68,71,73	0
22	CLA	BC	502	65/65	0.91	0.21	0.49	81,85,101,103	0
22	CLA	BC	511	65/65	0.89	0.25	0.45	91,99,104,105	0
29	SQD	BL	101	47/54	0.84	0.24	0.44	75,91,115,116	0
30	LMG	AM	101	42/55	0.80	0.29	0.41	68,86,93,95	0
22	CLA	AC	509	65/65	0.95	0.20	0.37	59,74,86,89	0
22	CLA	AB	603	65/65	0.94	0.17	0.33	54,60,72,74	0
22	CLA	AB	615	65/65	0.92	0.20	0.33	83,93,97,99	0
22	CLA	BC	506	65/65	0.86	0.24	0.33	81,85,97,99	0
33	BCT	AD	401	4/4	0.97	0.18	0.33	90,91,91,92	0
22	CLA	BC	509	65/65	0.92	0.21	0.32	73,83,93,94	0
26	BCR	AC	515	40/40	0.89	0.22	0.29	69,75,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	BC	501	65/65	0.93	0.19	0.28	76,80,87,88	0
23	PHO	BA	406	64/64	0.95	0.16	0.24	54,61,70,74	0
22	CLA	BC	503	65/65	0.91	0.20	0.15	82,97,100,101	0
22	CLA	BB	618	65/65	0.91	0.21	0.12	69,84,87,88	0
22	CLA	BA	404	65/65	0.95	0.16	0.10	55,60,68,70	0
22	CLA	BB	616	65/65	0.95	0.15	0.04	49,54,79,82	0
22	CLA	AB	607	65/65	0.95	0.15	0.02	50,55,74,74	0
22	CLA	BA	403	65/65	0.95	0.17	-0.06	57,64,71,75	0
26	BCR	AB	617	40/40	0.93	0.17	-0.07	56,67,75,76	0
22	CLA	AC	502	65/65	0.95	0.16	-0.07	50,58,81,84	0
22	CLA	BB	611	65/65	0.95	0.17	-0.07	67,74,81,85	0
22	CLA	BB	614	65/65	0.95	0.16	-0.25	59,68,75,77	0
25	OEC	BA	409	5/9	0.71	0.14	-0.51	30,74,79,92	0
25	OEC	AA	408	5/9	0.93	0.13	-0.71	56,62,67,75	0
22	CLA	AC	510	65/65	0.95	0.14	-0.79	48,56,70,72	0
21	FE2	AA	401	1/1	0.98	0.12	-1.91	69,69,69,69	0
21	FE2	BA	402	1/1	0.98	0.12	-2.36	81,81,81,81	0
32	LMT	AB	624	35/35	0.51	0.63	-	71,100,106,107	0
30	LMG	AI	101	43/55	0.63	0.46	-	83,92,97,98	0
35	CA	AO	301	1/1	0.91	0.23	-	87,87,87,87	0
35	CA	BO	301	1/1	0.76	0.34	-	100,100,100,100	0
32	LMT	BB	625	35/35	0.72	0.42	-	66,103,111,111	0
35	CA	BK	101	1/1	0.84	0.13	-	90,90,90,90	0
35	CA	AK	101	1/1	0.79	0.09	-	95,95,95,95	0
30	LMG	BI	101	43/55	0.73	0.37	-	84,90,99,100	0

## 6.5 Other polymers

There are no such residues in this entry.