



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:41 PM GMT

PDB ID : 4V82
Title : Crystal structure of cyanobacterial Photosystem II in complex with terbutryn
Authors : Gabdulkhakov, A.; Broser, M.; Guskov, A.; Kern, J.; Glockner, C.; Muh, F.;
Saenger, W.; Zouni, A.
Deposited on : 2010-11-30
Resolution : 3.20 Å(reported)

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

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

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

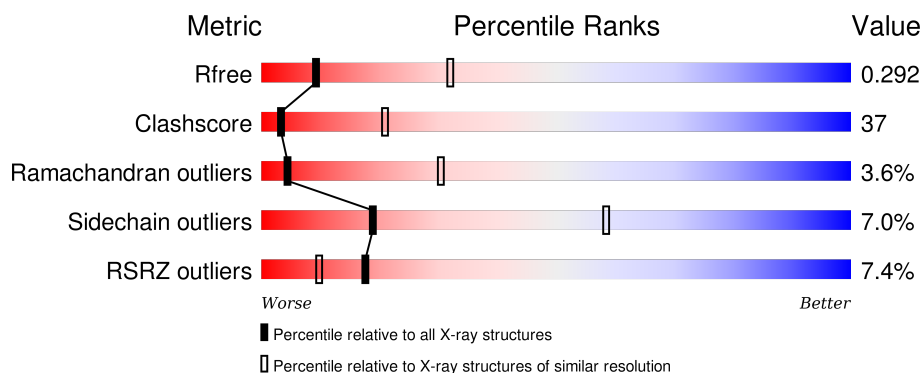
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	AA	344	<div> <div>3%</div> <div>40%</div> <div>53%</div> <div>5%</div> </div>
1	BA	344	<div> <div>5%</div> <div>39%</div> <div>53%</div> <div>5%</div> </div>
2	AB	510	<div> <div>3%</div> <div>46%</div> <div>45%</div> <div>5%</div> </div>
2	BB	510	<div> <div>5%</div> <div>46%</div> <div>45%</div> <div>5%</div> </div>
3	AC	461	<div> <div>5%</div> <div>40%</div> <div>51%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	BC	461	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	41	
18	BX	41	
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
23	CL	BA	5404[A]	-	-	-	X
24	CLA	AA	404	X	-	-	-
24	CLA	AA	405	X	-	-	-
24	CLA	AA	406	X	-	-	X
24	CLA	AA	407	X	-	-	X
24	CLA	AB	601	X	-	-	X
24	CLA	AB	602	X	-	-	-
24	CLA	AB	603	X	-	-	-
24	CLA	AB	604	X	-	-	-
24	CLA	AB	605	X	-	-	X
24	CLA	AB	606	X	-	-	-
24	CLA	AB	607	X	-	-	-
24	CLA	AB	608	X	-	-	X
24	CLA	AB	609	X	-	-	X
24	CLA	AB	610	X	-	-	-
24	CLA	AB	611	X	-	-	-
24	CLA	AB	612	X	-	-	-
24	CLA	AB	613	X	-	-	-
24	CLA	AB	614	X	-	-	-
24	CLA	AB	615	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AB	616	X	-	-	X
24	CLA	AC	501	X	-	-	-
24	CLA	AC	502	X	-	-	X
24	CLA	AC	503	X	-	-	X
24	CLA	AC	504	X	-	-	X
24	CLA	AC	505	X	-	-	X
24	CLA	AC	506	X	-	-	-
24	CLA	AC	507	X	-	-	-
24	CLA	AC	508	X	-	-	X
24	CLA	AC	509	X	-	-	-
24	CLA	AC	510	X	-	-	-
24	CLA	AC	511	X	-	X	-
24	CLA	AC	512	X	-	-	X
24	CLA	AC	513	X	-	-	X
24	CLA	AD	401	X	-	-	-
24	CLA	AD	404	X	-	-	X
24	CLA	BA	5405	X	-	-	-
24	CLA	BA	5406	X	-	X	-
24	CLA	BA	5407	X	-	-	-
24	CLA	BA	5408	X	-	-	-
24	CLA	BB	5605	X	-	-	X
24	CLA	BB	5606	X	-	-	-
24	CLA	BB	5607	X	-	-	-
24	CLA	BB	5608	X	-	-	-
24	CLA	BB	5609	X	-	-	X
24	CLA	BB	5610	X	-	-	-
24	CLA	BB	5611	X	-	-	-
24	CLA	BB	5612	X	-	-	X
24	CLA	BB	5613	X	-	-	-
24	CLA	BB	5614	X	-	-	-
24	CLA	BB	5615	X	-	-	-
24	CLA	BB	5616	X	-	-	-
24	CLA	BB	5617	X	-	-	X
24	CLA	BB	5618	X	-	-	-
24	CLA	BB	5619	X	-	-	-
24	CLA	BB	5620	X	-	-	-
24	CLA	BC	5501	X	-	-	-
24	CLA	BC	5502	X	-	-	-
24	CLA	BC	5503	X	-	-	-
24	CLA	BC	5504	X	-	-	X
24	CLA	BC	5505	X	-	-	-
24	CLA	BC	5506	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	BC	5507	X	-	-	-
24	CLA	BC	5508	X	-	-	-
24	CLA	BC	5509	X	-	-	-
24	CLA	BC	5510	X	-	-	-
24	CLA	BC	5511	X	-	X	X
24	CLA	BC	5512	X	-	-	-
24	CLA	BC	5513	X	-	-	X
24	CLA	BD	5402	X	-	-	-
24	CLA	BD	5405	X	-	-	-
25	MST	AA	408	-	-	X	-
25	MST	BA	5409	-	-	X	-
27	BCR	AB	617	-	-	-	X
27	BCR	AC	515	-	-	-	X
27	BCR	AC	516	-	-	-	X
27	BCR	AJ	101	-	-	-	X
27	BCR	AK	102	-	-	-	X
27	BCR	AT	101	-	-	-	X
27	BCR	AX	101	-	-	-	X
27	BCR	BB	5621	-	-	-	X
27	BCR	BB	5622	-	-	-	X
27	BCR	BC	5514	-	-	-	X
27	BCR	BC	5515	-	-	-	X
27	BCR	BC	5516	-	-	-	X
27	BCR	BD	5407	-	-	-	X
27	BCR	BJ	5101	-	-	-	X
27	BCR	BT	5101	-	-	-	X
27	BCR	BX	5101	-	-	-	X
28	DGD	AA	411	-	-	-	X
28	DGD	AB	628	-	-	-	X
28	DGD	AC	517	-	-	-	X
28	DGD	AC	518	X	-	-	X
28	DGD	AC	519	X	-	X	X
28	DGD	AE	101	-	-	-	X
28	DGD	BA	5412	-	-	-	X
28	DGD	BB	5602	-	-	-	X
28	DGD	BC	5518	X	-	-	X
28	DGD	BC	5519	X	-	X	X
28	DGD	BE	5102	-	-	-	X
28	DGD	BH	5101	-	-	-	X
29	LHG	BA	5415	-	-	-	X
30	SQD	AB	622	-	-	-	X
30	SQD	AF	102	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	BA	5401	-	-	-	X
30	SQD	BB	5625	-	-	-	X
30	SQD	BF	5102	-	-	-	X
31	LMG	AA	414	-	-	-	X
31	LMG	AA	417	-	-	-	X
31	LMG	AB	620	-	-	-	X
31	LMG	AB	621	-	-	-	X
31	LMG	AC	520	-	-	-	X
31	LMG	AC	521	-	-	-	X
31	LMG	AD	407	-	-	-	X
31	LMG	AD	408	-	-	-	X
31	LMG	AJ	102	-	-	-	X
31	LMG	AM	101	-	-	-	X
31	LMG	BA	5402	-	-	-	X
31	LMG	BB	5624	-	-	-	X
31	LMG	BC	5520	-	-	-	X
31	LMG	BC	5521	-	-	-	X
31	LMG	BD	5408	-	-	-	X
31	LMG	BD	5409	-	-	-	X
31	LMG	BD	5410	-	-	-	X
31	LMG	BE	5101	-	-	-	X
31	LMG	BL	5101	-	-	-	X
31	LMG	BM	5102	-	-	-	X
32	LMT	AB	624	-	-	-	X
32	LMT	AB	629	-	-	-	X
32	LMT	AB	630	-	-	-	X
32	LMT	AD	409	-	-	-	X
32	LMT	AI	102	-	-	-	X
32	LMT	AI	103	-	-	-	X
32	LMT	AM	102	-	-	-	X
32	LMT	BB	5603	-	-	-	X
32	LMT	BB	5604	-	-	-	X
32	LMT	BB	5627	-	-	-	X
32	LMT	BC	5522	-	-	-	X
32	LMT	BD	5411	-	-	-	X
32	LMT	BI	5102	-	-	-	X
32	LMT	BM	5101	-	-	-	X
33	DMS	AB	625	-	-	-	X
33	DMS	AU	201	-	-	-	X
33	DMS	AV	202	-	-	-	X
33	DMS	BB	5628	-	-	-	X
33	DMS	BB	5629	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	DMS	BV	5203	-	-	-	X
34	PHO	AD	402	X	-	-	-
34	PHO	AD	403	X	-	-	-
34	PHO	BD	5403	X	-	-	-
34	PHO	BD	5404	X	-	-	-
35	PL9	AD	405	-	-	-	X
36	HEM	BF	5101	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50266 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	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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			
4	BD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	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	38	Total	C	N	O	S	0	0	0
			271	182	42	46	1			
9	BJ	38	Total	C	N	O	S	0	0	0
			271	182	42	46	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			
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 Photosystem II reaction center 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 reaction center X 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 PSBX PROTEIN.

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				

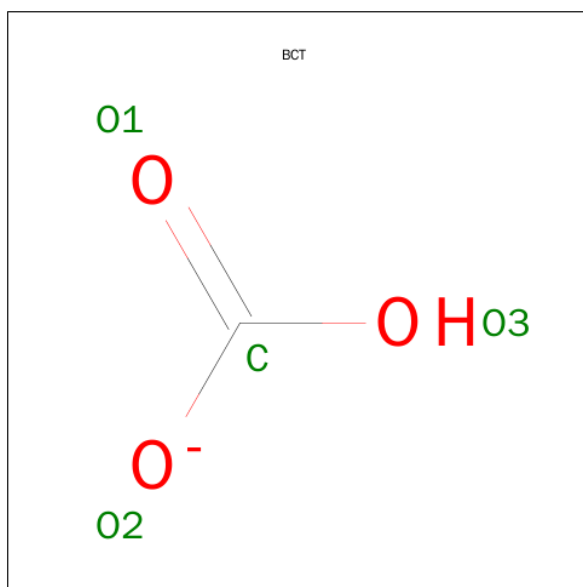
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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	BD	1	Total	Fe	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

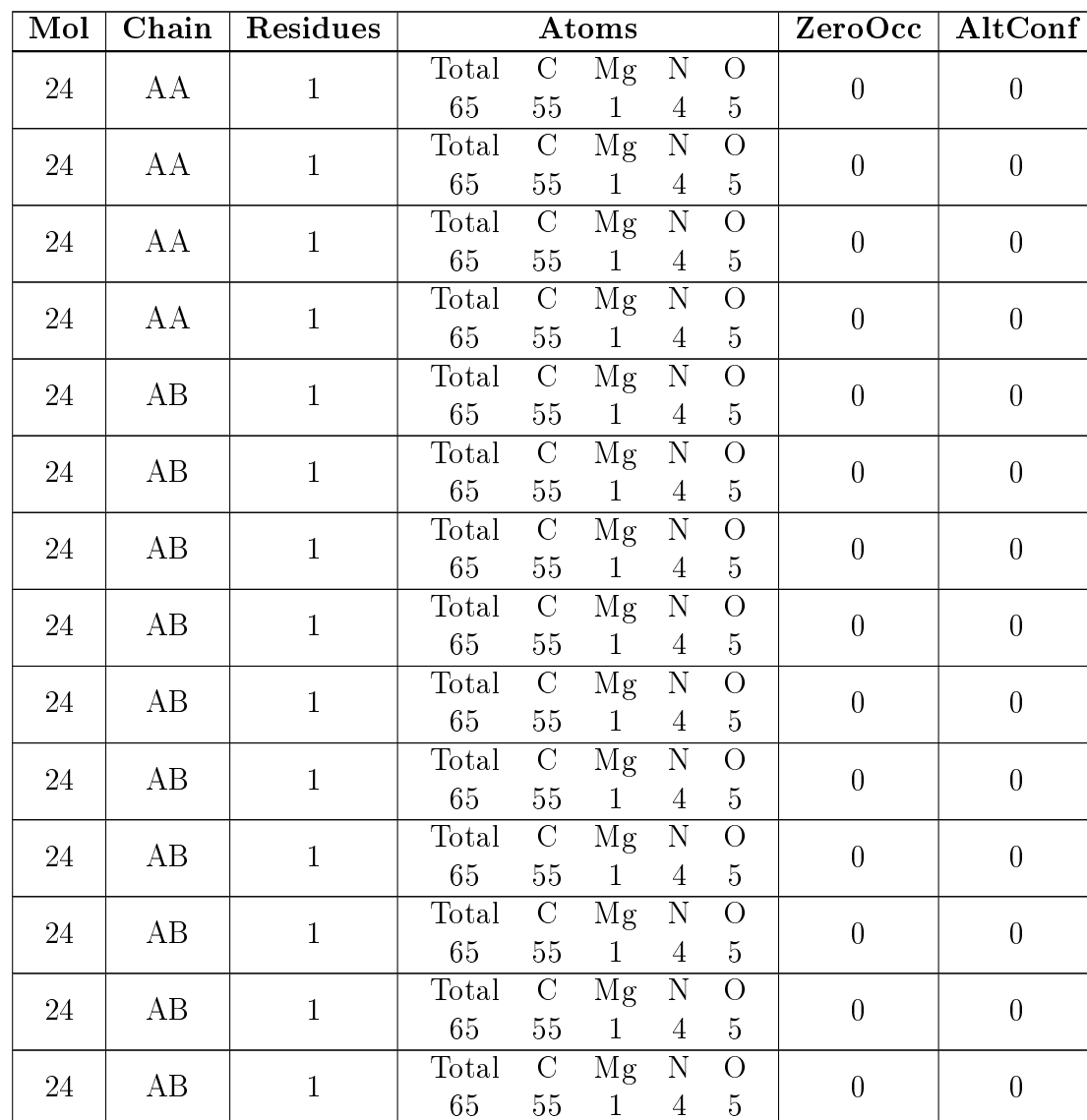


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	AA	1	Total	C	O	0	0
			4	1	3		
22	BA	1	Total	C	O	0	0
			4	1	3		

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	AA	1	Total	Cl	0	1
			2	2		
23	BA	1	Total	Cl	0	1
			2	2		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

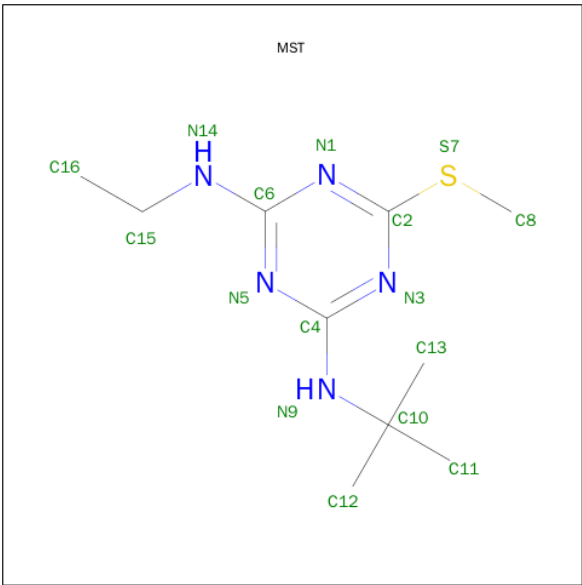
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55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

Continued on next page...

Continued from previous page...

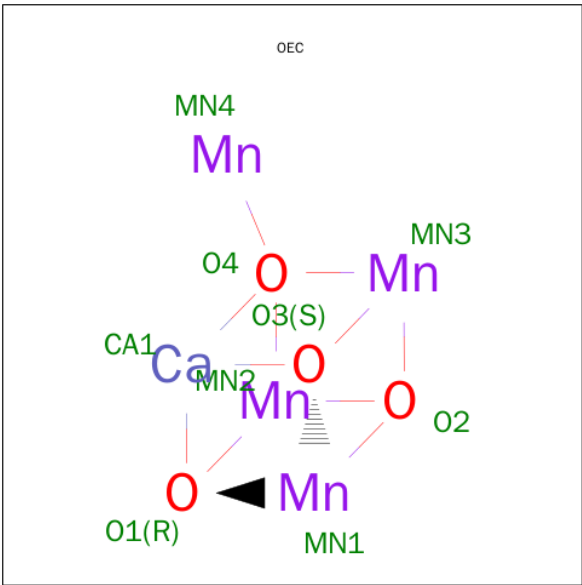
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55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

- Molecule 25 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (three-letter code: MST) (formula: C₁₀H₁₉N₅S).



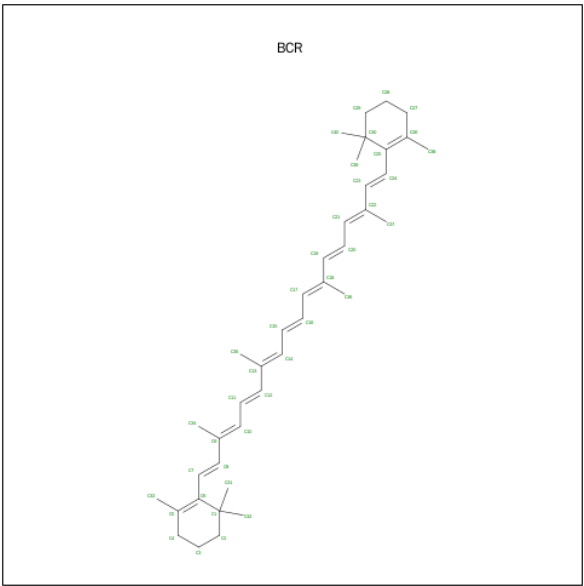
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



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

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



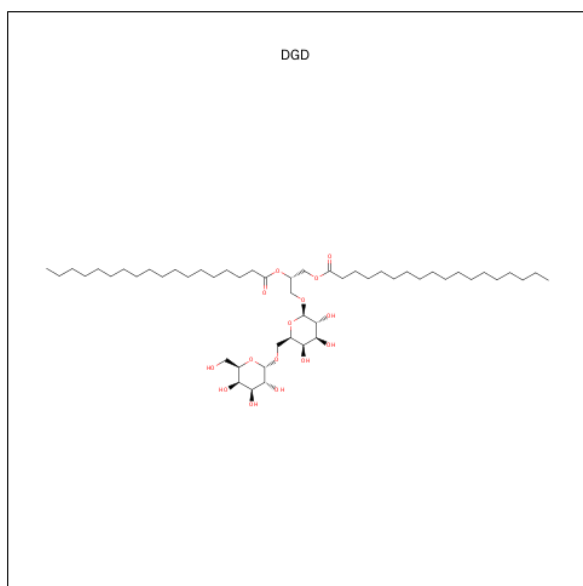
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0
27	AT	1	Total C 40 40	0	0
27	AX	1	Total C 40 40	0	0
27	BA	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

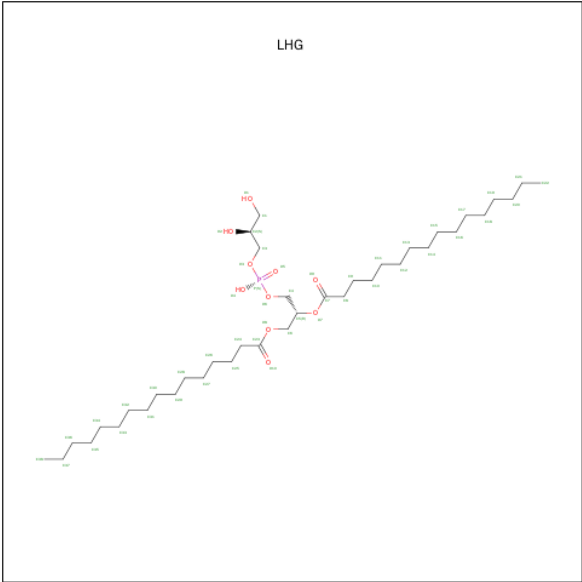
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0
27	BX	1	Total C 40 40	0	0

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



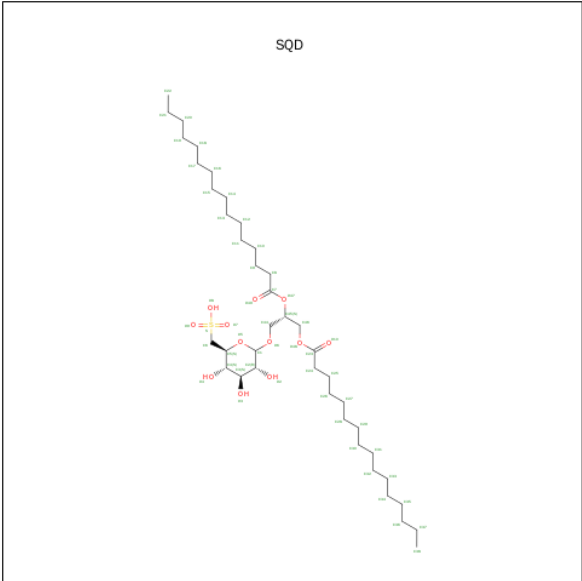
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	AA	1	Total	C	O	0	0
			56	41	15		
28	AB	1	Total	C	O	0	0
			52	37	15		
28	AC	1	Total	C	O	0	0
			53	38	15		
28	AC	1	Total	C	O	0	0
			62	47	15		
28	AC	1	Total	C	O	0	0
			66	51	15		
28	AE	1	Total	C	O	0	0
			63	48	15		
28	AH	1	Total	C	O	0	0
			58	43	15		
28	BA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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



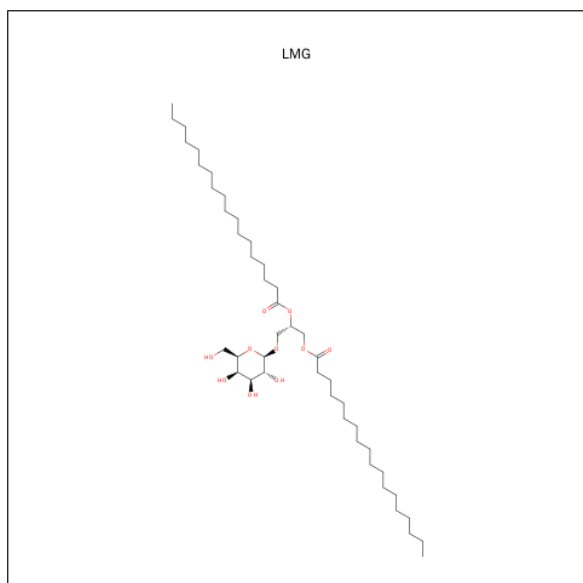
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	AA	1	Total	C	O	S	0	0
			51	38	12	1		
30	AA	1	Total	C	O	S	0	0
			54	41	12	1		
30	AB	1	Total	C	O	S	0	0
			43	30	12	1		
30	AB	1	Total	C	O	S	0	0
			47	34	12	1		
30	AF	1	Total	C	O	S	0	0
			45	32	12	1		
30	BA	1	Total	C	O	S	0	0
			54	41	12	1		
30	BA	1	Total	C	O	S	0	0
			51	38	12	1		
30	BB	1	Total	C	O	S	0	0
			47	34	12	1		
30	BB	1	Total	C	O	S	0	0
			43	30	12	1		
30	BF	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



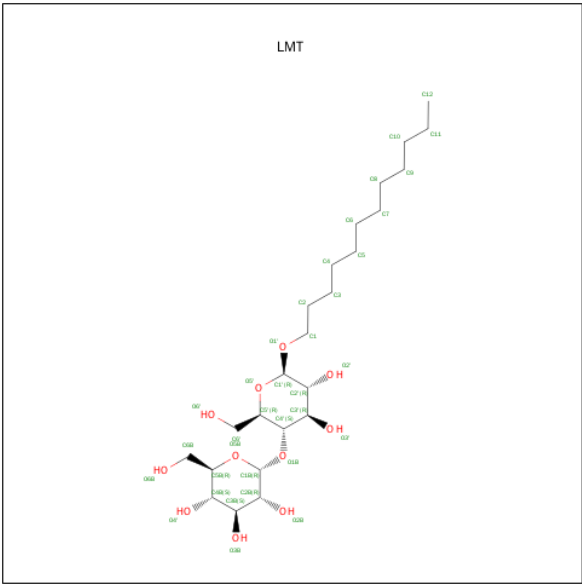
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			42	32	10		
31	AB	1	Total	C	O	0	0
			51	41	10		
31	AB	1	Total	C	O	0	0
			49	39	10		
31	AC	1	Total	C	O	0	0
			48	38	10		
31	AC	1	Total	C	O	0	0
			45	35	10		
31	AD	1	Total	C	O	0	0
			49	39	10		
31	AD	1	Total	C	O	0	0
			48	38	10		
31	AI	1	Total	C	O	0	0
			43	33	10		
31	AJ	1	Total	C	O	0	0
			46	36	10		
31	AM	1	Total	C	O	0	0
			42	32	10		
31	BA	1	Total	C	O	0	0
			42	32	10		
31	BB	1	Total	C	O	0	0
			49	39	10		
31	BC	1	Total	C	O	0	0
			48	38	10		
31	BC	1	Total	C	O	0	0
			45	35	10		
31	BD	1	Total	C	O	0	0
			46	36	10		
31	BD	1	Total	C	O	0	0
			49	39	10		
31	BD	1	Total	C	O	0	0
			48	38	10		
31	BE	1	Total	C	O	0	0
			44	34	10		
31	BI	1	Total	C	O	0	0
			43	33	10		
31	BL	1	Total	C	O	0	0
			51	41	10		
31	BM	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



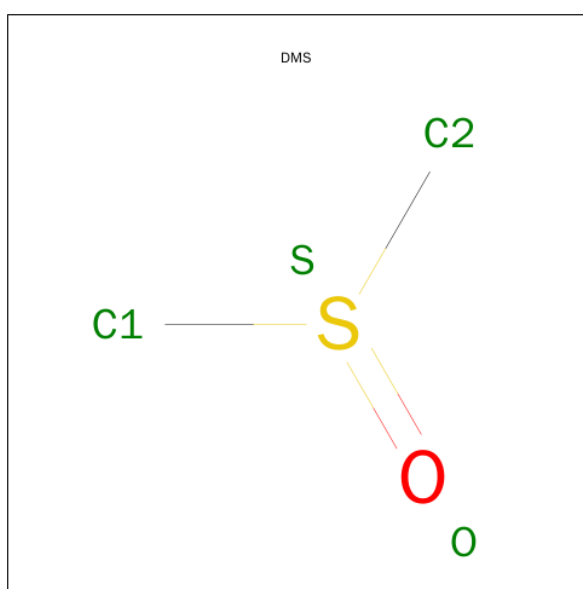
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM	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	BB	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	BC	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		

- Molecule 33 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



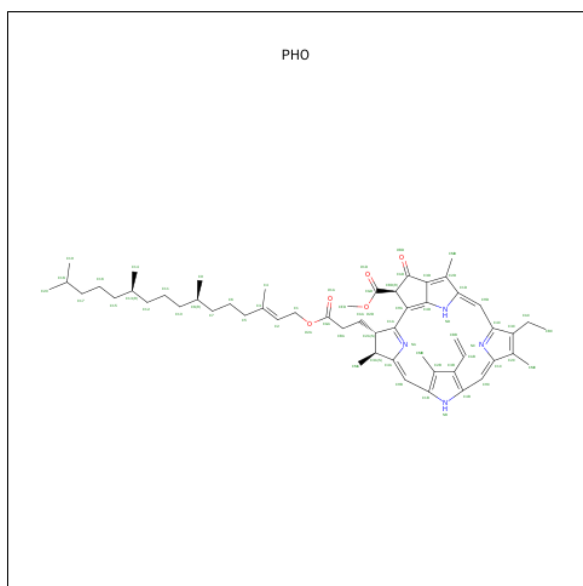
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AU	1	Total	C	O	S	0	0
			4	2	1	1		
33	AV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

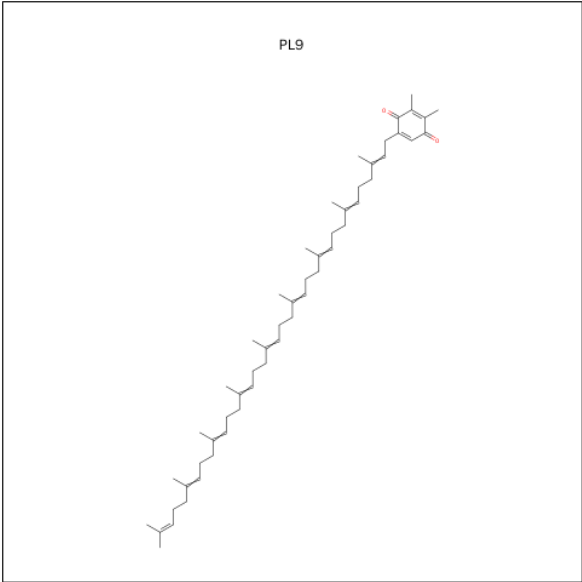
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



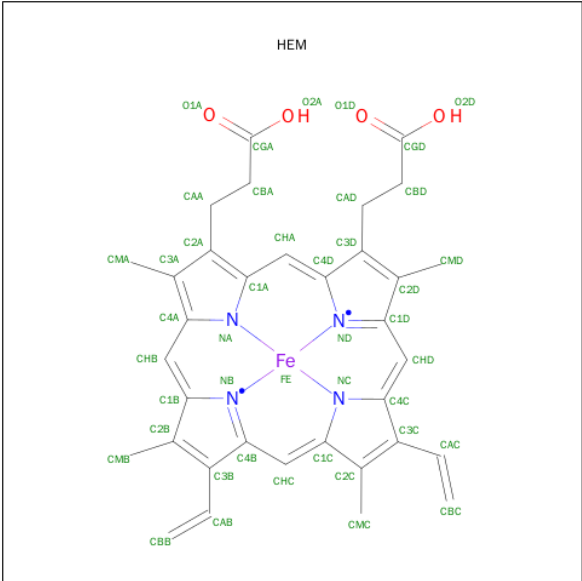
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 35 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
35	AD	1	Total	C	O	0	0
			55	53	2		
35	BD	1	Total	C	O	0	0
			55	53	2		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

Continued on next page...

Continued from previous page...

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

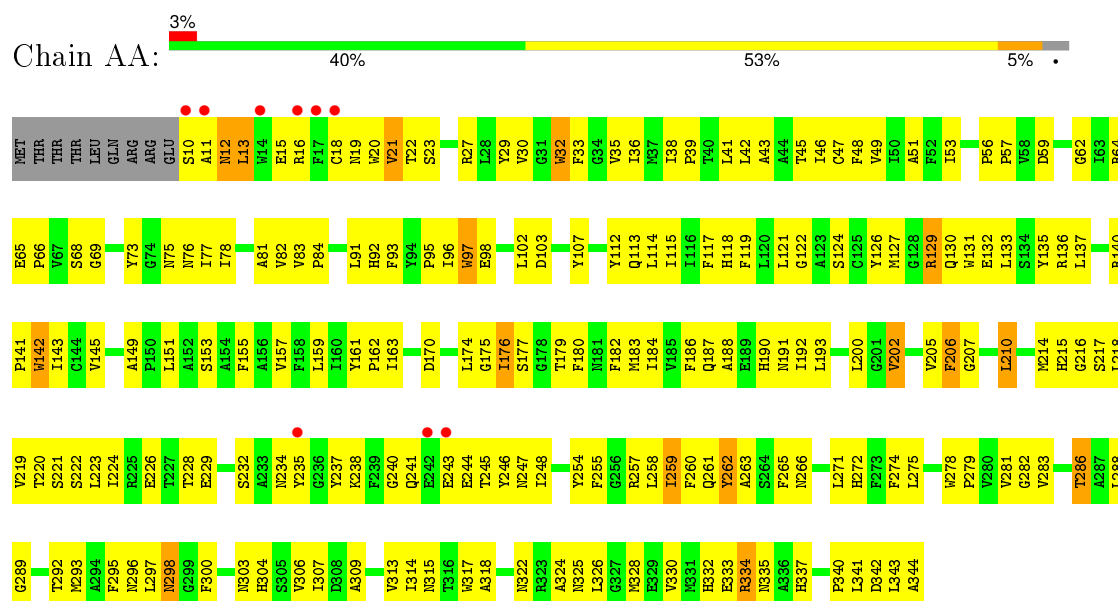
- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	BO	1	Total 1	Ca 1	0	0
37	AK	1	Total 1	Ca 1	0	0
37	BF	1	Total 1	Ca 1	0	0
37	BK	1	Total 1	Ca 1	0	0
37	AO	1	Total 1	Ca 1	0	0
37	AF	1	Total 1	Ca 1	0	0

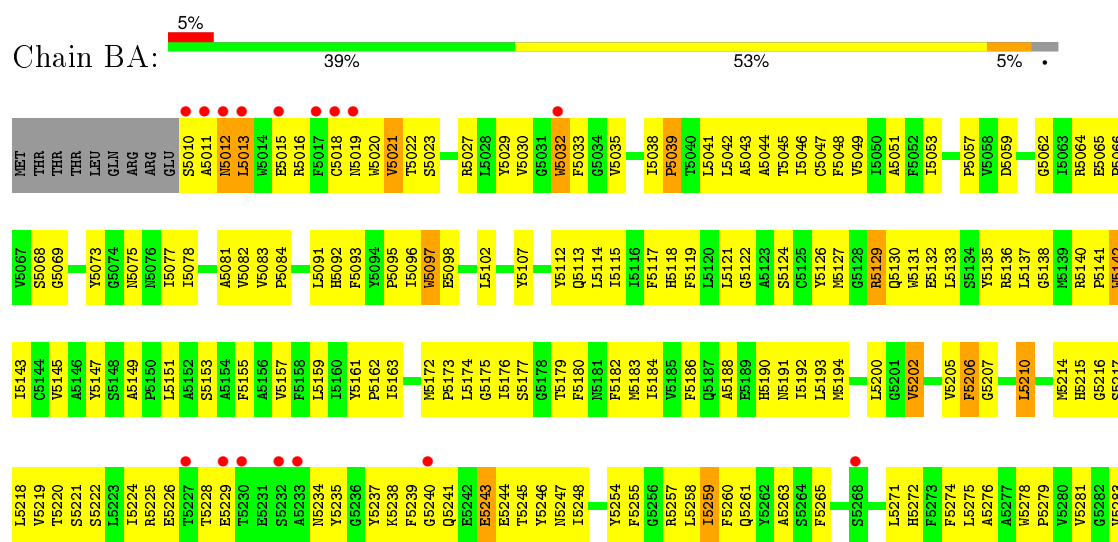
3 Residue-property plots

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 1

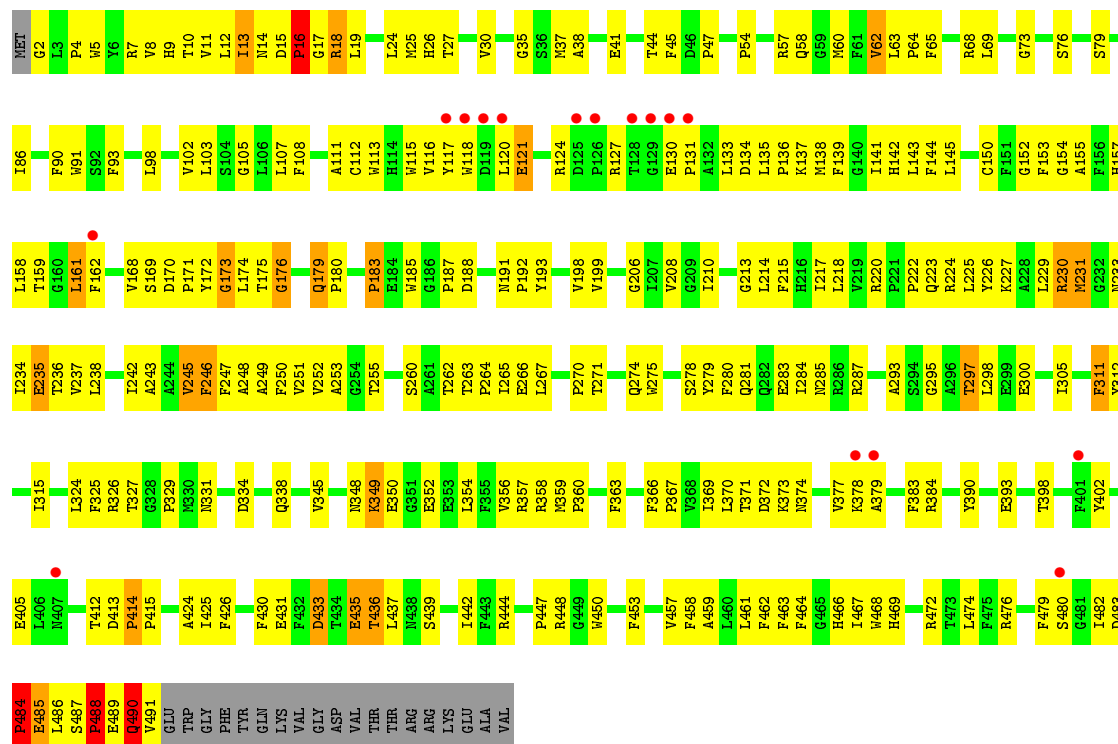


• Molecule 1: Photosystem Q(B) protein 1

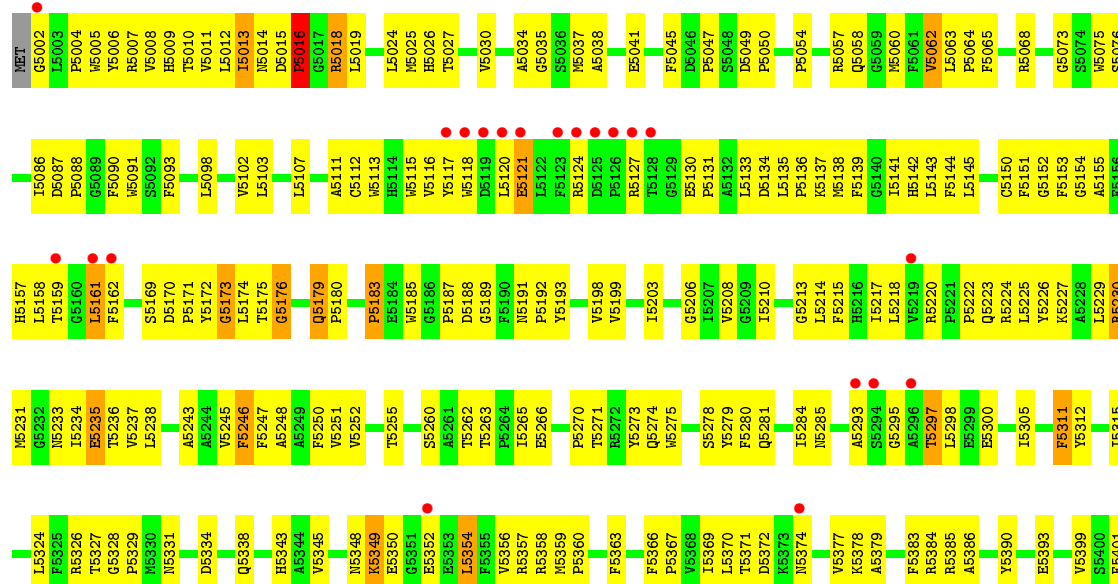


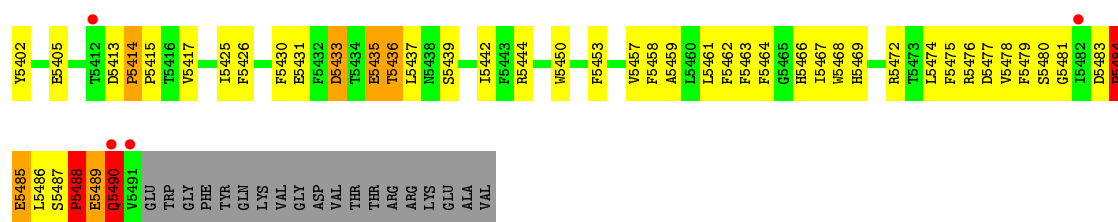


• Molecule 2: Photosystem II core light harvesting protein

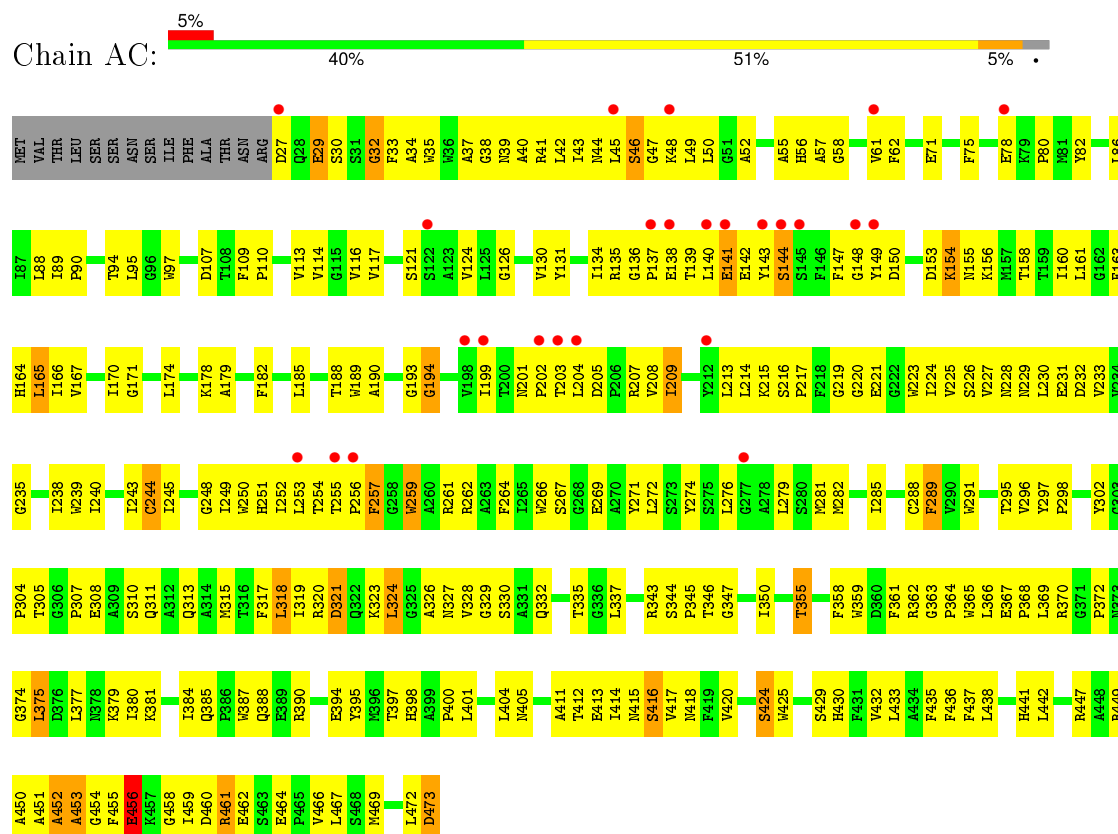


• Molecule 2: Photosystem II core light harvesting protein

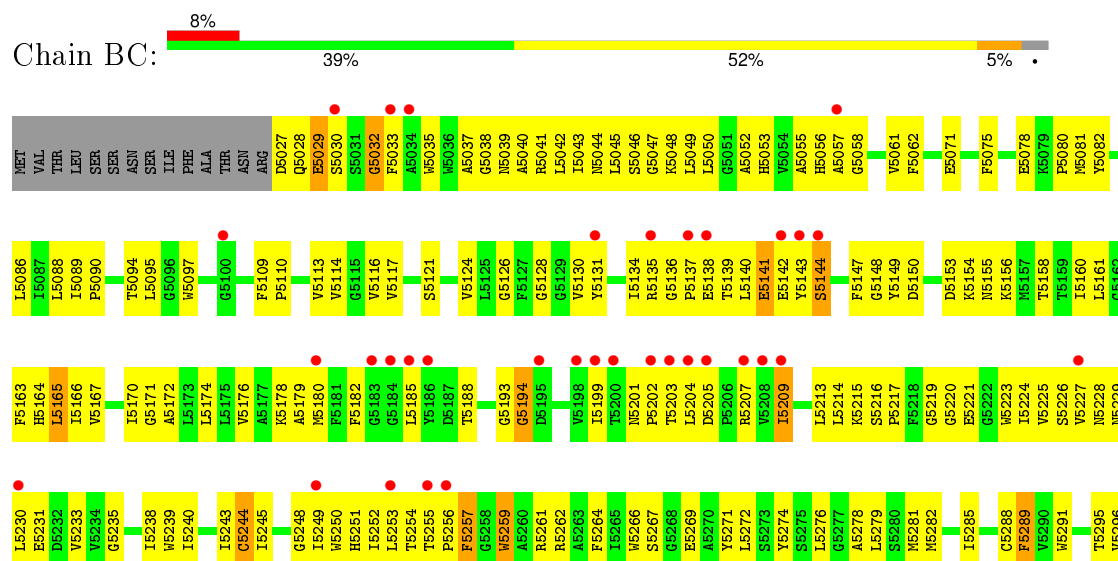


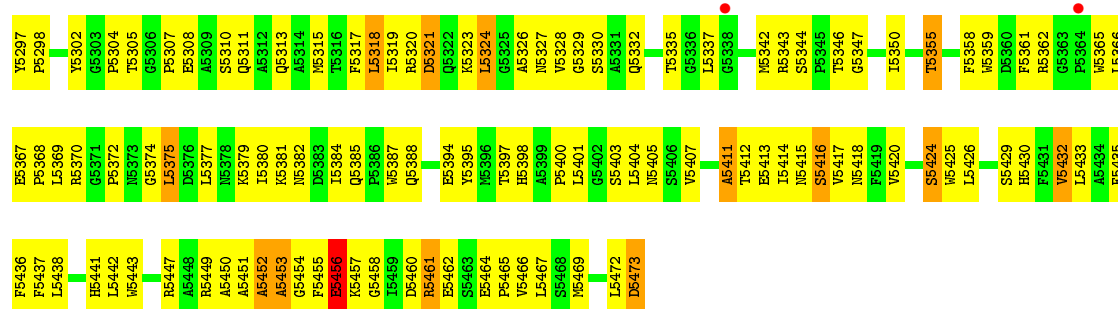


● Molecule 3: Photosystem II CP43 protein

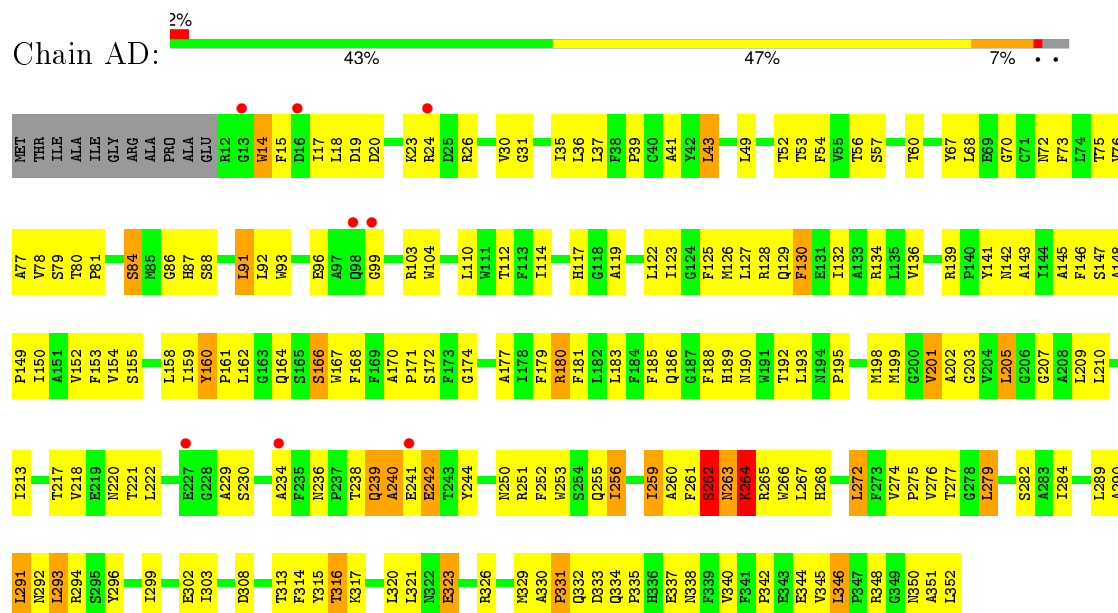


● Molecule 3: Photosystem II CP43 protein

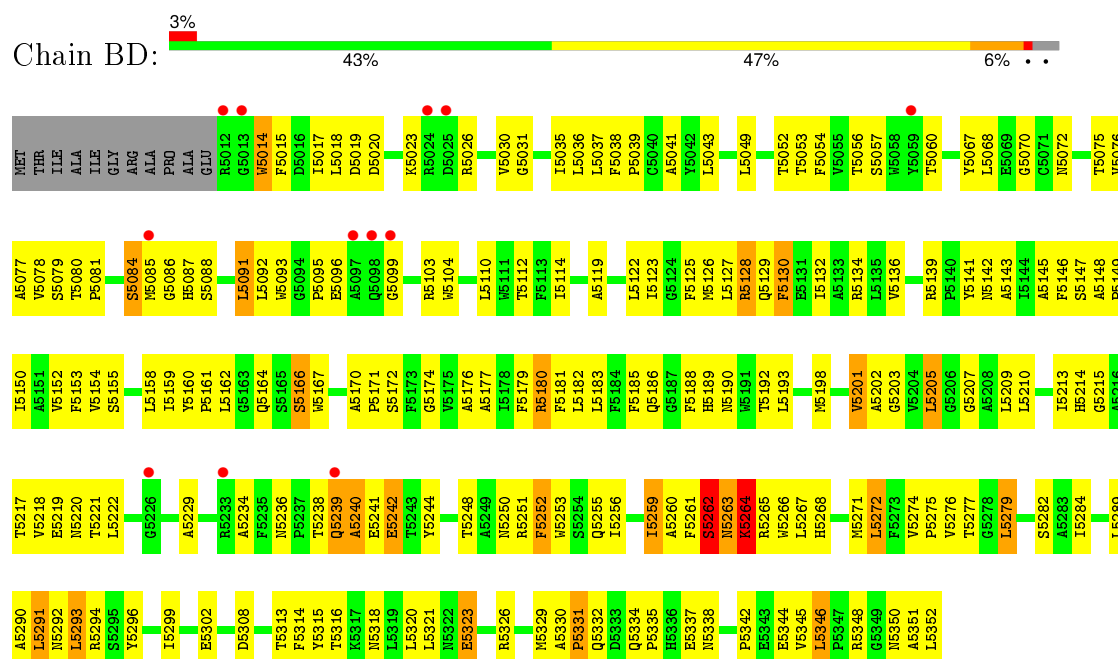




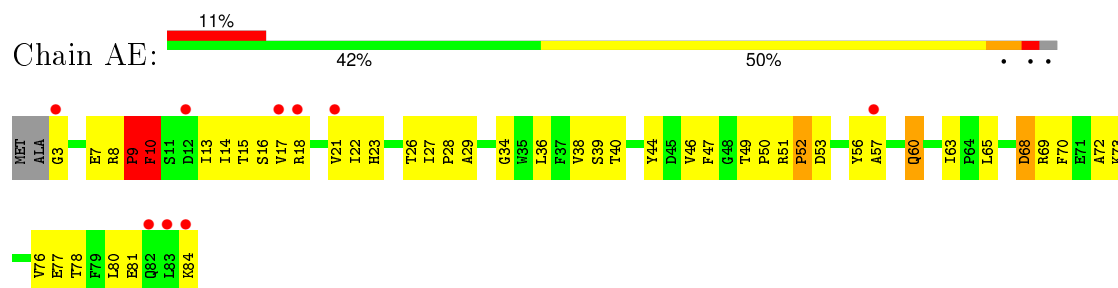
• Molecule 4: Photosystem II D2 protein



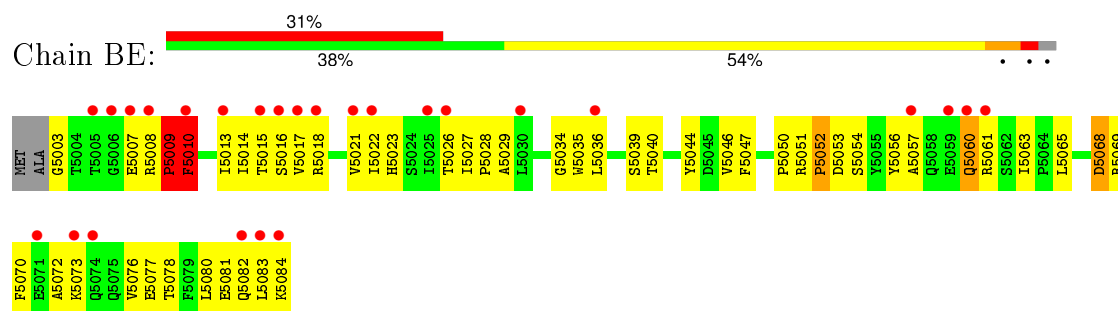
• Molecule 4: Photosystem II D2 protein



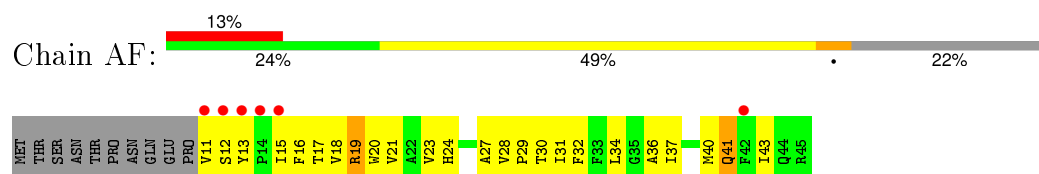
- Molecule 5: Cytochrome b559 subunit alpha



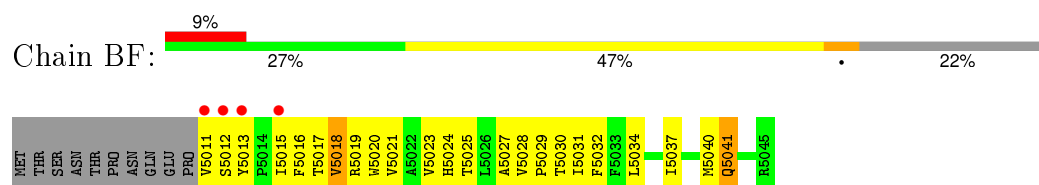
- Molecule 5: Cytochrome b559 subunit alpha



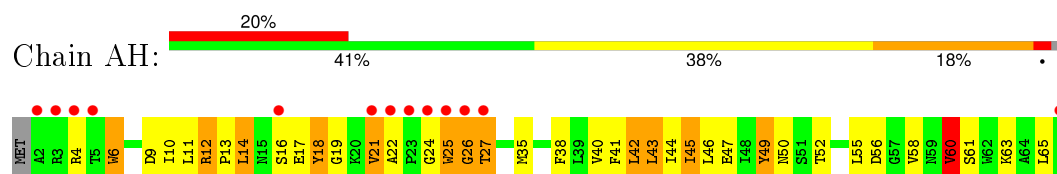
- Molecule 6: Cytochrome b559 subunit beta



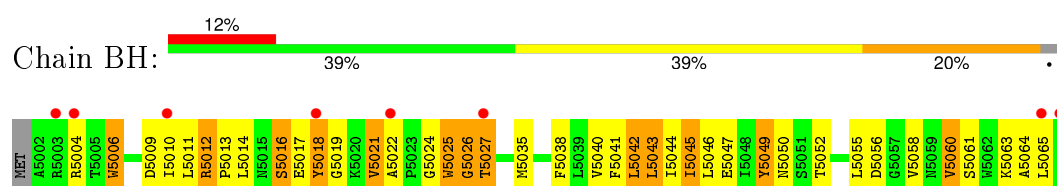
- Molecule 6: Cytochrome b559 subunit beta



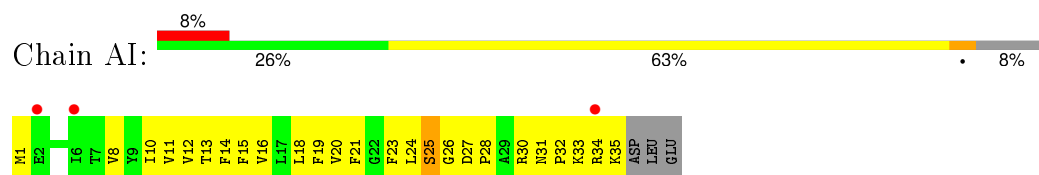
- Molecule 7: Photosystem II reaction center protein H



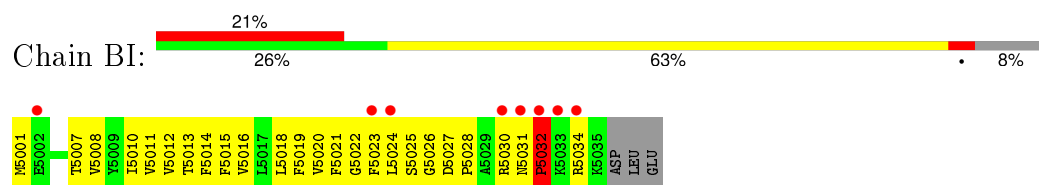
- Molecule 7: Photosystem II reaction center protein H



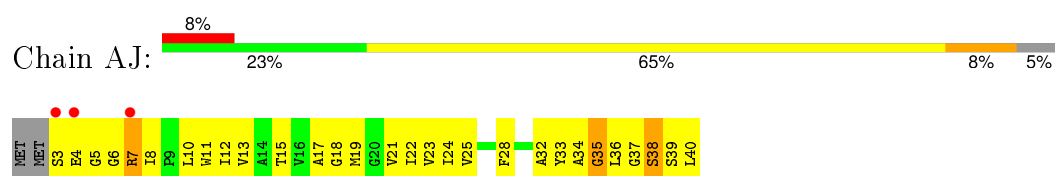
- Molecule 8: Photosystem II reaction center protein I



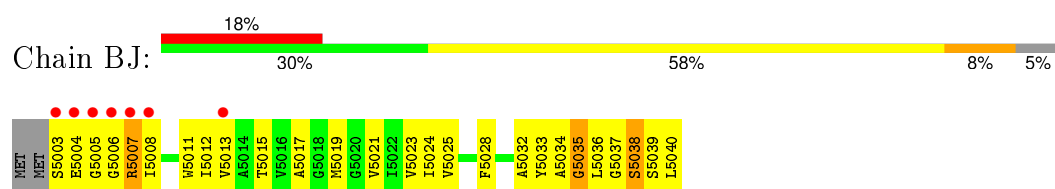
- Molecule 8: Photosystem II reaction center protein I



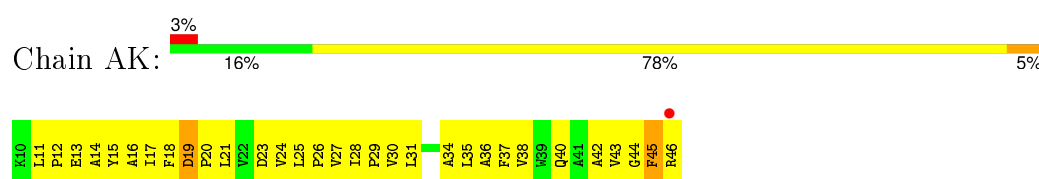
- Molecule 9: Photosystem II reaction center protein J



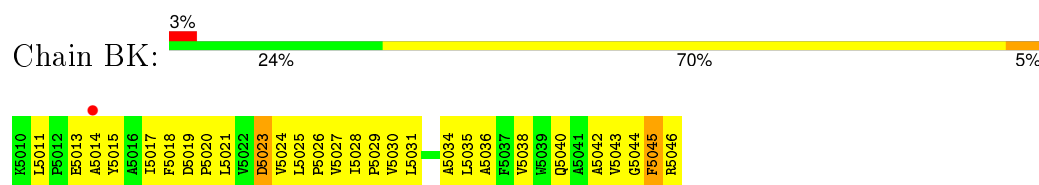
- Molecule 9: Photosystem II reaction center protein J



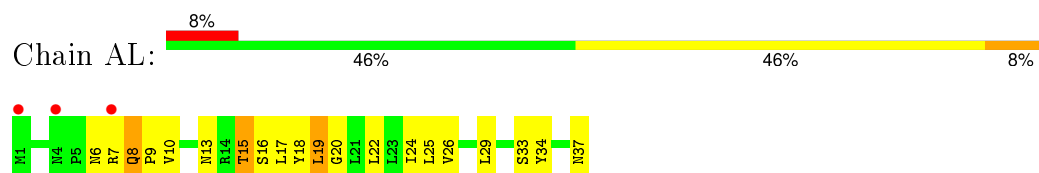
- Molecule 10: Photosystem II reaction center protein K



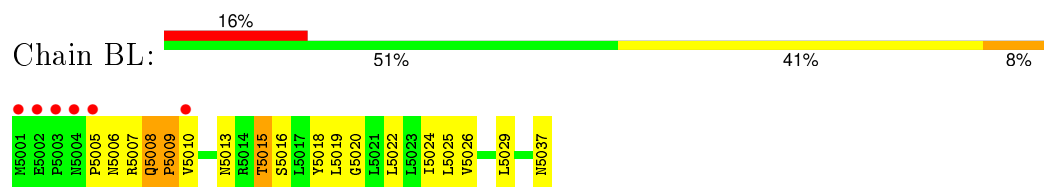
- Molecule 10: Photosystem II reaction center protein K



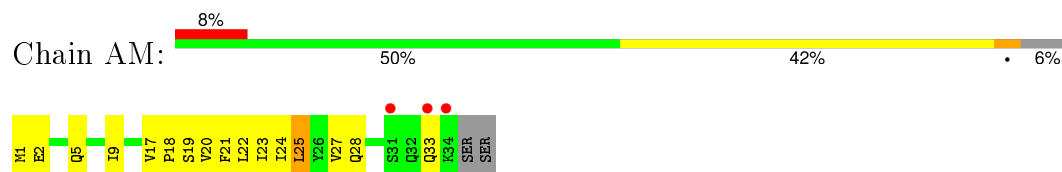
- Molecule 11: Photosystem II reaction center protein L



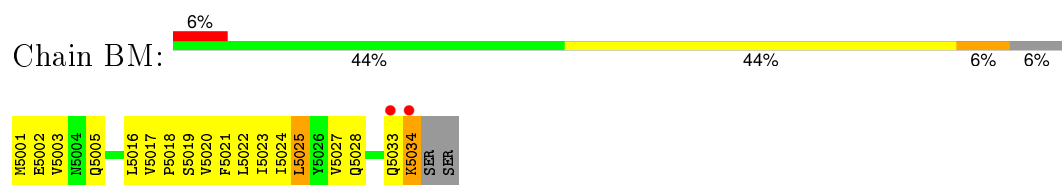
- Molecule 11: Photosystem II reaction center protein L



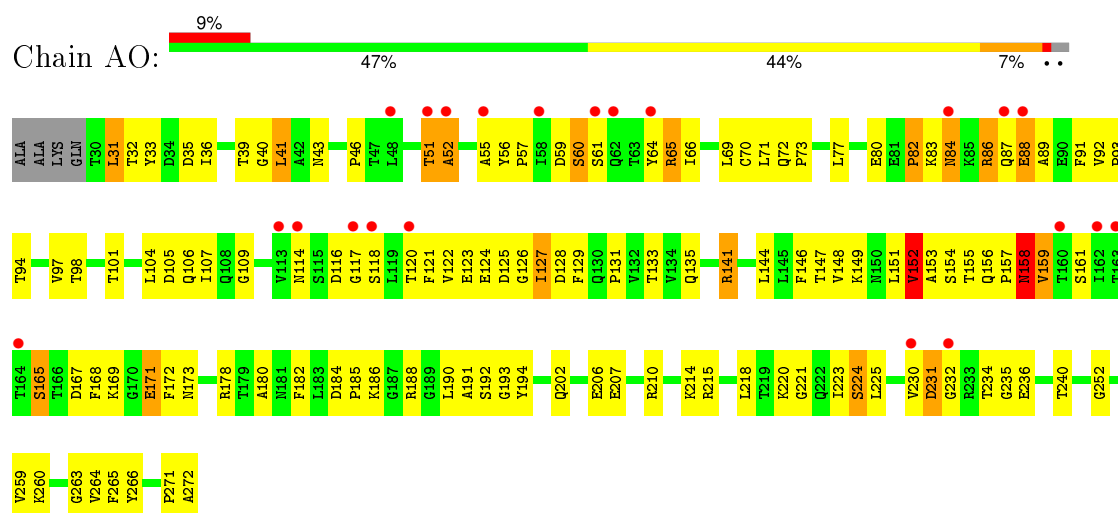
- Molecule 12: Photosystem II reaction center protein M



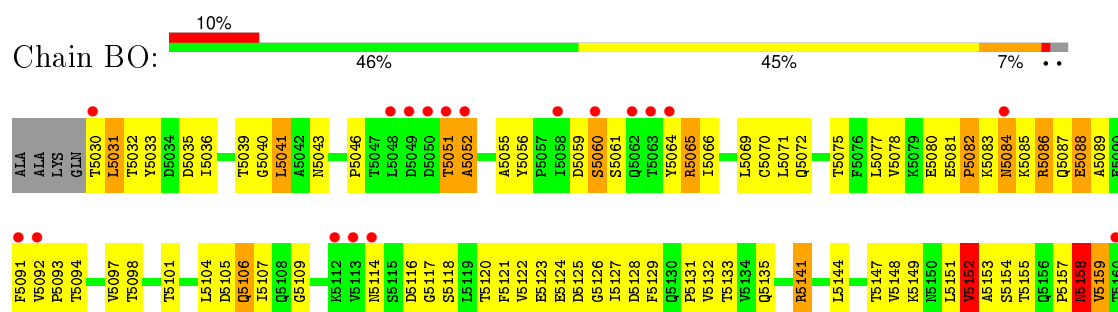
- Molecule 12: Photosystem II reaction center protein M

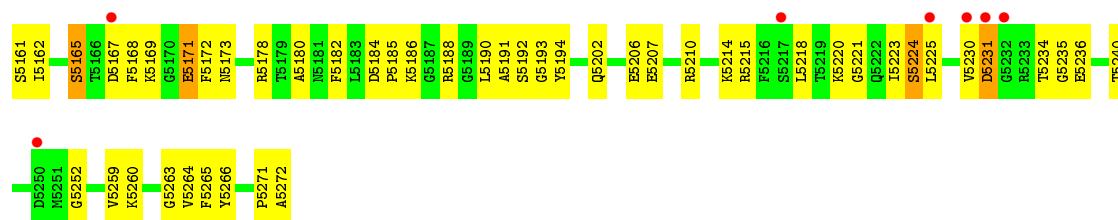


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

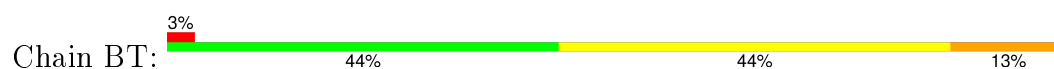




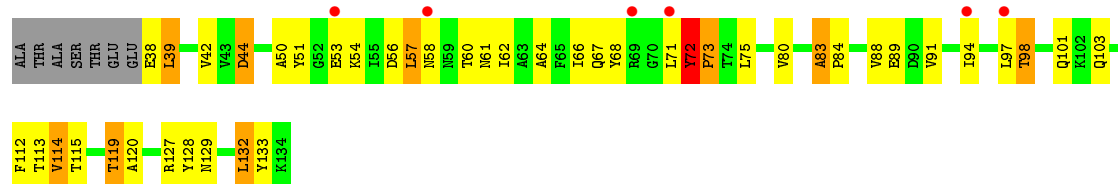
• Molecule 14: Photosystem II reaction center protein T



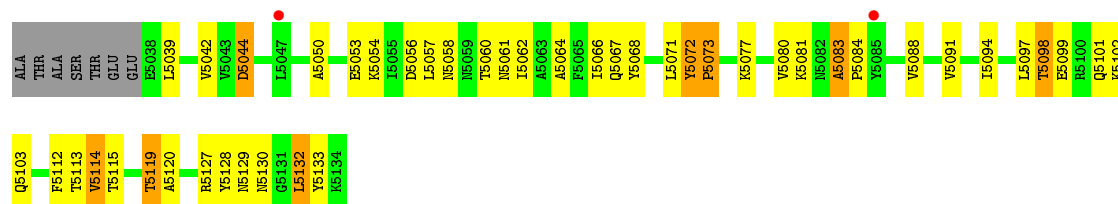
• Molecule 14: Photosystem II reaction center protein T



• Molecule 15: Photosystem II 12 kDa extrinsic protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

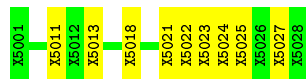


• Molecule 16: Cytochrome c-550



- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain BY:  68% 32%



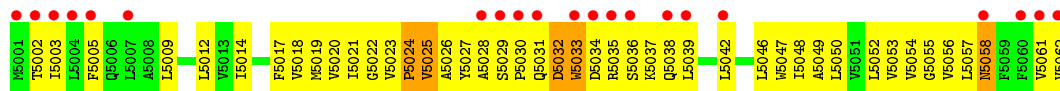
- Molecule 20: Photosystem II reaction center protein Z

Chain AZ:  18% 32% 60% 8%



- Molecule 20: Photosystem II reaction center protein Z

Chain BZ:  34% 29% 63% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.08Å 225.37Å 305.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 39.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.20) 99.1 (39.38-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.12Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.299 0.270 , 0.292	Depositor DCC
R_{free} test set	2899 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 159033 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	50266	wwPDB-VP
Average B, all atoms (Å ²)	119.0	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 ⓘ

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, MST, LMT, CLA, PL9, BCT, DMS, 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	0.50	0/2713	0.72	0/3700
1	BA	0.52	0/2713	0.72	0/3700
2	AB	0.51	0/3986	0.73	0/5433
2	BB	0.52	0/3986	0.73	3/5433 (0.1%)
3	AC	0.46	0/3556	0.71	1/4842 (0.0%)
3	BC	0.47	0/3556	0.71	1/4842 (0.0%)
4	AD	0.53	0/2806	0.73	0/3825
4	BD	0.55	0/2806	0.73	0/3825
5	AE	0.51	0/685	0.76	0/933
5	BE	0.54	0/685	0.77	0/933
6	AF	0.75	0/291	0.78	0/397
6	BF	0.71	0/291	0.74	0/397
7	AH	0.47	0/520	0.78	0/709
7	BH	0.49	0/520	0.79	0/709
8	AI	0.58	0/293	0.77	0/395
8	BI	0.64	0/293	0.81	0/395
9	AJ	0.55	0/277	0.86	0/375
9	BJ	0.67	0/277	0.88	0/375
10	AK	0.54	0/303	0.73	0/416
10	BK	0.62	0/303	0.73	0/416
11	AL	0.58	0/311	0.78	1/422 (0.2%)
11	BL	0.57	0/311	0.81	0/422
12	AM	0.65	0/270	0.87	0/367
12	BM	0.66	0/270	0.85	0/367
13	AO	0.49	0/1876	0.76	0/2548
13	BO	0.48	0/1876	0.76	1/2548 (0.0%)
14	AT	0.80	1/284 (0.4%)	0.82	0/381
14	BT	0.81	1/284 (0.4%)	0.87	2/381 (0.5%)
15	AU	0.54	0/785	0.84	2/1064 (0.2%)
15	BU	0.52	0/785	0.83	0/1064
16	AV	0.46	0/1081	0.70	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BV	0.46	0/1081	0.70	0/1468
17	Ay	1.12	1/202 (0.5%)	1.24	1/272 (0.4%)
17	By	1.03	1/202 (0.5%)	1.22	1/272 (0.4%)
18	AX	0.57	0/273	0.76	0/370
18	BX	0.63	0/273	0.69	0/370
20	AZ	0.53	0/490	0.75	1/669 (0.1%)
20	BZ	0.60	0/490	0.80	0/669
All	All	0.53	4/42004 (0.0%)	0.75	14/57172 (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
2	BB	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	By	5030	ILE	CA-CB	-5.67	1.41	1.54
14	BT	5032	LYS	C-OXT	5.50	1.33	1.23
17	Ay	35	ILE	CA-CB	-5.35	1.42	1.54
14	AT	32	LYS	CA-CB	5.19	1.65	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	BO	5030	THR	N-CA-CB	-5.76	99.35	110.30
2	BB	5488	PRO	N-CA-C	5.72	126.97	112.10
2	BB	5489	GLU	N-CA-C	5.65	126.27	111.00
14	BT	5004	ILE	CB-CA-C	-5.65	100.31	111.60
3	AC	32	GLY	N-CA-C	-5.56	99.19	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	262	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	BB	5273	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	300	0
1	BA	2628	0	2524	309	0
2	AB	3850	0	3718	344	0
2	BB	3850	0	3718	351	0
3	AC	3444	0	3365	350	0
3	BC	3444	0	3365	358	0
4	AD	2711	0	2610	245	0
4	BD	2711	0	2610	255	0
5	AE	666	0	651	68	0
5	BE	666	0	651	76	0
6	AF	282	0	291	36	0
6	BF	282	0	291	32	0
7	AH	507	0	521	65	0
7	BH	507	0	521	69	0
8	AI	286	0	308	34	0
8	BI	286	0	305	37	0
9	AJ	271	0	276	36	0
9	BJ	271	0	276	38	0
10	AK	293	0	305	48	0
10	BK	293	0	305	45	0
11	AL	304	0	316	34	0
11	BL	304	0	313	35	0
12	AM	267	0	289	26	0
12	BM	267	0	286	26	0
13	AO	1845	0	1801	137	0
13	BO	1845	0	1801	142	0
14	AT	275	0	288	28	0
14	BT	275	0	285	27	0
15	AU	774	0	773	52	0
15	BU	774	0	773	51	0
16	AV	1060	0	1068	48	0
16	BV	1060	0	1068	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	33	0
18	BX	270	0	299	27	0
19	AY	140	0	32	3	0
19	BY	140	0	32	7	0
20	AZ	479	0	516	53	0
20	BZ	479	0	513	55	0
21	AA	1	0	0	0	0
21	BD	1	0	0	0	0
22	AA	4	0	0	0	0
22	BA	4	0	0	0	0
23	AA	2	0	0	1	0
23	BA	2	0	0	0	0
24	AA	260	0	288	41	0
24	AB	1040	0	1152	133	0
24	AC	845	0	936	91	0
24	AD	130	0	144	17	0
24	BA	260	0	288	44	0
24	BB	1040	0	1152	142	0
24	BC	845	0	936	94	0
24	BD	130	0	144	18	0
25	AA	16	0	19	9	0
25	BA	16	0	19	9	0
26	AA	5	0	0	0	0
26	BA	5	0	0	0	0
27	AA	40	0	56	4	0
27	AB	120	0	168	8	0
27	AC	120	0	168	24	0
27	AD	40	0	56	2	0
27	AJ	40	0	56	4	0
27	AK	40	0	56	5	0
27	AT	40	0	56	10	0
27	AX	40	0	56	8	0
27	BA	40	0	56	3	0
27	BB	120	0	168	8	0
27	BC	120	0	168	25	0
27	BD	40	0	56	2	0
27	BJ	40	0	56	3	0
27	BK	40	0	56	5	0
27	BT	40	0	56	6	0
27	BX	40	0	56	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AA	56	0	70	9	0
28	AB	52	0	62	0	0
28	AC	181	0	243	63	0
28	AE	63	0	87	1	0
28	AH	58	0	74	9	0
28	BA	56	0	70	9	0
28	BB	52	0	62	5	0
28	BC	181	0	243	64	0
28	BE	63	0	87	1	0
28	BH	58	0	74	8	0
29	AA	76	0	95	7	0
29	BA	76	0	95	9	0
30	AA	105	0	145	2	0
30	AB	90	0	109	9	0
30	AF	45	0	53	1	0
30	BA	105	0	145	3	0
30	BB	90	0	109	11	0
30	BF	45	0	53	1	0
31	AA	86	0	111	17	0
31	AB	100	0	139	21	0
31	AC	93	0	125	11	0
31	AD	97	0	134	15	0
31	AI	43	0	56	3	0
31	AJ	46	0	61	2	0
31	AM	42	0	54	6	0
31	BA	42	0	53	3	0
31	BB	49	0	68	4	0
31	BC	93	0	125	10	0
31	BD	143	0	195	15	0
31	BE	44	0	58	4	0
31	BI	43	0	56	4	0
31	BL	51	0	71	18	0
31	BM	42	0	54	4	0
32	AB	140	0	184	15	0
32	AD	31	0	35	0	0
32	AI	70	0	92	9	0
32	AM	35	0	46	1	0
32	BB	140	0	184	16	0
32	BC	35	0	46	3	0
32	BD	31	0	35	1	0
32	BI	35	0	46	5	0
32	BM	35	0	46	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	AB	8	0	12	0	0
33	AU	4	0	6	0	0
33	AV	4	0	6	0	0
33	BB	8	0	12	0	0
33	BV	8	0	12	0	0
34	AD	128	0	148	14	0
34	BD	128	0	148	15	0
35	AD	55	0	80	15	0
35	BD	55	0	80	16	0
36	AF	43	0	30	8	0
36	AV	43	0	30	4	0
36	BF	43	0	30	7	0
36	BV	43	0	30	6	0
37	AF	1	0	0	0	0
37	AK	1	0	0	0	0
37	AO	1	0	0	0	0
37	BF	1	0	0	0	0
37	BK	1	0	0	0	0
37	BO	1	0	0	0	0
All	All	50266	0	51335	3700	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 37.

The worst 5 of 3700 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)
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG2	1.69	1.27
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG2	1.78	1.17
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.25	1.15
24:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.29	1.14
24:BB:5612:CLA:H42	4:BD:5127:LEU:HD11	1.29	1.14

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	AA	333/344 (97%)	284 (85%)	42 (13%)	7 (2%)	9	46
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	9	46
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	5	32
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	5	34
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	4	30
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	4	28
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	6	39
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	7	43
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	4	28
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	4	28
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	35
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	35
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1	8
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	2	13
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	15
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	15
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	1	7
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	1	7
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	17
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	17
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%)	24 (75%)	8 (25%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	198 (82%)	31 (13%)	12 (5%)	3	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	3	23
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	5	32
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	32
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	2	19
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	26
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	26	72
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	26	72
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0	1
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	0	3
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	0	3
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	0	3
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	21
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	21
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	4	30

5 of 183 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%)	250 (92%)	21 (8%)	16	54
1	BA	271/280 (97%)	253 (93%)	18 (7%)	21	61
2	AB	390/407 (96%)	372 (95%)	18 (5%)	33	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BB	390/407 (96%)	374 (96%)	16 (4%)	37	76
3	AC	347/362 (96%)	326 (94%)	21 (6%)	23	64
3	BC	347/362 (96%)	325 (94%)	22 (6%)	22	63
4	AD	275/283 (97%)	249 (90%)	26 (10%)	11	40
4	BD	275/283 (97%)	249 (90%)	26 (10%)	11	40
5	AE	72/73 (99%)	66 (92%)	6 (8%)	14	49
5	BE	72/73 (99%)	66 (92%)	6 (8%)	14	49
6	AF	29/39 (74%)	27 (93%)	2 (7%)	19	59
6	BF	29/39 (74%)	28 (97%)	1 (3%)	44	80
7	AH	53/55 (96%)	42 (79%)	11 (21%)	1	7
7	BH	53/55 (96%)	43 (81%)	10 (19%)	2	10
8	AI	32/35 (91%)	32 (100%)	0	100	100
8	BI	32/35 (91%)	31 (97%)	1 (3%)	47	82
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	38	77
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	38	77
10	AK	30/30 (100%)	29 (97%)	1 (3%)	45	81
10	BK	30/30 (100%)	29 (97%)	1 (3%)	45	81
11	AL	35/35 (100%)	33 (94%)	2 (6%)	25	67
11	BL	35/35 (100%)	32 (91%)	3 (9%)	13	46
12	AM	31/33 (94%)	30 (97%)	1 (3%)	46	81
12	BM	31/33 (94%)	29 (94%)	2 (6%)	21	61
13	AO	202/208 (97%)	187 (93%)	15 (7%)	17	56
13	BO	202/208 (97%)	187 (93%)	15 (7%)	17	56
14	AT	29/29 (100%)	28 (97%)	1 (3%)	44	80
14	BT	29/29 (100%)	27 (93%)	2 (7%)	19	59
15	AU	84/89 (94%)	76 (90%)	8 (10%)	11	40
15	BU	84/89 (94%)	76 (90%)	8 (10%)	11	40
16	AV	116/117 (99%)	111 (96%)	5 (4%)	35	75
16	BV	116/117 (99%)	110 (95%)	6 (5%)	29	69
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	1	2
17	By	20/37 (54%)	15 (75%)	5 (25%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	AX	30/34 (88%)	29 (97%)	1 (3%)	45 81
18	BX	30/34 (88%)	29 (97%)	1 (3%)	45 81
20	AZ	52/52 (100%)	49 (94%)	3 (6%)	25 66
20	BZ	52/52 (100%)	48 (92%)	4 (8%)	16 54
All	All	4246/4452 (95%)	3950 (93%)	296 (7%)	19 58

5 of 296 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	AU	132	LEU
1	BA	5335	ASN
15	BU	5053	GLU
16	AV	89	THR
1	BA	5032	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
18	AX	47	GLN
1	BA	5312	ASN
13	BO	5150	ASN
1	BA	5012	ASN
1	BA	5118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 196 ligands modelled in this entry, 12 are monoatomic - leaving 184 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	BCT	AA	402	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	AA	404	-	55,73,73	2.48	12 (21%)	61,113,113	1.58	15 (24%)
24	CLA	AA	405	-	55,73,73	2.54	16 (29%)	61,113,113	2.12	18 (29%)
24	CLA	AA	406	-	55,73,73	2.50	14 (25%)	61,113,113	1.98	16 (26%)
24	CLA	AA	407	-	55,73,73	2.49	13 (23%)	61,113,113	1.78	17 (27%)
25	MST	AA	408	-	16,16,16	0.52	0	21,22,22	4.03	8 (38%)
26	OEC	AA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	AA	410	-	41,41,41	1.62	7 (17%)	56,56,56	2.11	22 (39%)
28	DGD	AA	411	-	57,57,67	1.76	14 (24%)	71,71,81	3.75	25 (35%)
29	LHG	AA	412	-	38,38,48	1.91	5 (13%)	39,44,54	1.40	4 (10%)
30	SQD	AA	413	-	50,51,54	2.41	25 (50%)	58,62,65	3.03	20 (34%)
31	LMG	AA	414	-	44,44,55	1.08	3 (6%)	52,52,63	1.51	6 (11%)
29	LHG	AA	415	-	36,36,48	1.04	2 (5%)	37,42,54	1.15	3 (8%)
30	SQD	AA	416	-	53,54,54	2.40	29 (54%)	61,65,65	2.99	19 (31%)
31	LMG	AA	417	-	42,42,55	1.06	5 (11%)	50,50,63	2.37	12 (24%)
24	CLA	AB	601	-	55,73,73	2.85	15 (27%)	61,113,113	1.56	9 (14%)
24	CLA	AB	602	-	55,73,73	2.48	13 (23%)	61,113,113	1.60	12 (19%)
24	CLA	AB	603	-	55,73,73	2.61	13 (23%)	61,113,113	1.96	18 (29%)
24	CLA	AB	604	-	55,73,73	2.55	14 (25%)	61,113,113	1.58	15 (24%)
24	CLA	AB	605	-	55,73,73	2.67	13 (23%)	61,113,113	1.78	14 (22%)
24	CLA	AB	606	-	55,73,73	2.68	14 (25%)	61,113,113	1.72	16 (26%)
24	CLA	AB	607	-	55,73,73	2.59	16 (29%)	61,113,113	2.01	18 (29%)
24	CLA	AB	608	-	55,73,73	2.77	16 (29%)	61,113,113	2.04	17 (27%)
24	CLA	AB	609	-	55,73,73	2.64	12 (21%)	61,113,113	1.66	14 (22%)
24	CLA	AB	610	-	55,73,73	2.49	11 (20%)	61,113,113	1.62	11 (18%)
24	CLA	AB	611	-	55,73,73	2.52	13 (23%)	61,113,113	1.85	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AB	612	-	55,73,73	2.54	12 (21%)	61,113,113	1.76	12 (19%)
24	CLA	AB	613	-	55,73,73	2.31	11 (20%)	61,113,113	1.49	12 (19%)
24	CLA	AB	614	-	55,73,73	2.71	13 (23%)	61,113,113	1.90	15 (24%)
24	CLA	AB	615	-	55,73,73	2.51	12 (21%)	61,113,113	1.61	11 (18%)
24	CLA	AB	616	-	55,73,73	2.62	11 (20%)	61,113,113	1.54	9 (14%)
27	BCR	AB	617	-	41,41,41	1.58	6 (14%)	56,56,56	2.16	19 (33%)
27	BCR	AB	618	-	41,41,41	1.93	7 (17%)	56,56,56	2.13	16 (28%)
27	BCR	AB	619	-	41,41,41	1.84	8 (19%)	56,56,56	2.01	19 (33%)
31	LMG	AB	620	-	51,51,55	1.30	3 (5%)	59,59,63	2.01	13 (22%)
31	LMG	AB	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.90	15 (26%)
30	SQD	AB	622	-	42,43,54	2.62	20 (47%)	50,54,65	3.13	14 (28%)
32	LMT	AB	623	-	36,36,36	1.73	8 (22%)	47,47,47	0.98	2 (4%)
32	LMT	AB	624	-	36,36,36	1.62	7 (19%)	47,47,47	0.93	2 (4%)
33	DMS	AB	625	-	3,3,3	0.71	0	3,3,3	1.36	0
33	DMS	AB	626	-	3,3,3	0.66	0	3,3,3	0.99	0
30	SQD	AB	627	-	46,47,54	2.50	23 (50%)	54,58,65	2.97	14 (25%)
28	DGD	AB	628	-	53,53,67	1.42	7 (13%)	67,67,81	2.12	13 (19%)
32	LMT	AB	629	-	36,36,36	1.56	7 (19%)	47,47,47	1.38	5 (10%)
32	LMT	AB	630	-	36,36,36	1.70	9 (25%)	47,47,47	1.00	1 (2%)
24	CLA	AC	501	-	55,73,73	2.58	15 (27%)	61,113,113	1.75	13 (21%)
24	CLA	AC	502	-	55,73,73	2.52	12 (21%)	61,113,113	1.67	13 (21%)
24	CLA	AC	503	-	55,73,73	2.55	13 (23%)	61,113,113	1.80	16 (26%)
24	CLA	AC	504	-	55,73,73	2.47	15 (27%)	61,113,113	1.85	14 (22%)
24	CLA	AC	505	-	55,73,73	2.83	16 (29%)	61,113,113	1.85	13 (21%)
24	CLA	AC	506	-	55,73,73	2.71	14 (25%)	61,113,113	1.68	14 (22%)
24	CLA	AC	507	-	55,73,73	2.42	13 (23%)	61,113,113	1.62	12 (19%)
24	CLA	AC	508	-	55,73,73	2.49	12 (21%)	61,113,113	1.80	15 (24%)
24	CLA	AC	509	-	55,73,73	2.46	11 (20%)	61,113,113	1.69	12 (19%)
24	CLA	AC	510	-	55,73,73	2.48	11 (20%)	61,113,113	1.59	11 (18%)
24	CLA	AC	511	3	55,73,73	2.65	12 (21%)	61,113,113	1.92	15 (24%)
24	CLA	AC	512	-	55,73,73	2.58	12 (21%)	61,113,113	1.55	10 (16%)
24	CLA	AC	513	-	55,73,73	2.70	11 (20%)	61,113,113	1.69	14 (22%)
27	BCR	AC	514	-	41,41,41	1.62	7 (17%)	56,56,56	2.19	25 (44%)
27	BCR	AC	515	-	41,41,41	1.75	7 (17%)	56,56,56	2.29	22 (39%)
27	BCR	AC	516	-	41,41,41	1.64	8 (19%)	56,56,56	2.31	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	AC	517	-	54,54,67	1.32	7 (12%)	68,68,81	2.84	22 (32%)
28	DGD	AC	518	-	63,63,67	1.20	6 (9%)	77,77,81	2.94	25 (32%)
28	DGD	AC	519	-	67,67,67	1.47	11 (16%)	81,81,81	3.41	31 (38%)
31	LMG	AC	520	-	48,48,55	1.04	5 (10%)	56,56,63	1.93	18 (32%)
31	LMG	AC	521	-	45,45,55	1.07	2 (4%)	53,53,63	1.98	14 (26%)
24	CLA	AD	401	-	55,73,73	2.47	13 (23%)	61,113,113	1.67	14 (22%)
34	PHO	AD	402	-	67,69,69	2.30	13 (19%)	84,99,99	1.39	14 (16%)
34	PHO	AD	403	-	67,69,69	2.40	15 (22%)	84,99,99	1.52	15 (17%)
24	CLA	AD	404	-	55,73,73	2.60	15 (27%)	61,113,113	1.74	12 (19%)
35	PL9	AD	405	-	55,55,55	4.40	18 (32%)	68,69,69	2.90	24 (35%)
27	BCR	AD	406	-	41,41,41	1.65	7 (17%)	56,56,56	2.40	24 (42%)
31	LMG	AD	407	-	49,49,55	0.73	1 (2%)	57,57,63	2.72	20 (35%)
31	LMG	AD	408	-	48,48,55	0.94	4 (8%)	56,56,63	2.10	12 (21%)
32	LMT	AD	409	-	32,32,36	1.71	7 (21%)	43,43,47	1.23	2 (4%)
28	DGD	AE	101	-	64,64,67	1.52	13 (20%)	78,78,81	1.49	10 (12%)
36	HEM	AF	101	5,6	30,50,50	2.83	13 (43%)	24,82,82	3.89	13 (54%)
30	SQD	AF	102	-	44,45,54	2.53	21 (47%)	52,56,65	3.25	16 (30%)
28	DGD	AH	101	-	59,59,67	1.31	10 (16%)	73,73,81	2.10	19 (26%)
31	LMG	AI	101	-	43,43,55	1.01	2 (4%)	51,51,63	1.74	7 (13%)
32	LMT	AI	102	-	36,36,36	1.58	7 (19%)	47,47,47	1.00	2 (4%)
32	LMT	AI	103	-	36,36,36	1.42	6 (16%)	47,47,47	1.75	9 (19%)
27	BCR	AJ	101	-	41,41,41	2.47	13 (31%)	56,56,56	3.30	26 (46%)
31	LMG	AJ	102	-	46,46,55	0.95	3 (6%)	54,54,63	2.62	16 (29%)
27	BCR	AK	102	-	41,41,41	1.78	6 (14%)	56,56,56	2.52	25 (44%)
31	LMG	AM	101	-	42,42,55	0.94	2 (4%)	50,50,63	1.70	7 (14%)
32	LMT	AM	102	-	36,36,36	1.71	10 (27%)	47,47,47	0.90	1 (2%)
27	BCR	AT	101	-	41,41,41	1.63	6 (14%)	56,56,56	2.29	24 (42%)
33	DMS	AU	201	-	3,3,3	0.90	0	3,3,3	1.08	0
36	HEM	AV	201	16	30,50,50	2.80	14 (46%)	24,82,82	3.88	13 (54%)
33	DMS	AV	202	-	3,3,3	0.74	0	3,3,3	1.00	0
27	BCR	AX	101	-	41,41,41	1.86	8 (19%)	56,56,56	2.26	22 (39%)
30	SQD	BA	5401	-	53,54,54	2.43	28 (52%)	61,65,65	2.98	19 (31%)
31	LMG	BA	5402	-	42,42,55	1.06	3 (7%)	50,50,63	2.38	12 (24%)
22	BCT	BA	5403	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	BA	5405	-	55,73,73	2.47	13 (23%)	61,113,113	1.54	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BA	5406	-	55,73,73	2.64	15 (27%)	61,113,113	2.13	16 (26%)
24	CLA	BA	5407	-	55,73,73	2.61	15 (27%)	61,113,113	1.96	15 (24%)
24	CLA	BA	5408	-	55,73,73	2.59	13 (23%)	61,113,113	1.77	14 (22%)
25	MST	BA	5409	-	16,16,16	0.49	0	21,22,22	3.94	8 (38%)
26	OEC	BA	5410	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	BA	5411	-	41,41,41	1.68	7 (17%)	56,56,56	2.13	21 (37%)
28	DGD	BA	5412	-	57,57,67	1.79	12 (21%)	71,71,81	3.76	24 (33%)
29	LHG	BA	5413	-	38,38,48	1.90	5 (13%)	39,44,54	1.37	4 (10%)
30	SQD	BA	5414	-	50,51,54	2.50	26 (52%)	58,62,65	3.02	19 (32%)
29	LHG	BA	5415	-	36,36,48	1.04	2 (5%)	37,42,54	1.15	3 (8%)
30	SQD	BB	5601	-	46,47,54	2.50	23 (50%)	54,58,65	2.97	15 (27%)
28	DGD	BB	5602	-	53,53,67	1.46	7 (13%)	67,67,81	2.14	13 (19%)
32	LMT	BB	5603	-	36,36,36	1.56	7 (19%)	47,47,47	1.38	5 (10%)
32	LMT	BB	5604	-	36,36,36	1.68	9 (25%)	47,47,47	1.00	1 (2%)
24	CLA	BB	5605	-	55,73,73	2.86	14 (25%)	61,113,113	1.54	9 (14%)
24	CLA	BB	5606	-	55,73,73	2.51	12 (21%)	61,113,113	1.62	10 (16%)
24	CLA	BB	5607	-	55,73,73	2.57	12 (21%)	61,113,113	1.98	17 (27%)
24	CLA	BB	5608	-	55,73,73	2.49	13 (23%)	61,113,113	1.60	14 (22%)
24	CLA	BB	5609	-	55,73,73	2.60	14 (25%)	61,113,113	1.75	14 (22%)
24	CLA	BB	5610	-	55,73,73	2.71	15 (27%)	61,113,113	1.75	16 (26%)
24	CLA	BB	5611	-	55,73,73	2.51	14 (25%)	61,113,113	2.02	19 (31%)
24	CLA	BB	5612	-	55,73,73	2.74	16 (29%)	61,113,113	2.03	17 (27%)
24	CLA	BB	5613	-	55,73,73	2.64	13 (23%)	61,113,113	1.69	16 (26%)
24	CLA	BB	5614	-	55,73,73	2.47	11 (20%)	61,113,113	1.59	12 (19%)
24	CLA	BB	5615	-	55,73,73	2.58	13 (23%)	61,113,113	1.86	20 (32%)
24	CLA	BB	5616	-	55,73,73	2.60	12 (21%)	61,113,113	1.78	12 (19%)
24	CLA	BB	5617	-	55,73,73	2.34	13 (23%)	61,113,113	1.50	12 (19%)
24	CLA	BB	5618	-	55,73,73	2.70	12 (21%)	61,113,113	1.90	13 (21%)
24	CLA	BB	5619	-	55,73,73	2.46	12 (21%)	61,113,113	1.61	11 (18%)
24	CLA	BB	5620	-	55,73,73	2.63	12 (21%)	61,113,113	1.57	9 (14%)
27	BCR	BB	5621	-	41,41,41	1.51	7 (17%)	56,56,56	2.15	19 (33%)
27	BCR	BB	5622	-	41,41,41	1.88	7 (17%)	56,56,56	2.11	16 (28%)
27	BCR	BB	5623	-	41,41,41	1.71	8 (19%)	56,56,56	1.98	17 (30%)
31	LMG	BB	5624	-	49,49,55	0.79	1 (2%)	57,57,63	1.90	15 (26%)
30	SQD	BB	5625	-	42,43,54	2.63	20 (47%)	50,54,65	3.19	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BB	5626	-	36,36,36	1.73	9 (25%)	47,47,47	0.99	2 (4%)
32	LMT	BB	5627	-	36,36,36	1.58	8 (22%)	47,47,47	0.92	2 (4%)
33	DMS	BB	5628	-	3,3,3	0.69	0	3,3,3	1.08	0
33	DMS	BB	5629	-	3,3,3	0.67	0	3,3,3	1.14	0
24	CLA	BC	5501	-	55,73,73	2.68	13 (23%)	61,113,113	1.75	13 (21%)
24	CLA	BC	5502	-	55,73,73	2.60	13 (23%)	61,113,113	1.69	13 (21%)
24	CLA	BC	5503	-	55,73,73	2.62	13 (23%)	61,113,113	1.76	16 (26%)
24	CLA	BC	5504	-	55,73,73	2.60	14 (25%)	61,113,113	1.86	14 (22%)
24	CLA	BC	5505	-	55,73,73	2.87	15 (27%)	61,113,113	1.81	13 (21%)
24	CLA	BC	5506	-	55,73,73	2.73	14 (25%)	61,113,113	1.68	15 (24%)
24	CLA	BC	5507	-	55,73,73	2.50	12 (21%)	61,113,113	1.64	11 (18%)
24	CLA	BC	5508	-	55,73,73	2.57	13 (23%)	61,113,113	1.84	14 (22%)
24	CLA	BC	5509	-	55,73,73	2.65	14 (25%)	61,113,113	1.67	13 (21%)
24	CLA	BC	5510	-	55,73,73	2.53	11 (20%)	61,113,113	1.60	11 (18%)
24	CLA	BC	5511	3	55,73,73	2.76	15 (27%)	61,113,113	1.90	14 (22%)
24	CLA	BC	5512	-	55,73,73	2.66	12 (21%)	61,113,113	1.52	10 (16%)
24	CLA	BC	5513	-	55,73,73	2.77	14 (25%)	61,113,113	1.68	11 (18%)
27	BCR	BC	5514	-	41,41,41	1.80	6 (14%)	56,56,56	2.14	24 (42%)
27	BCR	BC	5515	-	41,41,41	1.89	8 (19%)	56,56,56	2.29	23 (41%)
27	BCR	BC	5516	-	41,41,41	1.78	7 (17%)	56,56,56	2.27	20 (35%)
28	DGD	BC	5517	-	54,54,67	1.41	8 (14%)	68,68,81	2.84	21 (30%)
28	DGD	BC	5518	-	63,63,67	1.23	6 (9%)	77,77,81	2.91	24 (31%)
28	DGD	BC	5519	-	67,67,67	1.50	12 (17%)	81,81,81	3.41	30 (37%)
31	LMG	BC	5520	-	48,48,55	1.08	3 (6%)	56,56,63	1.90	17 (30%)
31	LMG	BC	5521	-	45,45,55	1.01	2 (4%)	53,53,63	1.98	13 (24%)
32	LMT	BC	5522	-	36,36,36	1.48	7 (19%)	47,47,47	1.74	8 (17%)
24	CLA	BD	5402	-	55,73,73	2.55	13 (23%)	61,113,113	1.69	14 (22%)
34	PHO	BD	5403	-	67,69,69	2.40	14 (20%)	84,99,99	1.41	16 (19%)
34	PHO	BD	5404	-	67,69,69	2.44	14 (20%)	84,99,99	1.57	17 (20%)
24	CLA	BD	5405	-	55,73,73	2.63	13 (23%)	61,113,113	1.72	11 (18%)
35	PL9	BD	5406	-	55,55,55	4.52	20 (36%)	68,69,69	2.92	24 (35%)
27	BCR	BD	5407	-	41,41,41	1.82	9 (21%)	56,56,56	2.38	24 (42%)
31	LMG	BD	5408	-	46,46,55	0.95	3 (6%)	54,54,63	2.61	16 (29%)
31	LMG	BD	5409	-	49,49,55	0.70	0	57,57,63	2.73	21 (36%)
31	LMG	BD	5410	-	48,48,55	0.93	2 (4%)	56,56,63	2.11	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BD	5411	-	32,32,36	1.69	7 (21%)	43,43,47	1.24	2 (4%)
31	LMG	BE	5101	-	44,44,55	1.07	2 (4%)	52,52,63	1.52	6 (11%)
28	DGD	BE	5102	-	64,64,67	1.49	13 (20%)	78,78,81	1.48	10 (12%)
36	HEM	BF	5101	5,6	30,50,50	2.91	14 (46%)	24,82,82	3.93	13 (54%)
30	SQD	BF	5102	-	44,45,54	2.54	21 (47%)	52,56,65	3.27	17 (32%)
28	DGD	BH	5101	-	59,59,67	1.29	8 (13%)	73,73,81	2.11	19 (26%)
31	LMG	BI	5101	-	43,43,55	1.00	3 (6%)	51,51,63	1.72	7 (13%)
32	LMT	BI	5102	-	36,36,36	1.62	8 (22%)	47,47,47	1.00	2 (4%)
27	BCR	BJ	5101	-	41,41,41	2.41	14 (34%)	56,56,56	3.28	25 (44%)
27	BCR	BK	5102	-	41,41,41	1.91	8 (19%)	56,56,56	2.48	24 (42%)
31	LMG	BL	5101	-	51,51,55	1.34	3 (5%)	59,59,63	2.00	13 (22%)
32	LMT	BM	5101	-	36,36,36	1.72	9 (25%)	47,47,47	0.90	2 (4%)
31	LMG	BM	5102	-	42,42,55	0.99	3 (7%)	50,50,63	1.70	8 (16%)
27	BCR	BT	5101	-	41,41,41	1.77	6 (14%)	56,56,56	2.29	24 (42%)
36	HEM	BV	5201	16	30,50,50	2.96	14 (46%)	24,82,82	3.84	13 (54%)
33	DMS	BV	5202	-	3,3,3	0.84	0	3,3,3	0.93	0
33	DMS	BV	5203	-	3,3,3	0.82	0	3,3,3	1.12	0
27	BCR	BX	5101	-	41,41,41	1.89	9 (21%)	56,56,56	2.29	22 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCT	AA	402	21	-	0/0/0/0	0/0/0/0
24	CLA	AA	404	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	405	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	406	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	407	-	4/4/20/25	0/37/135/135	0/0/9/9
25	MST	AA	408	-	-	0/10/10/10	0/1/1/1
26	OEC	AA	409	1,3	-	0/0/0/54	0/0/0/5
27	BCR	AA	410	-	-	0/29/63/63	0/2/2/2
28	DGD	AA	411	-	-	0/45/85/95	0/2/2/2
29	LHG	AA	412	-	-	0/43/43/53	0/0/0/0
30	SQD	AA	413	-	-	0/46/66/69	0/1/1/1
31	LMG	AA	414	-	-	0/39/59/70	0/1/1/1
29	LHG	AA	415	-	-	0/41/41/53	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	AA	416	-	-	0/49/69/69	0/1/1/1
31	LMG	AA	417	-	-	0/37/57/70	0/1/1/1
24	CLA	AB	601	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	602	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	603	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	604	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	605	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	606	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	607	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	608	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	609	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	610	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	611	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	612	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	613	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	614	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	615	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	616	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	AB	617	-	-	0/29/63/63	0/2/2/2
27	BCR	AB	618	-	-	0/29/63/63	0/2/2/2
27	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
31	LMG	AB	620	-	-	0/46/66/70	0/1/1/1
31	LMG	AB	621	-	-	0/44/64/70	0/1/1/1
30	SQD	AB	622	-	-	0/38/58/69	0/1/1/1
32	LMT	AB	623	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	624	-	-	0/21/61/61	0/2/2/2
33	DMS	AB	625	-	-	0/0/0/0	0/0/0/0
33	DMS	AB	626	-	-	0/0/0/0	0/0/0/0
30	SQD	AB	627	-	-	0/42/62/69	0/1/1/1
28	DGD	AB	628	-	-	0/41/81/95	0/2/2/2
32	LMT	AB	629	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	630	-	-	0/21/61/61	0/2/2/2
24	CLA	AC	501	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	502	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	503	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	504	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	505	-	4/4/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AC	506	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	507	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	508	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	509	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	510	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	511	3	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	512	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	513	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	AC	514	-	-	0/29/63/63	0/2/2/2
27	BCR	AC	515	-	-	0/29/63/63	0/2/2/2
27	BCR	AC	516	-	-	0/29/63/63	0/2/2/2
28	DGD	AC	517	-	-	0/42/82/95	0/2/2/2
28	DGD	AC	518	-	1/1/13/13	0/51/91/95	0/2/2/2
28	DGD	AC	519	-	1/1/13/13	0/55/95/95	0/2/2/2
31	LMG	AC	520	-	-	0/43/63/70	0/1/1/1
31	LMG	AC	521	-	-	0/40/60/70	0/1/1/1
24	CLA	AD	401	-	4/4/20/25	0/37/135/135	0/0/9/9
34	PHO	AD	402	-	1/1/17/22	0/53/103/103	0/1/6/6
34	PHO	AD	403	-	1/1/17/22	0/53/103/103	0/1/6/6
24	CLA	AD	404	-	4/4/20/25	0/37/135/135	0/0/9/9
35	PL9	AD	405	-	-	2/53/73/73	0/1/1/1
27	BCR	AD	406	-	-	0/29/63/63	0/2/2/2
31	LMG	AD	407	-	-	0/44/64/70	0/1/1/1
31	LMG	AD	408	-	-	0/43/63/70	0/1/1/1
32	LMT	AD	409	-	-	0/17/57/61	0/2/2/2
28	DGD	AE	101	-	-	0/52/92/95	0/2/2/2
36	HEM	AF	101	5,6	-	0/10/54/54	0/0/8/8
30	SQD	AF	102	-	-	0/40/60/69	0/1/1/1
28	DGD	AH	101	-	-	0/47/87/95	0/2/2/2
31	LMG	AI	101	-	-	0/38/58/70	0/1/1/1
32	LMT	AI	102	-	-	0/21/61/61	0/2/2/2
32	LMT	AI	103	-	-	0/21/61/61	0/2/2/2
27	BCR	AJ	101	-	-	0/29/63/63	0/2/2/2
31	LMG	AJ	102	-	-	0/41/61/70	0/1/1/1
27	BCR	AK	102	-	-	0/29/63/63	0/2/2/2
31	LMG	AM	101	-	-	0/37/57/70	0/1/1/1
32	LMT	AM	102	-	-	0/21/61/61	0/2/2/2
27	BCR	AT	101	-	-	0/29/63/63	0/2/2/2
33	DMS	AU	201	-	-	0/0/0/0	0/0/0/0
36	HEM	AV	201	16	-	0/10/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DMS	AV	202	-	-	0/0/0/0	0/0/0/0
27	BCR	AX	101	-	-	0/29/63/63	0/2/2/2
30	SQD	BA	5401	-	-	0/49/69/69	0/1/1/1
31	LMG	BA	5402	-	-	0/37/57/70	0/1/1/1
22	BCT	BA	5403	21	-	0/0/0/0	0/0/0/0
24	CLA	BA	5405	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5406	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5407	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5408	-	4/4/20/25	0/37/135/135	0/0/9/9
25	MST	BA	5409	-	-	0/10/10/10	0/1/1/1
26	OEC	BA	5410	1,3	-	0/0/0/54	0/0/0/5
27	BCR	BA	5411	-	-	0/29/63/63	0/2/2/2
28	DGD	BA	5412	-	-	0/45/85/95	0/2/2/2
29	LHG	BA	5413	-	-	0/43/43/53	0/0/0/0
30	SQD	BA	5414	-	-	0/46/66/69	0/1/1/1
29	LHG	BA	5415	-	-	0/41/41/53	0/0/0/0
30	SQD	BB	5601	-	-	0/42/62/69	0/1/1/1
28	DGD	BB	5602	-	-	0/41/81/95	0/2/2/2
32	LMT	BB	5603	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	5604	-	-	0/21/61/61	0/2/2/2
24	CLA	BB	5605	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5606	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5607	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5608	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5609	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5610	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5611	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5612	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5613	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5614	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5615	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5616	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5617	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5618	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5619	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5620	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	BB	5621	-	-	0/29/63/63	0/2/2/2
27	BCR	BB	5622	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	BB	5623	-	-	0/29/63/63	0/2/2/2
31	LMG	BB	5624	-	-	0/44/64/70	0/1/1/1
30	SQD	BB	5625	-	-	0/38/58/69	0/1/1/1
32	LMT	BB	5626	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	5627	-	-	0/21/61/61	0/2/2/2
33	DMS	BB	5628	-	-	0/0/0/0	0/0/0/0
33	DMS	BB	5629	-	-	0/0/0/0	0/0/0/0
24	CLA	BC	5501	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5502	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5503	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5504	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5505	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5506	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5507	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5508	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5509	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5510	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5511	3	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5512	-	4/4/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5513	-	4/4/20/25	0/37/135/135	0/0/9/9
27	BCR	BC	5514	-	-	0/29/63/63	0/2/2/2
27	BCR	BC	5515	-	-	0/29/63/63	0/2/2/2
27	BCR	BC	5516	-	-	0/29/63/63	0/2/2/2
28	DGD	BC	5517	-	-	0/42/82/95	0/2/2/2
28	DGD	BC	5518	-	1/1/13/13	0/51/91/95	0/2/2/2
28	DGD	BC	5519	-	1/1/13/13	0/55/95/95	0/2/2/2
31	LMG	BC	5520	-	-	0/43/63/70	0/1/1/1
31	LMG	BC	5521	-	-	0/40/60/70	0/1/1/1
32	LMT	BC	5522	-	-	0/21/61/61	0/2/2/2
24	CLA	BD	5402	-	4/4/20/25	0/37/135/135	0/0/9/9
34	PHO	BD	5403	-	1/1/17/22	0/53/103/103	0/1/6/6
34	PHO	BD	5404	-	1/1/17/22	0/53/103/103	0/1/6/6
24	CLA	BD	5405	-	4/4/20/25	0/37/135/135	0/0/9/9
35	PL9	BD	5406	-	-	1/53/73/73	0/1/1/1
27	BCR	BD	5407	-	-	0/29/63/63	0/2/2/2
31	LMG	BD	5408	-	-	0/41/61/70	0/1/1/1
31	LMG	BD	5409	-	-	0/44/64/70	0/1/1/1
31	LMG	BD	5410	-	-	0/43/63/70	0/1/1/1
32	LMT	BD	5411	-	-	0/17/57/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	BE	5101	-	-	0/39/59/70	0/1/1/1
28	DGD	BE	5102	-	-	0/52/92/95	0/2/2/2
36	HEM	BF	5101	5,6	-	0/10/54/54	0/0/8/8
30	SQD	BF	5102	-	-	0/40/60/69	0/1/1/1
28	DGD	BH	5101	-	-	0/47/87/95	0/2/2/2
31	LMG	BI	5101	-	-	0/38/58/70	0/1/1/1
32	LMT	BI	5102	-	-	0/21/61/61	0/2/2/2
27	BCR	BJ	5101	-	-	0/29/63/63	0/2/2/2
27	BCR	BK	5102	-	-	0/29/63/63	0/2/2/2
31	LMG	BL	5101	-	-	0/46/66/70	0/1/1/1
32	LMT	BM	5101	-	-	0/21/61/61	0/2/2/2
31	LMG	BM	5102	-	-	0/37/57/70	0/1/1/1
27	BCR	BT	5101	-	-	0/29/63/63	0/2/2/2
36	HEM	BV	5201	16	-	0/10/54/54	0/0/8/8
33	DMS	BV	5202	-	-	0/0/0/0	0/0/0/0
33	DMS	BV	5203	-	-	0/0/0/0	0/0/0/0
27	BCR	BX	5101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 1822 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BV	5201	HEM	C3B-C4B	-7.11	1.45	1.51
36	BF	5101	HEM	C3B-C4B	-6.40	1.46	1.51
36	AF	101	HEM	C3B-C4B	-6.34	1.46	1.51
36	BF	5101	HEM	C2D-C3D	-6.13	1.36	1.54
36	BV	5201	HEM	C2D-C3D	-5.81	1.37	1.54

The worst 5 of 2457 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BJ	5101	BCR	C32-C1-C6	-10.33	94.11	110.30
27	AJ	101	BCR	C32-C1-C6	-10.27	94.20	110.30
28	BA	5412	DGD	O3G-C1D-C2D	-9.80	95.67	108.04
28	AC	519	DGD	C3G-O3G-C1D	-9.79	93.25	113.82
28	AA	411	DGD	O3G-C1D-C2D	-9.69	95.80	108.04

5 of 288 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	BC	5502	CLA	C8
24	BC	5502	CLA	NC
24	BC	5502	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	BC	5502	CLA	NA
24	BC	5511	CLA	C8

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	AD	405	PL9	C29-C28-C27-C26
35	BD	5406	PL9	C49-C48-C47-C46
35	AD	405	PL9	C49-C48-C47-C46

There are no ring outliers.

167 monomers are involved in 1068 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AA	404	CLA	12	0
24	AA	405	CLA	20	0
24	AA	406	CLA	1	0
24	AA	407	CLA	9	0
25	AA	408	MST	9	0
27	AA	410	BCR	4	0
28	AA	411	DGD	9	0
29	AA	412	LHG	5	0
31	AA	414	LMG	11	0
29	AA	415	LHG	2	0
30	AA	416	SQD	2	0
31	AA	417	LMG	6	0
24	AB	601	CLA	5	0
24	AB	602	CLA	7	0
24	AB	603	CLA	15	0
24	AB	604	CLA	12	0
24	AB	605	CLA	10	0
24	AB	606	CLA	9	0
24	AB	607	CLA	10	0
24	AB	608	CLA	15	0
24	AB	609	CLA	7	0
24	AB	610	CLA	8	0
24	AB	611	CLA	15	0
24	AB	612	CLA	12	0
24	AB	613	CLA	9	0
24	AB	614	CLA	10	0
24	AB	615	CLA	8	0
24	AB	616	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	AB	617	BCR	3	0
27	AB	618	BCR	2	0
27	AB	619	BCR	3	0
31	AB	620	LMG	17	0
31	AB	621	LMG	4	0
30	AB	622	SQD	6	0
32	AB	624	LMT	9	0
30	AB	627	SQD	3	0
32	AB	629	LMT	4	0
32	AB	630	LMT	2	0
24	AC	501	CLA	5	0
24	AC	502	CLA	6	0
24	AC	503	CLA	6	0
24	AC	504	CLA	10	0
24	AC	505	CLA	9	0
24	AC	506	CLA	5	0
24	AC	507	CLA	5	0
24	AC	508	CLA	10	0
24	AC	509	CLA	6	0
24	AC	510	CLA	6	0
24	AC	511	CLA	22	0
24	AC	512	CLA	4	0
24	AC	513	CLA	3	0
27	AC	514	BCR	6	0
27	AC	515	BCR	6	0
27	AC	516	BCR	12	0
28	AC	517	DGD	10	0
28	AC	518	DGD	12	0
28	AC	519	DGD	42	0
31	AC	520	LMG	4	0
31	AC	521	LMG	7	0
24	AD	401	CLA	9	0
34	AD	402	PHO	11	0
34	AD	403	PHO	3	0
24	AD	404	CLA	8	0
35	AD	405	PL9	15	0
27	AD	406	BCR	2	0
31	AD	407	LMG	4	0
31	AD	408	LMG	11	0
28	AE	101	DGD	1	0
36	AF	101	HEM	8	0
30	AF	102	SQD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	AH	101	DGD	9	0
31	AI	101	LMG	3	0
32	AI	102	LMT	5	0
32	AI	103	LMT	4	0
27	AJ	101	BCR	4	0
31	AJ	102	LMG	2	0
27	AK	102	BCR	5	0
31	AM	101	LMG	6	0
32	AM	102	LMT	1	0
27	AT	101	BCR	10	0
36	AV	201	HEM	4	0
27	AX	101	BCR	8	0
30	BA	5401	SQD	3	0
31	BA	5402	LMG	3	0
24	BA	5405	CLA	11	0
24	BA	5406	CLA	22	0
24	BA	5407	CLA	1	0
24	BA	5408	CLA	11	0
25	BA	5409	MST	9	0
27	BA	5411	BCR	3	0
28	BA	5412	DGD	9	0
29	BA	5413	LHG	6	0
29	BA	5415	LHG	3	0
30	BB	5601	SQD	5	0
28	BB	5602	DGD	5	0
32	BB	5603	LMT	2	0
32	BB	5604	LMT	2	0
24	BB	5605	CLA	5	0
24	BB	5606	CLA	7	0
24	BB	5607	CLA	15	0
24	BB	5608	CLA	12	0
24	BB	5609	CLA	12	0
24	BB	5610	CLA	9	0
24	BB	5611	CLA	10	0
24	BB	5612	CLA	14	0
24	BB	5613	CLA	7	0
24	BB	5614	CLA	9	0
24	BB	5615	CLA	19	0
24	BB	5616	CLA	12	0
24	BB	5617	CLA	8	0
24	BB	5618	CLA	14	0
24	BB	5619	CLA	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	BB	5620	CLA	4	0
27	BB	5621	BCR	3	0
27	BB	5622	BCR	1	0
27	BB	5623	BCR	4	0
31	BB	5624	LMG	4	0
30	BB	5625	SQD	6	0
32	BB	5626	LMT	2	0
32	BB	5627	LMT	10	0
24	BC	5501	CLA	6	0
24	BC	5502	CLA	6	0
24	BC	5503	CLA	5	0
24	BC	5504	CLA	8	0
24	BC	5505	CLA	9	0
24	BC	5506	CLA	4	0
24	BC	5507	CLA	7	0
24	BC	5508	CLA	9	0
24	BC	5509	CLA	8	0
24	BC	5510	CLA	6	0
24	BC	5511	CLA	23	0
24	BC	5512	CLA	5	0
24	BC	5513	CLA	5	0
27	BC	5514	BCR	6	0
27	BC	5515	BCR	6	0
27	BC	5516	BCR	13	0
28	BC	5517	DGD	10	0
28	BC	5518	DGD	10	0
28	BC	5519	DGD	45	0
31	BC	5520	LMG	3	0
31	BC	5521	LMG	7	0
32	BC	5522	LMT	3	0
24	BD	5402	CLA	10	0
34	BD	5403	PHO	12	0
34	BD	5404	PHO	3	0
24	BD	5405	CLA	8	0
35	BD	5406	PL9	16	0
27	BD	5407	BCR	2	0
31	BD	5408	LMG	1	0
31	BD	5409	LMG	4	0
31	BD	5410	LMG	10	0
32	BD	5411	LMT	1	0
31	BE	5101	LMG	4	0
28	BE	5102	DGD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	BF	5101	HEM	7	0
30	BF	5102	SQD	1	0
28	BH	5101	DGD	8	0
31	BI	5101	LMG	4	0
32	BI	5102	LMT	5	0
27	BJ	5101	BCR	3	0
27	BK	5102	BCR	5	0
31	BL	5101	LMG	18	0
32	BM	5101	LMT	2	0
31	BM	5102	LMG	4	0
27	BT	5101	BCR	6	0
36	BV	5201	HEM	6	0
27	BX	5101	BCR	4	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	AA	335/344 (97%)	0.05	9 (2%) 58 44	82, 104, 147, 160	0
1	BA	335/344 (97%)	0.04	17 (5%) 32 18	86, 106, 148, 160	0
2	AB	490/510 (96%)	0.07	16 (3%) 50 35	81, 103, 136, 152	0
2	BB	490/510 (96%)	0.16	25 (5%) 32 18	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.36	25 (5%) 28 16	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.32	36 (8%) 15 8	91, 124, 149, 159	0
4	AD	341/352 (96%)	0.05	8 (2%) 64 49	81, 105, 139, 153	0
4	BD	341/352 (96%)	0.04	12 (3%) 48 32	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.58	9 (10%) 7 4	104, 126, 151, 155	0
5	BE	82/84 (97%)	1.39	26 (31%) 1 0	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.48	6 (17%) 2 1	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.31	4 (11%) 7 4	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.59	13 (20%) 1 1	113, 124, 140, 147	0
7	BH	65/66 (98%)	0.63	8 (12%) 5 3	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.18	3 (8%) 13 7	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.84	8 (22%) 1 1	108, 116, 142, 147	0
9	AJ	38/40 (95%)	0.10	3 (7%) 15 9	109, 122, 157, 159	0
9	BJ	38/40 (95%)	0.57	7 (18%) 2 1	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.02	1 (2%) 58 44	121, 135, 145, 147	0
10	BK	37/37 (100%)	0.18	1 (2%) 58 44	123, 136, 147, 148	0
11	AL	37/37 (100%)	0.29	3 (8%) 15 8	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.54	6 (16%) 3 2	90, 104, 158, 160	0
12	AM	34/36 (94%)	0.29	3 (8%) 12 7	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.07	2 (5%) 26 14	90, 99, 140, 153	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.43	22 (9%) 11 6	83, 116, 148, 160	0
13	BO	243/247 (98%)	0.38	25 (10%) 9 5	85, 117, 147, 160	0
14	AT	32/32 (100%)	0.41	3 (9%) 11 6	92, 106, 158, 160	0
14	BT	32/32 (100%)	0.04	1 (3%) 52 38	93, 106, 158, 160	0
15	AU	97/104 (93%)	0.34	6 (6%) 24 13	93, 105, 116, 125	0
15	BU	97/104 (93%)	0.21	2 (2%) 67 52	94, 106, 116, 127	0
16	AV	137/137 (100%)	0.19	3 (2%) 65 50	96, 112, 128, 132	0
16	BV	137/137 (100%)	0.54	15 (10%) 7 4	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.72	4 (14%) 4 2	141, 154, 160, 160	0
17	By	28/46 (60%)	0.93	7 (25%) 1 1	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.51	7 (18%) 2 1	121, 129, 147, 150	0
18	BX	37/41 (90%)	0.53	6 (16%) 3 2	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.78	11 (17%) 2 1	134, 148, 160, 160	0
20	BZ	62/62 (100%)	1.61	21 (33%) 0 0	135, 150, 160, 160	0
All	All	5224/5494 (95%)	0.28	384 (7%) 17 10	81, 113, 149, 160	0

The worst 5 of 384 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BZ	5062	VAL	10.1
20	BZ	5061	VAL	8.2
13	BO	5084	ASN	7.8
7	BH	5066	GLY	7.0
20	BZ	5001	MET	7.0

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
28	DGD	AE	101	63/66	0.35	0.72	13.63	146,160,160,160	0
27	BCR	AJ	101	40/40	0.53	0.65	13.18	158,160,160,160	0
27	BCR	BJ	5101	40/40	0.64	0.51	7.31	160,160,160,160	0
31	LMG	BA	5402	42/55	0.61	0.50	7.22	144,157,160,160	0
31	LMG	AD	407	49/55	0.77	0.48	7.10	126,133,143,145	0
28	DGD	BB	5602	52/66	0.46	0.55	6.46	152,160,160,160	0
33	DMS	AV	202	4/4	0.83	0.66	6.16	148,148,148,149	0
33	DMS	BV	5203	4/4	0.92	0.69	5.97	160,160,160,160	0
28	DGD	BC	5518	62/66	0.69	0.50	5.90	147,156,160,160	0
32	LMT	AB	629	35/35	0.67	0.48	5.03	133,160,160,160	0
28	DGD	AC	518	62/66	0.76	0.41	5.03	146,155,160,160	0
31	LMG	BD	5410	48/55	0.65	0.58	5.01	126,131,141,141	0
32	LMT	BB	5603	35/35	0.64	0.46	4.94	132,160,160,160	0
31	LMG	AA	417	42/55	0.68	0.45	4.72	145,157,160,160	0
33	DMS	BB	5628	4/4	0.86	0.60	4.64	156,157,157,157	0
29	LHG	BA	5415	37/49	0.45	0.63	4.63	151,160,160,160	0
27	BCR	AT	101	40/40	0.83	0.40	4.43	126,140,146,147	0
31	LMG	AB	620	51/55	0.72	0.50	4.29	125,139,150,151	0
28	DGD	AB	628	52/66	0.53	0.60	4.14	154,160,160,160	0
31	LMG	AB	621	49/55	0.67	0.45	4.09	145,150,157,160	0
31	LMG	BB	5624	49/55	0.74	0.41	4.06	145,150,157,160	0
27	BCR	BT	5101	40/40	0.77	0.40	4.03	124,143,147,147	0
28	DGD	BE	5102	63/66	0.42	0.70	4.01	145,160,160,160	0
31	LMG	AD	408	48/55	0.75	0.48	3.98	121,130,139,139	0
31	LMG	BC	5520	48/55	0.55	0.56	3.87	138,159,160,160	0
31	LMG	BD	5408	46/55	0.68	0.49	3.72	139,145,160,160	0
31	LMG	BL	5101	51/55	0.79	0.48	3.63	122,138,151,152	0
27	BCR	BB	5622	40/40	0.92	0.36	3.63	110,117,120,121	0
33	DMS	BB	5629	4/4	0.93	0.29	3.55	125,126,127,127	0
23	CL	BA	5404[A]	1/1	0.72	0.33	3.54	29,29,29,29	1
33	DMS	AB	625	4/4	0.89	0.45	3.51	156,157,157,157	0
31	LMG	AJ	102	46/55	0.72	0.44	3.36	139,144,160,160	0
28	DGD	BC	5519	66/66	0.79	0.37	3.31	112,121,158,159	0
27	BCR	BD	5407	40/40	0.88	0.31	3.30	112,127,132,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	LMG	AC	520	48/55	0.57	0.59	3.27	136,157,160,160	0
24	CLA	BB	5617	65/65	0.91	0.33	3.24	98,102,138,141	0
32	LMT	BI	5102	35/35	0.62	0.85	3.17	151,160,160,160	0
24	CLA	BC	5504	65/65	0.88	0.34	3.14	132,135,160,160	0
28	DGD	AC	519	66/66	0.84	0.36	3.13	110,120,157,158	0
24	CLA	AB	608	65/65	0.88	0.41	3.13	123,127,135,140	0
32	LMT	BB	5604	35/35	0.70	0.53	3.12	131,160,160,160	0
32	LMT	AB	624	35/35	0.69	0.62	3.11	156,160,160,160	0
27	BCR	AK	102	40/40	0.80	0.39	3.06	133,139,151,152	0
31	LMG	AA	414	44/55	0.61	0.46	3.05	140,160,160,160	0
28	DGD	BH	5101	58/66	0.82	0.39	3.01	107,118,156,160	0
28	DGD	BA	5412	56/66	0.50	0.61	2.97	150,160,160,160	0
24	CLA	BB	5609	65/65	0.91	0.34	2.95	103,110,124,124	0
24	CLA	AB	601	65/65	0.70	0.56	2.95	146,159,160,160	0
31	LMG	BD	5409	49/55	0.79	0.42	2.93	128,133,144,146	0
24	CLA	AA	406	65/65	0.86	0.35	2.93	105,112,138,139	0
28	DGD	AC	517	53/66	0.81	0.40	2.92	121,128,135,140	0
30	SQD	BB	5625	43/54	0.57	0.48	2.89	132,148,160,160	0
28	DGD	AA	411	56/66	0.54	0.55	2.83	148,158,160,160	0
32	LMT	AM	102	35/35	0.79	0.42	2.81	126,149,154,154	0
24	CLA	AA	407	65/65	0.91	0.34	2.80	93,101,150,151	0
24	CLA	AD	404	65/65	0.87	0.36	2.70	126,130,148,149	0
24	CLA	AC	505	65/65	0.87	0.41	2.67	121,146,150,151	0
24	CLA	BB	5612	65/65	0.91	0.40	2.65	122,127,136,139	0
24	CLA	AC	504	65/65	0.89	0.34	2.60	129,134,160,160	0
32	LMT	BB	5627	35/35	0.74	0.45	2.53	156,160,160,160	0
30	SQD	BA	5401	54/54	0.64	0.47	2.53	136,160,160,160	0
35	PL9	AD	405	55/55	0.90	0.36	2.53	99,109,113,113	0
24	CLA	AC	503	65/65	0.88	0.49	2.50	137,144,147,152	0
24	CLA	AB	605	65/65	0.89	0.29	2.36	105,113,122,124	0
27	BCR	BB	5621	40/40	0.88	0.32	2.34	112,120,124,125	0
32	LMT	AI	103	35/35	0.71	0.49	2.28	156,158,160,160	0
24	CLA	AC	508	65/65	0.89	0.36	2.28	140,144,157,158	0
27	BCR	AX	101	40/40	0.60	0.50	2.24	135,143,158,159	0
27	BCR	AC	515	40/40	0.71	0.45	2.24	149,152,155,155	0
32	LMT	BM	5101	35/35	0.73	0.38	2.20	126,149,154,155	0
32	LMT	AB	630	35/35	0.73	0.50	2.19	132,160,160,160	0
24	CLA	BB	5605	65/65	0.71	0.59	2.13	146,159,160,160	0
24	CLA	AC	502	65/65	0.91	0.36	2.12	103,109,142,143	0
32	LMT	AI	102	35/35	0.70	0.60	2.07	149,158,160,160	0
27	BCR	BX	5101	40/40	0.61	0.50	2.06	136,143,157,158	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	BCR	AB	617	40/40	0.86	0.31	2.05	112,121,125,125	0
31	LMG	BE	5101	44/55	0.65	0.46	2.02	140,160,160,160	0
32	LMT	BC	5522	35/35	0.75	0.67	2.00	157,160,160,160	0
24	CLA	BA	5408	65/65	0.89	0.31	1.99	95,103,150,150	0
24	CLA	BB	5608	65/65	0.94	0.32	1.96	96,103,124,125	0
27	BCR	AC	516	40/40	0.69	0.48	1.94	135,138,143,143	0
24	CLA	BB	5614	65/65	0.89	0.33	1.93	117,123,124,128	0
24	CLA	AB	609	65/65	0.70	0.41	1.92	126,136,141,143	0
33	DMS	AU	201	4/4	0.75	0.40	1.89	160,160,160,160	0
28	DGD	AH	101	58/66	0.86	0.31	1.87	108,120,155,157	0
24	CLA	AC	507	65/65	0.88	0.38	1.86	137,149,152,153	0
24	CLA	BC	5502	65/65	0.89	0.33	1.85	108,111,143,144	0
24	CLA	AC	501	65/65	0.88	0.38	1.84	133,136,139,143	0
24	CLA	BD	5405	65/65	0.84	0.34	1.79	125,131,148,149	0
30	SQD	AB	622	43/54	0.62	0.43	1.78	133,149,160,160	0
24	CLA	AB	610	65/65	0.90	0.34	1.78	117,121,123,127	0
24	CLA	BB	5616	65/65	0.91	0.31	1.77	108,110,120,122	0
24	CLA	BB	5611	65/65	0.90	0.28	1.77	95,102,132,136	0
24	CLA	AB	611	65/65	0.94	0.30	1.73	99,113,116,122	0
34	PHO	BD	5403	64/64	0.88	0.34	1.72	102,109,118,118	0
27	BCR	BC	5514	40/40	0.80	0.41	1.72	123,126,129,129	0
27	BCR	AD	406	40/40	0.87	0.32	1.72	110,126,131,131	0
34	PHO	AD	403	64/64	0.93	0.28	1.72	119,123,128,129	0
31	LMG	AC	521	45/55	0.41	0.62	1.70	154,160,160,160	0
24	CLA	BC	5508	65/65	0.83	0.34	1.69	142,146,157,159	0
35	PL9	BD	5406	55/55	0.85	0.35	1.68	103,110,115,116	0
24	CLA	BA	5406	65/65	0.89	0.28	1.65	89,94,108,112	0
24	CLA	AD	401	65/65	0.92	0.28	1.63	93,100,115,119	0
33	DMS	AB	626	4/4	0.89	0.26	1.63	129,130,130,130	0
23	CL	BA	5404[B]	1/1	0.72	0.33	1.61	115,115,115,115	1
24	CLA	AB	603	65/65	0.88	0.38	1.59	107,109,119,121	0
30	SQD	BF	5102	45/54	0.67	0.56	1.56	154,160,160,160	0
24	CLA	AB	607	65/65	0.91	0.27	1.53	94,100,132,135	0
34	PHO	AD	402	64/64	0.92	0.31	1.52	99,109,116,117	0
27	BCR	BK	5102	40/40	0.79	0.37	1.52	136,140,152,152	0
27	BCR	BB	5623	40/40	0.82	0.37	1.47	111,116,131,131	0
24	CLA	BA	5407	65/65	0.87	0.30	1.47	110,114,138,139	0
27	BCR	AB	618	40/40	0.86	0.28	1.45	109,117,122,122	0
24	CLA	AC	509	65/65	0.88	0.39	1.42	115,128,135,137	0
24	CLA	AB	606	65/65	0.82	0.33	1.36	120,133,140,141	0
24	CLA	BC	5510	65/65	0.91	0.33	1.36	113,116,130,131	0
27	BCR	BC	5515	40/40	0.70	0.43	1.35	150,152,155,156	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	SQD	AF	102	45/54	0.73	0.46	1.34	154,160,160,160	0
24	CLA	AB	602	65/65	0.85	0.34	1.32	124,127,129,132	0
24	CLA	BC	5503	65/65	0.83	0.36	1.31	137,147,148,152	0
23	CL	AA	403[A]	1/1	0.87	0.32	1.30	33,33,33,33	1
23	CL	AA	403[B]	1/1	0.87	0.32	1.29	108,108,108,108	1
33	DMS	BV	5202	4/4	0.91	0.29	1.29	148,149,149,150	0
24	CLA	BC	5507	65/65	0.83	0.36	1.23	136,150,153,154	0
31	LMG	AM	101	42/55	0.66	0.53	1.21	136,158,160,160	0
29	LHG	AA	415	37/49	0.75	0.36	1.20	149,160,160,160	0
24	CLA	BB	5615	65/65	0.92	0.26	1.19	101,113,117,120	0
24	CLA	BC	5505	65/65	0.81	0.36	1.17	123,148,152,153	0
30	SQD	AA	416	54/54	0.75	0.33	1.16	136,160,160,160	0
24	CLA	BB	5613	65/65	0.73	0.39	1.16	127,135,140,142	0
24	CLA	AB	613	65/65	0.92	0.27	1.16	99,102,136,140	0
24	CLA	AB	614	65/65	0.83	0.38	1.14	129,133,160,160	0
32	LMT	AD	409	31/35	0.71	0.43	1.12	139,154,160,160	0
24	CLA	AB	604	65/65	0.93	0.30	1.12	96,104,125,127	0
24	CLA	AC	512	65/65	0.79	0.45	1.12	154,158,160,160	0
24	CLA	BB	5607	65/65	0.89	0.29	1.08	108,111,120,123	0
24	CLA	AB	612	65/65	0.93	0.29	1.06	107,111,120,121	0
24	CLA	AB	615	65/65	0.88	0.32	1.05	134,139,155,157	0
24	CLA	AB	616	65/65	0.85	0.41	1.04	143,147,160,160	0
24	CLA	BA	5405	65/65	0.86	0.31	1.03	90,101,105,109	0
32	LMT	BD	5411	31/35	0.66	0.51	0.99	140,152,160,160	0
27	BCR	BC	5516	40/40	0.63	0.48	0.98	136,140,145,145	0
24	CLA	AC	506	65/65	0.73	0.39	0.97	136,143,160,160	0
24	CLA	BC	5513	65/65	0.71	0.51	0.95	158,160,160,160	0
27	BCR	AC	514	40/40	0.88	0.34	0.93	120,123,127,128	0
24	CLA	BB	5619	65/65	0.90	0.35	0.92	135,137,155,157	0
31	LMG	BM	5102	42/55	0.72	0.47	0.88	136,160,160,160	0
30	SQD	AB	627	47/54	0.77	0.36	0.85	138,157,160,160	0
24	CLA	AA	404	65/65	0.91	0.27	0.83	89,99,106,108	0
27	BCR	BA	5411	40/40	0.90	0.29	0.83	94,122,132,132	0
28	DGD	BC	5517	53/66	0.86	0.28	0.82	124,130,136,139	0
24	CLA	AA	405	65/65	0.94	0.27	0.81	88,93,108,111	0
36	HEM	AF	101	43/43	0.94	0.40	0.80	148,152,159,160	0
24	CLA	BB	5606	65/65	0.84	0.31	0.79	124,127,130,131	0
24	CLA	BC	5511	65/65	0.80	0.42	0.79	154,158,159,160	0
34	PHO	BD	5404	64/64	0.90	0.28	0.78	123,125,129,130	0
24	CLA	AC	510	65/65	0.92	0.33	0.75	110,113,129,130	0
27	BCR	AB	619	40/40	0.84	0.30	0.75	111,117,131,131	0
24	CLA	BD	5402	65/65	0.90	0.27	0.72	97,101,117,119	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
29	LHG	AA	412	39/49	0.89	0.29	0.71	110,118,128,132	0
24	CLA	BC	5506	65/65	0.74	0.40	0.70	136,143,160,160	0
24	CLA	BC	5509	65/65	0.89	0.30	0.66	116,128,138,138	0
30	SQD	BA	5414	51/54	0.72	0.37	0.65	145,150,160,160	0
24	CLA	BC	5501	65/65	0.89	0.31	0.65	134,137,141,144	0
30	SQD	BB	5601	47/54	0.73	0.38	0.65	137,156,160,160	0
31	LMG	BC	5521	45/55	0.62	0.56	0.64	154,160,160,160	0
24	CLA	AC	513	65/65	0.72	0.44	0.60	158,160,160,160	0
30	SQD	AA	413	51/54	0.84	0.32	0.58	143,150,160,160	0
27	BCR	AA	410	40/40	0.91	0.27	0.52	91,122,130,130	0
24	CLA	BB	5610	65/65	0.82	0.31	0.47	121,132,140,141	0
24	CLA	BC	5512	65/65	0.81	0.36	0.47	157,160,160,160	0
24	CLA	BB	5618	65/65	0.87	0.32	0.46	128,133,160,160	0
29	LHG	BA	5413	39/49	0.87	0.28	0.42	113,122,128,129	0
36	HEM	BV	5201	43/43	0.92	0.28	0.38	97,102,106,109	0
36	HEM	AV	201	43/43	0.96	0.27	0.36	94,100,102,103	0
25	MST	AA	408	16/16	0.93	0.26	0.31	123,126,129,130	0
26	OEC	AA	409	5/9	0.95	0.28	0.29	82,83,90,110	0
36	HEM	BF	5101	43/43	0.91	0.46	0.22	148,152,160,160	0
24	CLA	AC	511	65/65	0.87	0.33	0.13	152,155,157,158	0
25	MST	BA	5409	16/16	0.92	0.23	0.08	124,129,131,132	0
24	CLA	BB	5620	65/65	0.83	0.30	-0.04	143,147,160,160	0
26	OEC	BA	5410	5/9	0.73	0.22	-0.53	23,88,99,134	0
22	BCT	AA	402	4/4	0.99	0.20	-0.79	135,136,137,137	0
21	FE2	AA	401	1/1	0.98	0.18	-0.91	115,115,115,115	0
22	BCT	BA	5403	4/4	0.97	0.16	-1.22	135,136,136,137	0
21	FE2	BD	5401	1/1	0.94	0.12	-2.42	119,119,119,119	0
32	LMT	AB	623	35/35	0.53	0.74	-	135,160,160,160	0
31	LMG	AI	101	43/55	0.35	0.80	-	159,160,160,160	0
32	LMT	BB	5626	35/35	0.38	0.63	-	131,160,160,160	0
37	CA	AK	101	1/1	0.84	0.12	-	146,146,146,146	0
37	CA	BO	5301	1/1	0.65	0.30	-	160,160,160,160	0
31	LMG	BI	5101	43/55	0.55	0.70	-	160,160,160,160	0
37	CA	BF	5103	1/1	0.14	0.16	-	146,146,146,146	0
37	CA	AO	301	1/1	0.50	0.21	-	152,152,152,152	0
37	CA	AF	103	1/1	0.36	0.23	-	150,150,150,150	0
37	CA	BK	5101	1/1	0.62	0.22	-	145,145,145,145	0

6.5 Other polymers ⓘ

There are no such residues in this entry.