



wwPDB X-ray Structure Validation Summary Report

Jun 17, 2014 – 05:46 AM BST

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 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/ValidationPDFNotes.html>

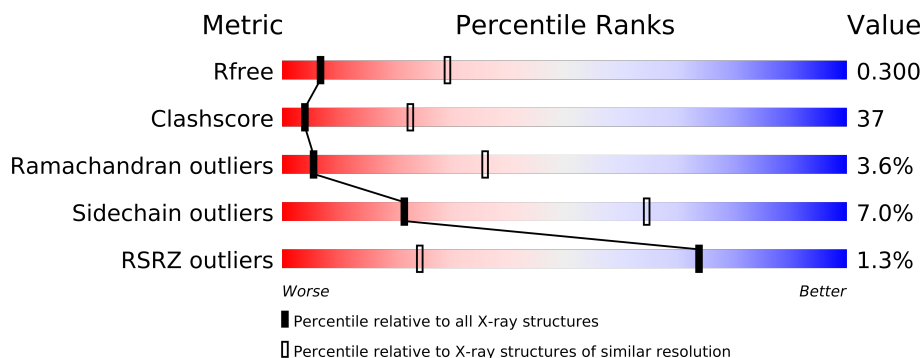
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	344	
1	BA	344	
2	AB	510	
2	BB	510	
3	AC	461	
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	

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Mol	Chain	Length	Quality of chain
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	
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
24	CLA	AA	406	-	X
24	CLA	AA	407	-	X
24	CLA	AB	601	-	X
24	CLA	AB	605	-	X
24	CLA	AB	608	-	X
24	CLA	AB	615	-	X
24	CLA	AB	616	-	X
24	CLA	AC	504	-	X
24	CLA	AD	404	-	X
24	CLA	BA	5408	-	X
24	CLA	BB	5605	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
24	CLA	BB	5609	-	X
24	CLA	BB	5612	-	X
24	CLA	BC	5504	-	X
24	CLA	BC	5513	-	X
24	CLA	BD	5405	-	X
27	BCR	AB	617	-	X
27	BCR	AC	515	-	X
27	BCR	AC	516	-	X
27	BCR	AD	406	-	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	5623	-	X
27	BCR	BC	5515	-	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
28	DGD	AC	519	-	X
28	DGD	AE	101	-	X
28	DGD	BA	5412	-	X
28	DGD	BB	5602	-	X
28	DGD	BC	5518	-	X
28	DGD	BC	5519	-	X
28	DGD	BE	5102	-	X
29	LHG	BA	5415	-	X
30	SQD	AB	622	-	X
30	SQD	AF	102	-	X
30	SQD	BA	5401	-	X
30	SQD	BB	5625	-	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

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Mol	Type	Chain	Res	Geometry	Electron density
31	LMG	AD	407	-	X
31	LMG	AD	408	-	X
31	LMG	AI	101	-	X
31	LMG	AJ	102	-	X
31	LMG	BA	5402	-	X
31	LMG	BB	5624	-	X
31	LMG	BC	5520	-	X
31	LMG	BD	5408	-	X
31	LMG	BD	5410	-	X
31	LMG	BE	5101	-	X
31	LMG	BI	5101	-	X
31	LMG	BL	5101	-	X
32	LMT	AB	623	-	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	5626	-	X
32	LMT	BB	5627	-	X
32	LMT	BC	5522	-	X
32	LMT	BI	5102	-	X
32	LMT	BM	5101	-	X
33	DMS	AB	625	-	X
33	DMS	AB	626	-	X
33	DMS	AV	202	-	X
33	DMS	BB	5628	-	X
33	DMS	BV	5203	-	X
35	PL9	AD	405	-	X
37	CA	BO	5301	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 50266 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

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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				

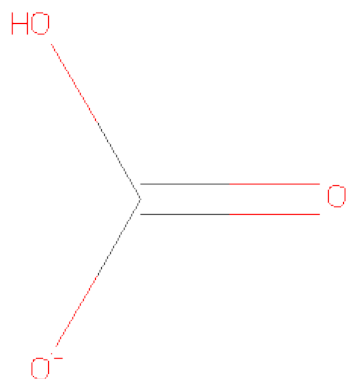
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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).

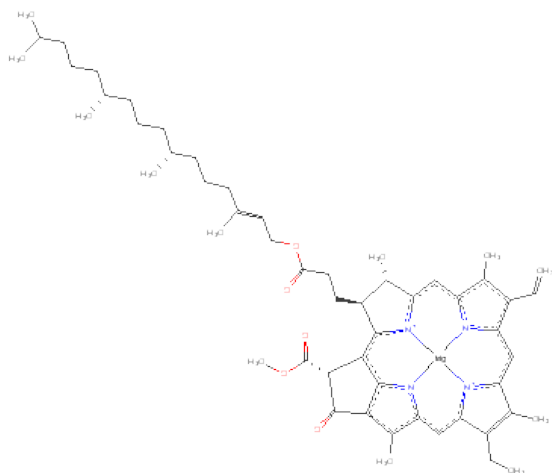


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	AA	1	Total	C	O	0	0
			4	1	3		
22	BA	1	Total	C	O	0	0
			4	1	3		

- 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: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

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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

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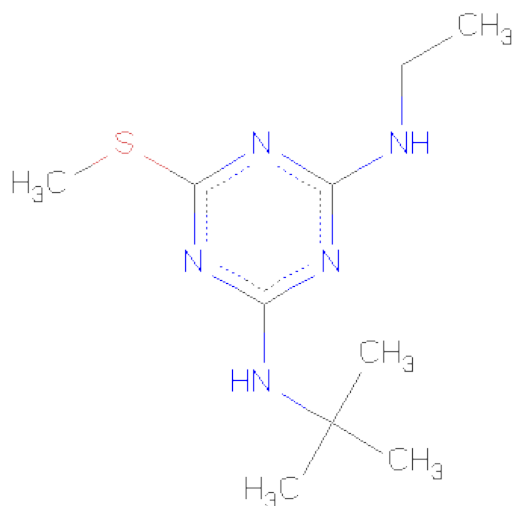
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BB	1	Total 65	C 55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

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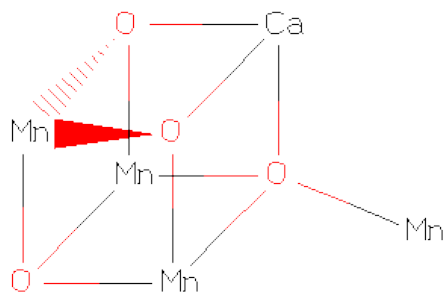
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	BC	1	Total 65	C 55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



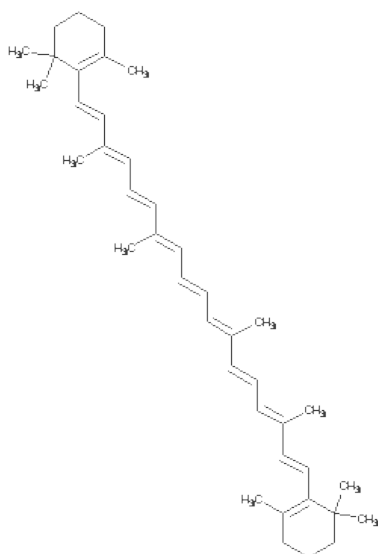
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

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



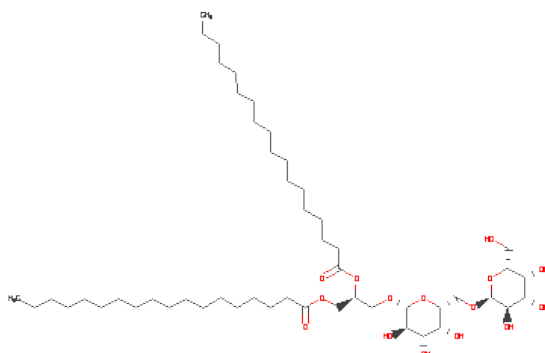
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0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

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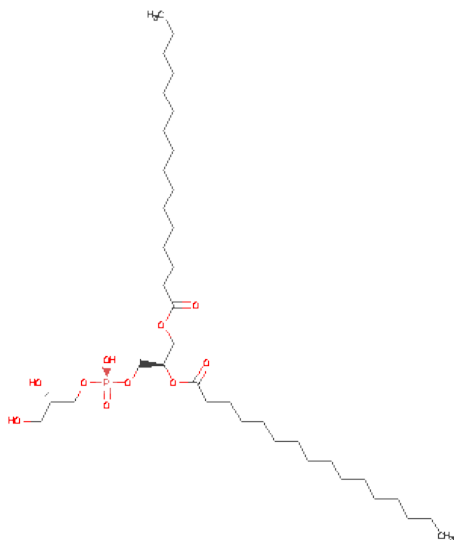
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0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

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



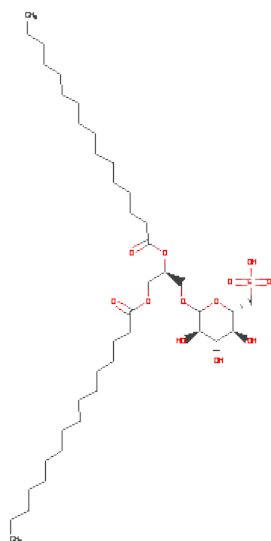
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	AA	1	Total	C	O	0	0
			56	41	15		
28	AB	1	Total	C	O	0	0
			52	37	15		
28	AC	1	Total	C	O	0	0
			53	38	15		
28	AC	1	Total	C	O	0	0
			62	47	15		
28	AC	1	Total	C	O	0	0
			66	51	15		
28	AE	1	Total	C	O	0	0
			63	48	15		
28	AH	1	Total	C	O	0	0
			58	43	15		
28	BA	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: $C_{38}H_{75}O_{10}P$).



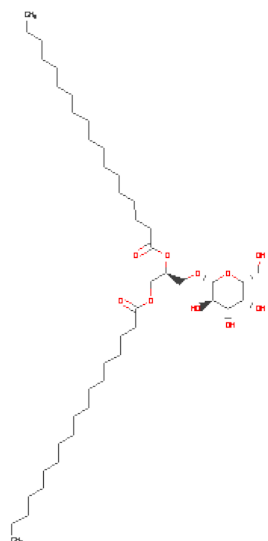
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-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).



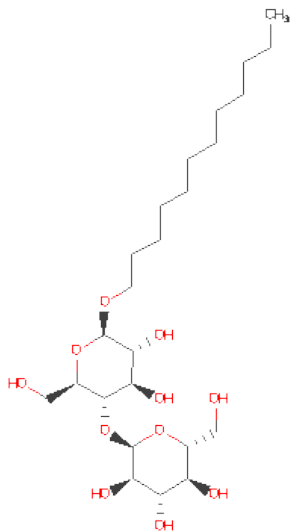
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

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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-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



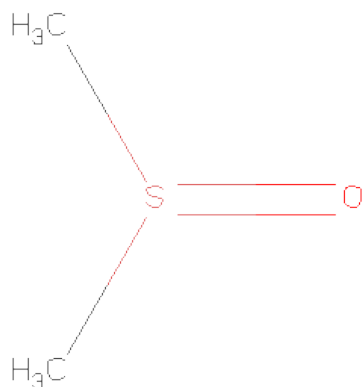
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM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

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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).



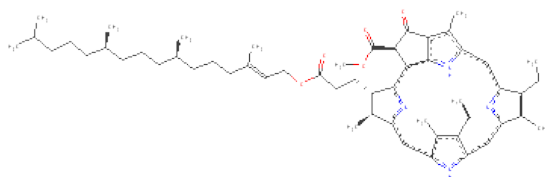
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AB	1	Total	C	O	S	0	0
			4	2	1	1		
33	AU	1	Total	C	O	S	0	0
			4	2	1	1		
33	AV	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BB	1	Total	C	O	S	0	0
			4	2	1	1		
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

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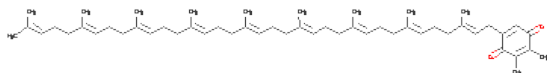
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	BV	1	Total	C	O	S	0	0
			4	2	1	1		

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



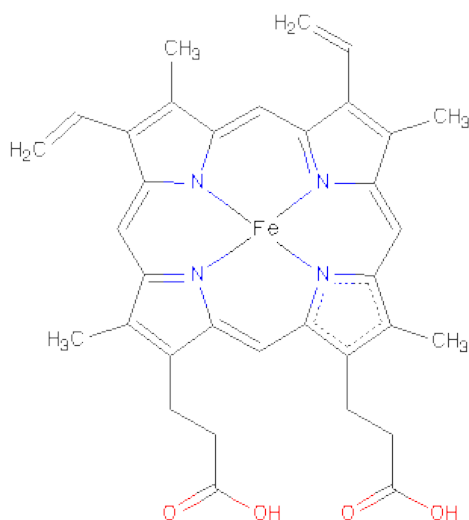
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	AD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		
34	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- 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		

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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

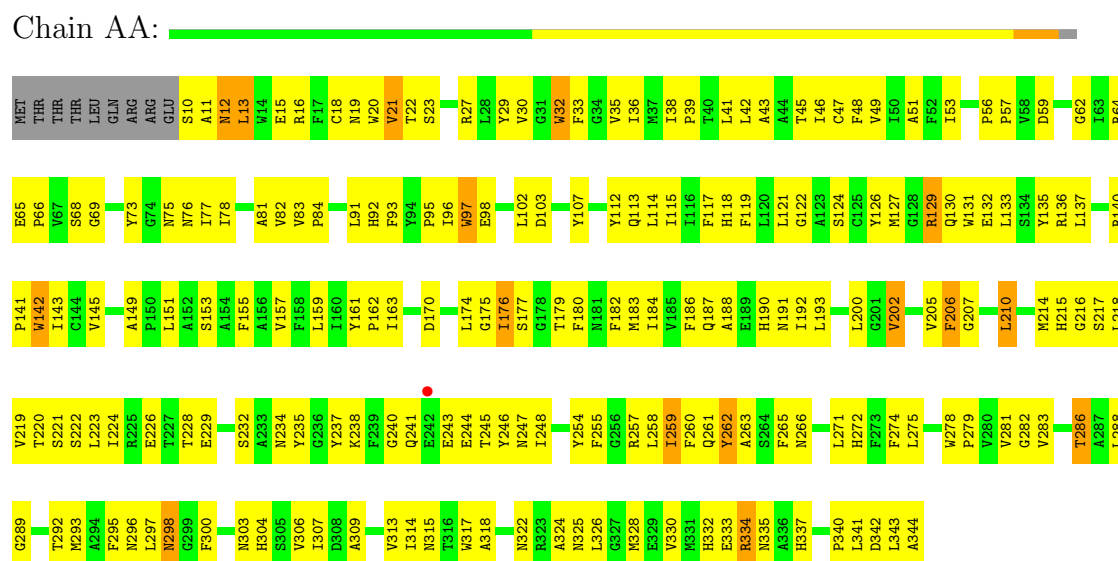
- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

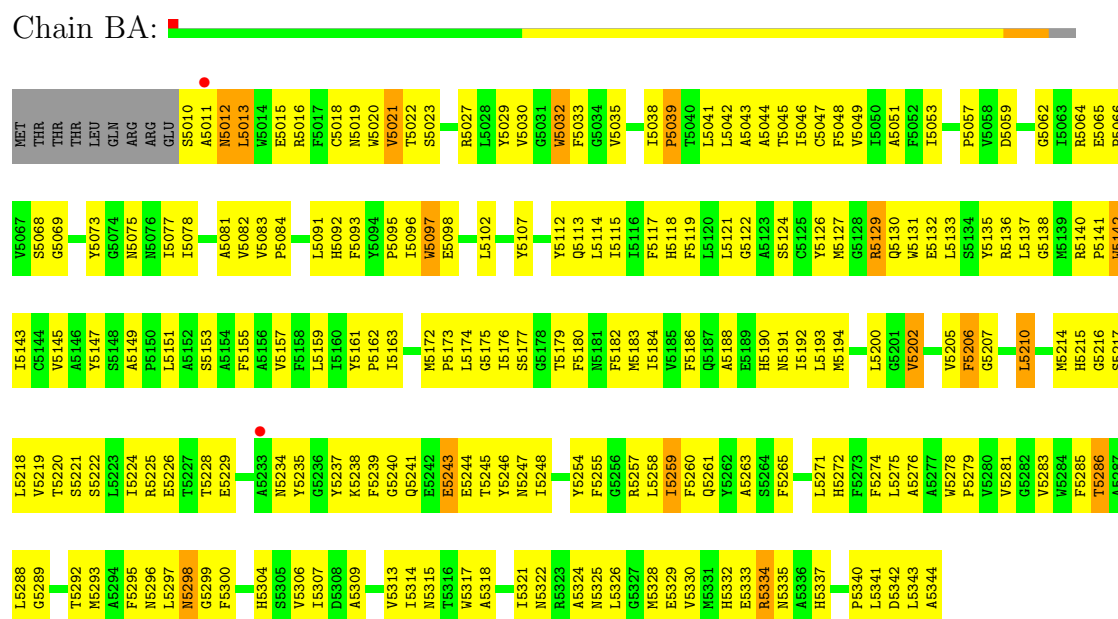
3 Residue-property plots

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

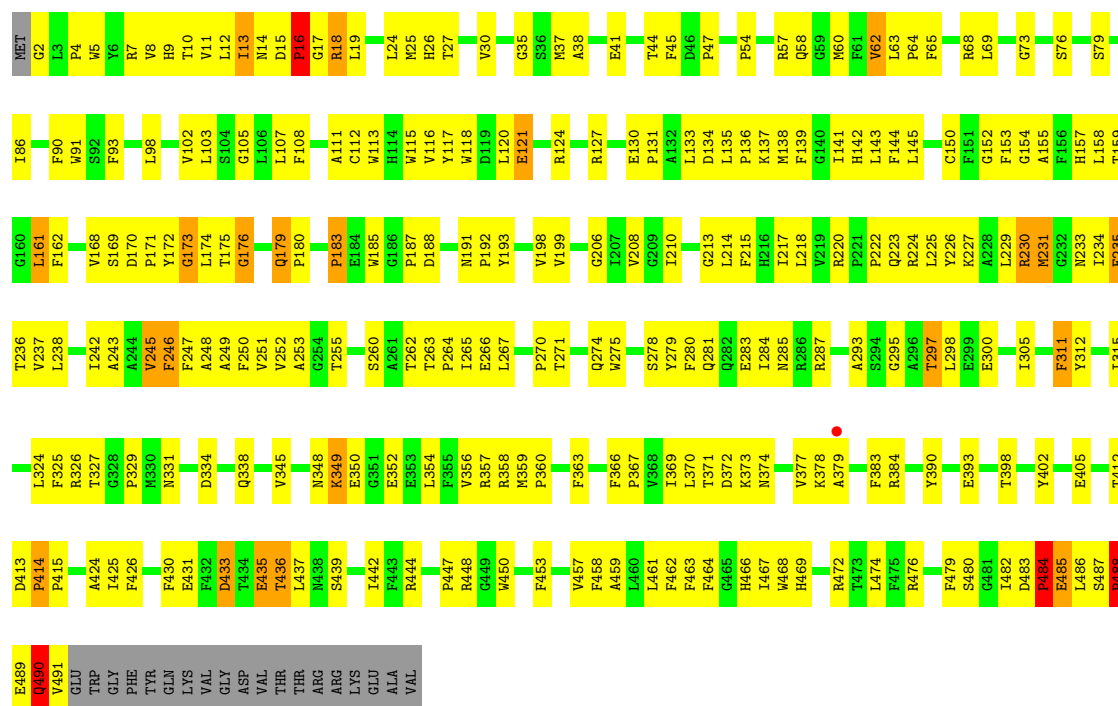


• Molecule 1: Photosystem Q(B) protein 1



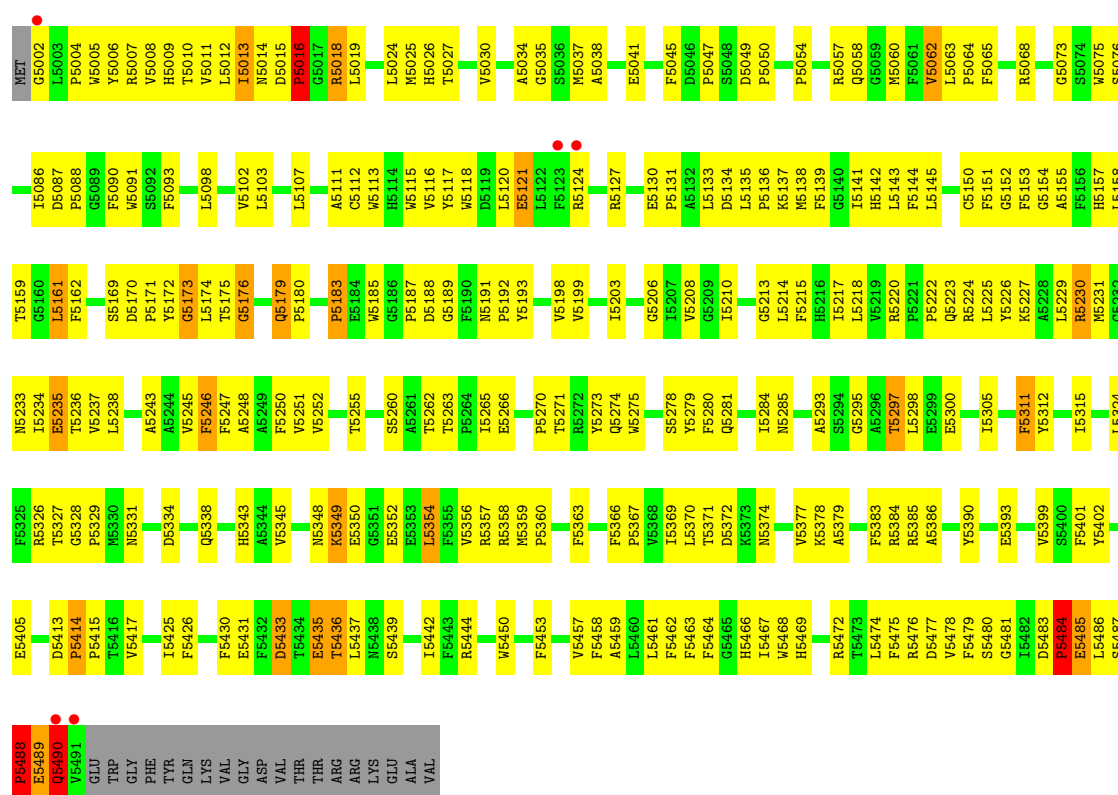
• Molecule 2: Photosystem II core light harvesting protein

Chain AB:



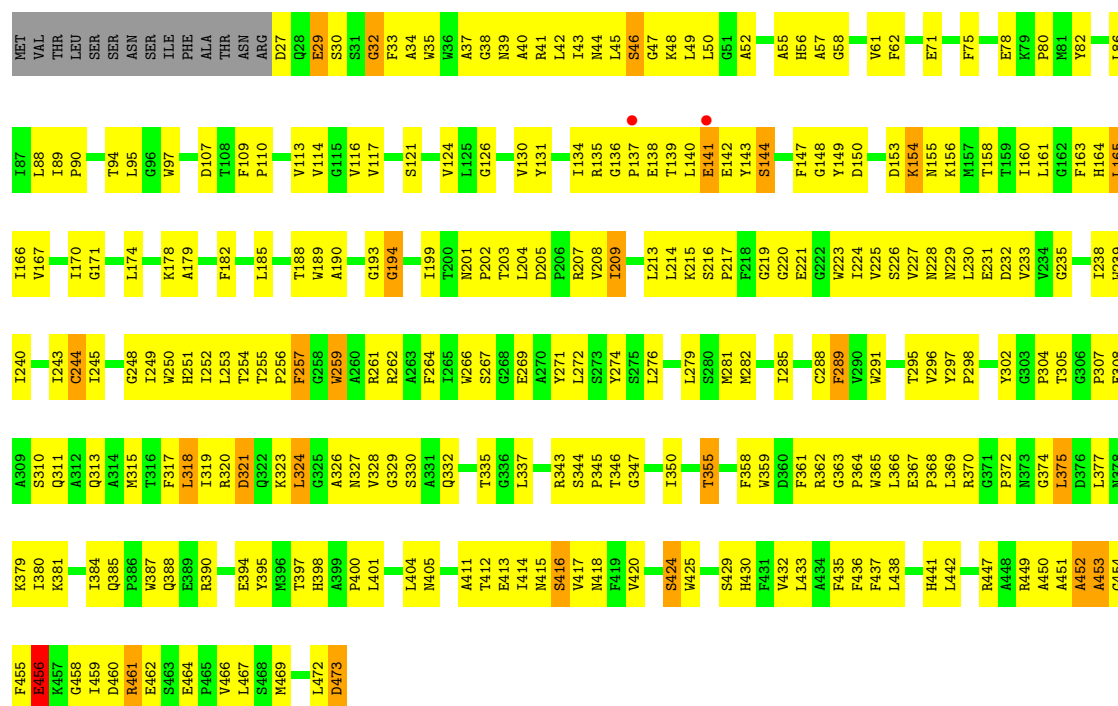
• Molecule 2: Photosystem II core light harvesting protein

Chain BB:



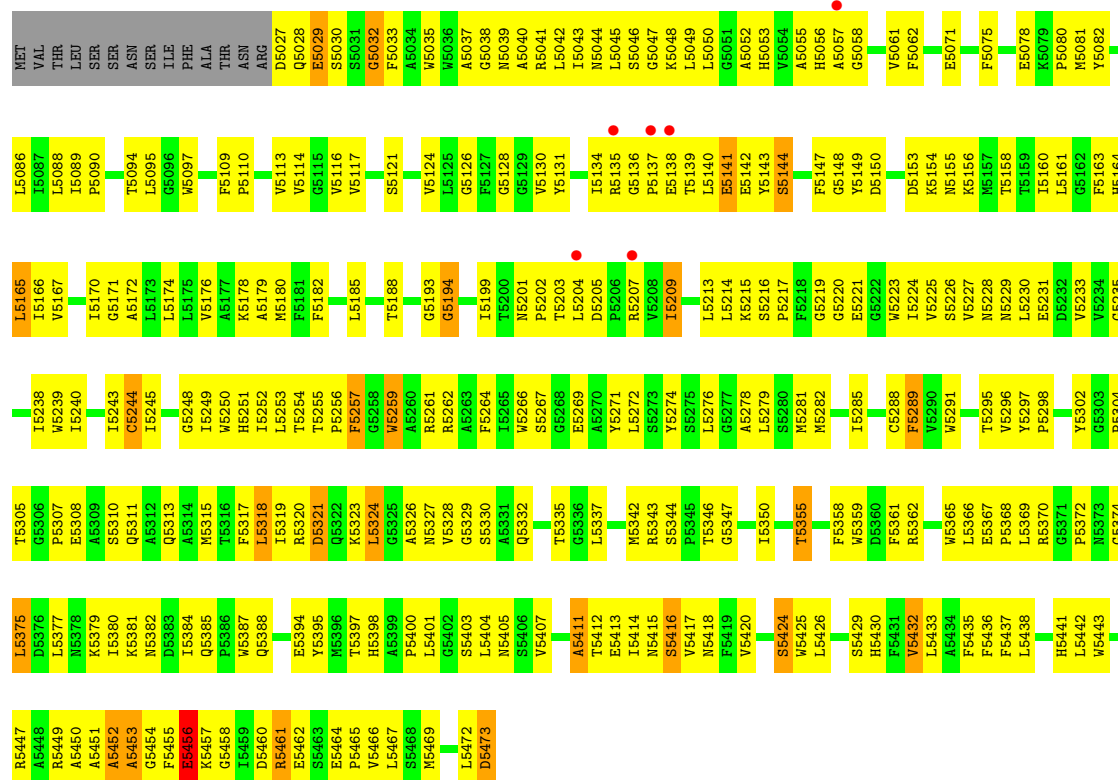
• Molecule 3: Photosystem II CP43 protein

Chain AC:



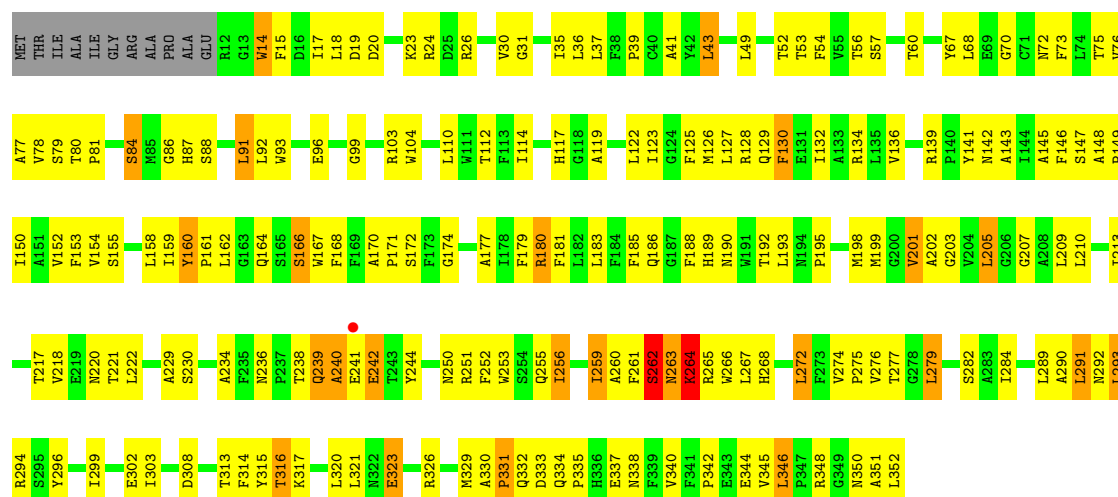
- Molecule 3: Photosystem II CP43 protein

Chain BC:



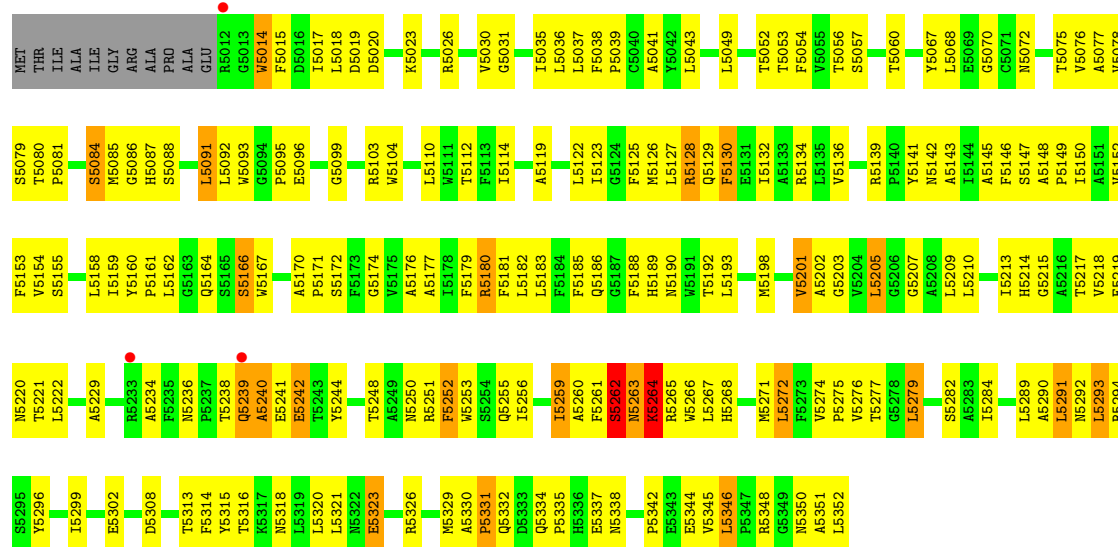
- Molecule 4: Photosystem II D2 protein

Chain AD:



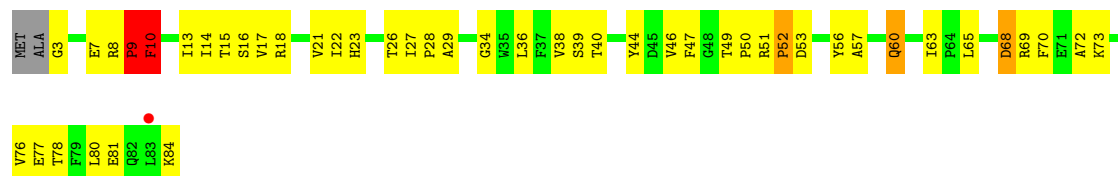
- Molecule 4: Photosystem II D2 protein

Chain BD:



- Molecule 5: Cytochrome b559 subunit alpha

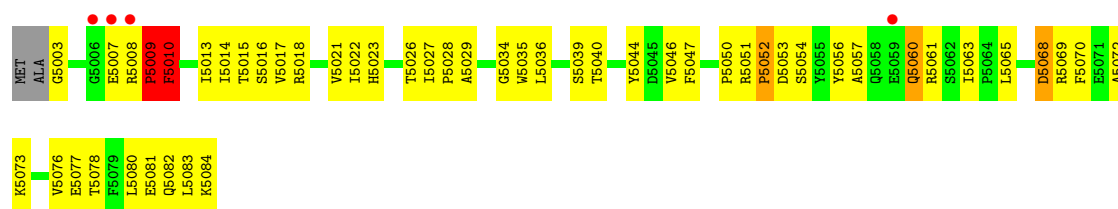
Chain AE:



- Molecule 5: Cytochrome b559 subunit alpha

Chain BE:





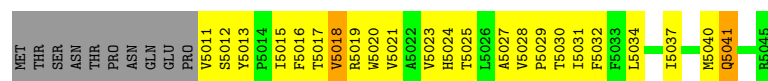
- Molecule 6: Cytochrome b559 subunit beta

Chain AF:



- Molecule 6: Cytochrome b559 subunit beta

Chain BF:



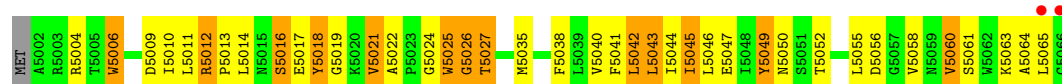
- Molecule 7: Photosystem II reaction center protein H

Chain AH:



- Molecule 7: Photosystem II reaction center protein H

Chain BH:



- Molecule 8: Photosystem II reaction center protein I

Chain AI:



- Molecule 8: Photosystem II reaction center protein I

Chain BI:



- Molecule 9: Photosystem II reaction center protein J

Chain AJ:



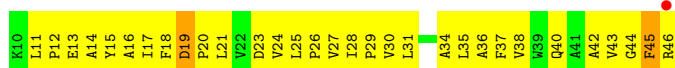
- Molecule 9: Photosystem II reaction center protein J

Chain BJ:



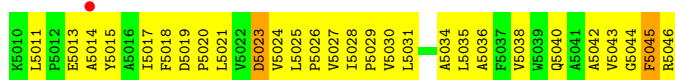
- Molecule 10: Photosystem II reaction center protein K

Chain AK:



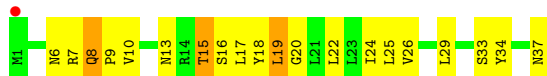
- Molecule 10: Photosystem II reaction center protein K

Chain BK:



- Molecule 11: Photosystem II reaction center protein L

Chain AL:



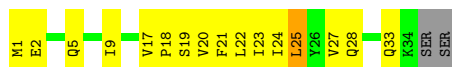
- Molecule 11: Photosystem II reaction center protein L

Chain BL:



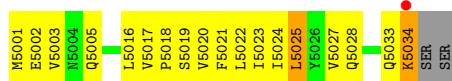
- Molecule 12: Photosystem II reaction center protein M

Chain AM:



- Molecule 12: Photosystem II reaction center protein M

Chain BM:



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Y266	P271	A272	G170	E171	N173	R178	T179	A180	N181	F182	L183	D184	P185	K186	G187	R188	G189	L190	A191	S192	G193	Y194	Q202	E206	E207	R210	K214	R215	L218	T219	K220	G221	Q222	I223	S224	L225	V230	D231	G232	R233	T234	G235	E236	T240	G252	V259	K260	G263	V264	T265	T98	T101	L104	D105	Q106	T107	Q108	G109	M114	S115	D116	G117	S118	L119	T120	F121	V122	E123	E124	D125	G126	I127	D128	F129	Q130	P131	V132	T133	V134	Q135	R141	L144	F145	T146	T147	V148	K149	N150	L151	V152	A153	K154	T155	Q156	P157	N158	V159	T160	S161	S165	T166	D167	F168	V169	A1A	L1A	G1A	T30	L31	T32	Y33	D34	D35	I36	T39	G40	L41	A42	M43	P46	T51	A52	A55	Y56	P57	L58	D59	S60	S61	Y64	R65	I66	L69	C70	L71	Q72	P73	L77	E80	E81	P82	K83	N84	K85	R86	Q87	O88	A89	E90	F91	V92	P93	T94	V07
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|-------|------------------------|------------------------|------------------------|
| V5264 | D5167 | V5097 | ALA |
| F5265 | K5168 | T5098 | ALA |
| Y5266 | K5169 | <div><div></div></div> | LYS |
| P5271 | <div><div></div></div> | T5101 | GLN |
| | G5170 | | T5030 |
| A5272 | F5172 | L5104 | L5031 |
| | N5173 | D5105 | T5032 |
| | | <div><div></div></div> | Y5033 |
| | R5178 | <div><div></div></div> | D5034 |
| | T5179 | T5107 | D5035 |
| | A5180 | <div><div></div></div> | I5036 |
| | N5181 | G5109 | |
| | F5182 | <div><div></div></div> | T5039 |
| | L5183 | K5112 | G5040 |
| | D5184 | N5114 | L5041 |
| | P5185 | S5115 | A5042 |
| | K5186 | D5116 | N5043 |
| | G5187 | G5117 | |
| | R5188 | S5118 | P5046 |
| | G5189 | L5119 | |
| | L5190 | T5120 | T5061 |
| | A5191 | F5121 | A5062 |
| | S5192 | V5122 | |
| | G5193 | E5123 | A5065 |
| | Y5194 | E5124 | Y5066 |
| | | D5125 | |
| | Q5202 | G5126 | D5069 |
| | | T5127 | S5060 |
| | E5206 | D5128 | S5061 |
| | E5207 | F5129 | |
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| | K5214 | V5132 | I5066 |
| | R5215 | T5133 | |
| | | V5134 | L5069 |
| | | Q5135 | G5070 |
| | L5218 | | L5071 |
| | T5219 | <div><div></div></div> | Q5072 |
| | K5220 | R5141 | |
| | Q5221 | L5144 | T5075 |
| | S5223 | | <div><div></div></div> |
| | <div><div></div></div> | T5147 | F5076 |
| | S5224 | V5148 | L5077 |
| | E5225 | K5149 | V5078 |
| | | N5150 | <div><div></div></div> |
| | V5230 | L5151 | E5080 |
| | <div><div></div></div> | <div><div></div></div> | E5081 |
| | T5234 | V5152 | V5082 |
| | G5235 | A5153 | K5083 |
| | E5236 | S5154 | N5084 |
| | | T5155 | K5085 |
| | | <div><div></div></div> | R5086 |
| | | P5157 | Q5087 |
| | T5240 | <div><div></div></div> | E5088 |
| | | V5159 | A5089 |
| | G5252 | T5160 | <div><div></div></div> |
| | V5259 | S5161 | F5091 |
| | K5260 | T5162 | V5092 |
| | | | P5093 |
| | | <div><div></div></div> | T5094 |
| | C5263 | S5166 | |

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|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | I4 | I14 | I15 | I16 | I17 | I18 | I19 | A20 | I21 | F22 | F23 | R24 | E25 | P26 | I29 | T30 | K31 | K32 |
|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

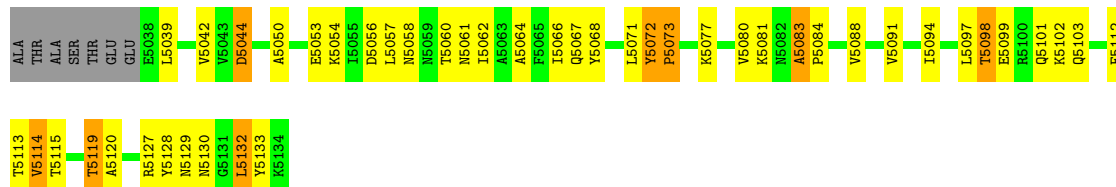
- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|--|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| M5001 | E5002 | T5003 | I5004 | T5005 | Y5006 | | I5014 | A5015 | L5016 | F5017 | F5018 | F5019 | A5020 | I5021 | F5022 | F5023 | R5024 | E5025 | P5026 | P5027 | R5028 | I5029 | T5030 | K5031 | K5032 |
|-------|-------|-------|-------|-------|-------|--|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|
| ALA | THR | ALA | SER | THR | GLU | GLU | E38 | L39 | V42 | V43 | D44 | A50 | Y51 | G52 | E53 | K54 | I55 | D56 | L57 | N58 | N59 | T60 | N61 | I62 | A63 | A64 | F65 | I66 | Q67 | Y68 | L71 | Y72 | P73 | T74 | L75 | V80 | A83 | P84 | V88 | E89 | D90 | V91 | I94 | L97 | T98 | Q101 | K102 | Q103 | F104 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|



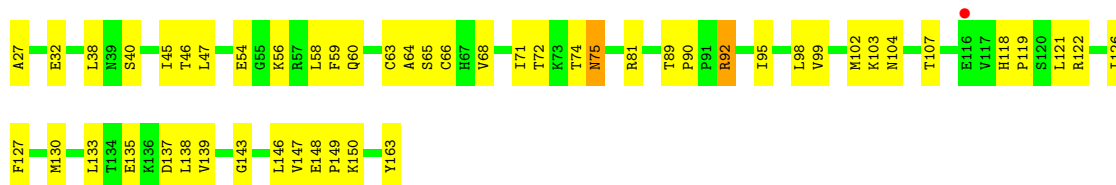
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain BU:



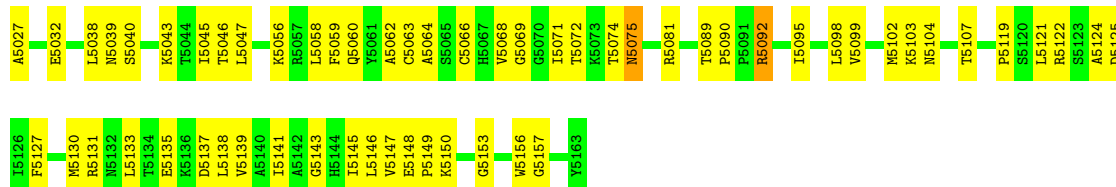
- Molecule 16: Cytochrome c-550

Chain AV:



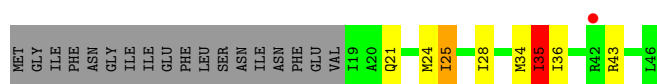
- Molecule 16: Cytochrome c-550

Chain BV:



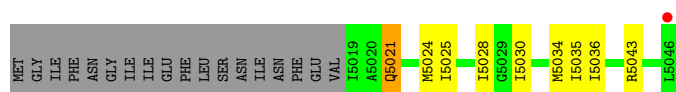
- Molecule 17: Photosystem II reaction center protein ycf12

Chain Ay:



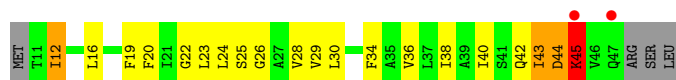
- Molecule 17: Photosystem II reaction center protein ycf12

Chain By:



- Molecule 18: Photosystem II reaction center X protein

Chain AX:



- Molecule 18: Photosystem II reaction center X protein

Chain BX:



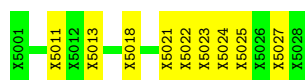
- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain AY:



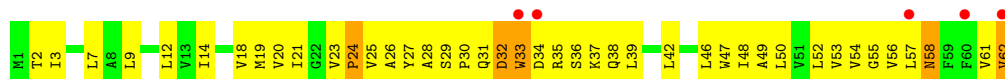
- Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain BY:



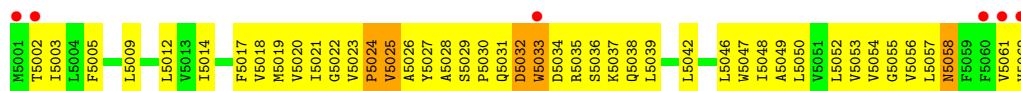
- Molecule 20: Photosystem II reaction center protein Z

Chain AZ:



- Molecule 20: Photosystem II reaction center protein Z

Chain BZ:



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 0.281 , 0.300	Depositor DCC
R_{free} test set	3179 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 , 67.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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.

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

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Mol	Chain	Res	Type	Group
2	BB	5273	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AV	1060	0	1068	48	0
16	BV	1060	0	1068	48	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BT	40	0	56	6	0
27	BX	40	0	56	4	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BI	35	0	46	5	0
32	BM	35	0	46	2	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

The worst 5 of 3700 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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%)	11	55
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	11	55
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	6	38
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	7	41
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	5	36
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	5	34
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	8	46
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	9	51
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	5	34
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	5	34
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	42
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	42
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1	11
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	2	18
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	19
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	19
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	1	9
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	1	9
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	22
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	22
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	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	4	28
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	6	38
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	6	38
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	3	24
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	4	31
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	30	80
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	30	80
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0	1
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	1	4
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	1	4
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	1	4
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	26
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	26
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	5	36

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%)	18	59
1	BA	271/280 (97%)	253 (93%)	18 (7%)	24	67
2	AB	390/407 (96%)	372 (95%)	18 (5%)	37	80
2	BB	390/407 (96%)	374 (96%)	16 (4%)	41	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	347/362 (96%)	326 (94%)	21 (6%)	26	71
3	BC	347/362 (96%)	325 (94%)	22 (6%)	25	69
4	AD	275/283 (97%)	249 (90%)	26 (10%)	12	45
4	BD	275/283 (97%)	249 (90%)	26 (10%)	12	45
5	AE	72/73 (99%)	66 (92%)	6 (8%)	16	55
5	BE	72/73 (99%)	66 (92%)	6 (8%)	16	55
6	AF	29/39 (74%)	27 (93%)	2 (7%)	22	65
6	BF	29/39 (74%)	28 (97%)	1 (3%)	49	86
7	AH	53/55 (96%)	42 (79%)	11 (21%)	2	8
7	BH	53/55 (96%)	43 (81%)	10 (19%)	2	11
8	AI	32/35 (91%)	32 (100%)	0	100	100
8	BI	32/35 (91%)	31 (97%)	1 (3%)	52	88
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	42	83
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	42	83
10	AK	30/30 (100%)	29 (97%)	1 (3%)	50	87
10	BK	30/30 (100%)	29 (97%)	1 (3%)	50	87
11	AL	35/35 (100%)	33 (94%)	2 (6%)	29	74
11	BL	35/35 (100%)	32 (91%)	3 (9%)	15	52
12	AM	31/33 (94%)	30 (97%)	1 (3%)	51	87
12	BM	31/33 (94%)	29 (94%)	2 (6%)	24	68
13	AO	202/208 (97%)	187 (93%)	15 (7%)	20	62
13	BO	202/208 (97%)	187 (93%)	15 (7%)	20	62
14	AT	29/29 (100%)	28 (97%)	1 (3%)	49	86
14	BT	29/29 (100%)	27 (93%)	2 (7%)	22	65
15	AU	84/89 (94%)	76 (90%)	8 (10%)	12	45
15	BU	84/89 (94%)	76 (90%)	8 (10%)	12	45
16	AV	116/117 (99%)	111 (96%)	5 (4%)	40	81
16	BV	116/117 (99%)	110 (95%)	6 (5%)	32	76
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	1	3
17	By	20/37 (54%)	15 (75%)	5 (25%)	1	3
18	AX	30/34 (88%)	29 (97%)	1 (3%)	50	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	BX	30/34 (88%)	29 (97%)	1 (3%)	50 87
20	AZ	52/52 (100%)	49 (94%)	3 (6%)	28 73
20	BZ	52/52 (100%)	48 (92%)	4 (8%)	18 59
All	All	4246/4452 (95%)	3950 (93%)	296 (7%)	21 64

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 chains 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	-	73,73,73	2.53	21 (28%)	96,113,113	1.93	22 (22%)
24	CLA	AA	405	-	73,73,73	2.57	26 (35%)	96,113,113	2.28	31 (32%)
24	CLA	AA	406	-	73,73,73	2.56	22 (30%)	96,113,113	2.16	27 (28%)
24	CLA	AA	407	-	73,73,73	2.57	22 (30%)	96,113,113	2.04	26 (27%)
25	MST	AA	408	-	16,16,16	0.52	0	22,22,22	3.87	8 (36%)
26	OEC	AA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	AA	410	-	41,41,41	1.60	7 (17%)	56,56,56	2.04	21 (37%)
28	DGD	AA	411	-	57,57,67	1.84	15 (26%)	71,71,81	3.79	25 (35%)
29	LHG	AA	412	-	38,38,48	1.95	6 (15%)	44,44,54	1.40	4 (9%)
30	SQD	AA	413	-	51,51,54	7.21	28 (54%)	62,62,65	3.42	23 (37%)
31	LMG	AA	414	-	44,44,55	1.41	3 (6%)	52,52,63	1.68	8 (15%)
29	LHG	AA	415	-	36,36,48	1.72	4 (11%)	42,42,54	1.10	3 (7%)
30	SQD	AA	416	-	54,54,54	2.69	29 (53%)	65,65,65	3.22	22 (33%)
31	LMG	AA	417	-	42,42,55	1.62	7 (16%)	50,50,63	2.41	12 (24%)
24	CLA	AB	601	-	73,73,73	2.93	25 (34%)	96,113,113	1.79	18 (18%)
24	CLA	AB	602	-	73,73,73	2.58	23 (31%)	96,113,113	1.89	22 (22%)
24	CLA	AB	603	-	73,73,73	2.71	21 (28%)	96,113,113	2.23	29 (30%)
24	CLA	AB	604	-	73,73,73	2.59	25 (34%)	96,113,113	1.91	23 (23%)
24	CLA	AB	605	-	73,73,73	2.79	25 (34%)	96,113,113	2.00	27 (28%)
24	CLA	AB	606	-	73,73,73	2.69	24 (32%)	96,113,113	1.97	26 (27%)
24	CLA	AB	607	-	73,73,73	2.56	26 (35%)	96,113,113	2.24	29 (30%)
24	CLA	AB	608	-	73,73,73	2.77	25 (34%)	96,113,113	2.24	29 (30%)
24	CLA	AB	609	-	73,73,73	2.70	23 (31%)	96,113,113	1.90	23 (23%)
24	CLA	AB	610	-	73,73,73	2.51	20 (27%)	96,113,113	1.84	23 (23%)
24	CLA	AB	611	-	73,73,73	2.60	22 (30%)	96,113,113	2.08	31 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	AB	612	-	73,73,73	2.68	22 (30%)	96,113,113	1.94	26 (27%)
24	CLA	AB	613	-	73,73,73	2.43	19 (26%)	96,113,113	1.87	23 (23%)
24	CLA	AB	614	-	73,73,73	2.98	24 (32%)	96,113,113	2.10	23 (23%)
24	CLA	AB	615	-	73,73,73	2.65	23 (31%)	96,113,113	1.91	20 (20%)
24	CLA	AB	616	-	73,73,73	2.67	21 (28%)	96,113,113	1.80	20 (20%)
27	BCR	AB	617	-	41,41,41	1.57	6 (14%)	56,56,56	2.09	21 (37%)
27	BCR	AB	618	-	41,41,41	1.91	7 (17%)	56,56,56	2.05	16 (28%)
27	BCR	AB	619	-	41,41,41	1.82	8 (19%)	56,56,56	1.94	18 (32%)
31	LMG	AB	620	-	51,51,55	5.72	5 (9%)	59,59,63	2.03	15 (25%)
31	LMG	AB	621	-	49,49,55	1.41	3 (6%)	57,57,63	1.90	14 (24%)
30	SQD	AB	622	-	43,43,54	7.89	23 (53%)	54,54,65	3.49	18 (33%)
32	LMT	AB	623	-	36,36,36	1.73	7 (19%)	47,47,47	0.99	2 (4%)
32	LMT	AB	624	-	36,36,36	1.61	6 (16%)	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	-	47,47,54	3.10	25 (53%)	58,58,65	3.31	15 (25%)
28	DGD	AB	628	-	53,53,67	1.47	6 (11%)	67,67,81	2.15	15 (22%)
32	LMT	AB	629	-	36,36,36	1.56	7 (19%)	47,47,47	1.38	6 (12%)
32	LMT	AB	630	-	36,36,36	1.70	8 (22%)	47,47,47	1.00	1 (2%)
24	CLA	AC	501	-	73,73,73	2.68	23 (31%)	96,113,113	2.03	24 (25%)
24	CLA	AC	502	-	73,73,73	2.59	22 (30%)	96,113,113	1.91	22 (22%)
24	CLA	AC	503	-	73,73,73	2.64	24 (32%)	96,113,113	2.06	27 (28%)
24	CLA	AC	504	-	73,73,73	2.54	24 (32%)	96,113,113	2.09	24 (25%)
24	CLA	AC	505	-	73,73,73	2.89	26 (35%)	96,113,113	2.06	23 (23%)
24	CLA	AC	506	-	73,73,73	2.79	24 (32%)	96,113,113	1.96	24 (25%)
24	CLA	AC	507	-	73,73,73	2.43	23 (31%)	96,113,113	1.82	20 (20%)
24	CLA	AC	508	-	73,73,73	2.62	23 (31%)	96,113,113	2.08	27 (28%)
24	CLA	AC	509	-	73,73,73	2.69	21 (28%)	96,113,113	1.93	22 (22%)
24	CLA	AC	510	-	73,73,73	2.60	22 (30%)	96,113,113	1.83	21 (21%)
24	CLA	AC	511	3	73,73,73	2.87	21 (28%)	96,113,113	2.05	25 (26%)
24	CLA	AC	512	-	73,73,73	2.76	23 (31%)	96,113,113	1.88	22 (22%)
24	CLA	AC	513	-	73,73,73	2.87	21 (28%)	96,113,113	1.89	21 (21%)
27	BCR	AC	514	-	41,41,41	1.60	7 (17%)	56,56,56	2.13	23 (41%)
27	BCR	AC	515	-	41,41,41	1.74	7 (17%)	56,56,56	2.22	21 (37%)
27	BCR	AC	516	-	41,41,41	1.63	8 (19%)	56,56,56	2.23	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	1.73	9 (16%)	68,68,81	2.88	23 (33%)
28	DGD	AC	518	-	63,63,67	1.30	7 (11%)	77,77,81	2.95	25 (32%)
28	DGD	AC	519	-	67,67,67	1.45	10 (14%)	81,81,81	3.46	29 (35%)
31	LMG	AC	520	-	48,48,55	1.83	7 (14%)	56,56,63	1.94	18 (32%)
31	LMG	AC	521	-	45,45,55	1.40	4 (8%)	53,53,63	2.05	15 (28%)
24	CLA	AD	401	-	73,73,73	2.54	24 (32%)	96,113,113	1.95	24 (25%)
34	PHO	AD	402	-	69,69,69	2.89	17 (24%)	92,99,99	1.75	19 (20%)
34	PHO	AD	403	-	69,69,69	3.08	19 (27%)	92,99,99	1.81	22 (23%)
24	CLA	AD	404	-	73,73,73	2.66	25 (34%)	96,113,113	1.97	22 (22%)
35	PL9	AD	405	-	55,55,55	4.31	18 (32%)	69,69,69	3.01	24 (34%)
27	BCR	AD	406	-	41,41,41	1.64	7 (17%)	56,56,56	2.33	24 (42%)
31	LMG	AD	407	-	49,49,55	5.81	3 (6%)	57,57,63	2.72	21 (36%)
31	LMG	AD	408	-	48,48,55	5.81	6 (12%)	56,56,63	2.17	13 (23%)
32	LMT	AD	409	-	32,32,36	1.77	8 (25%)	43,43,47	1.31	2 (4%)
28	DGD	AE	101	-	64,64,67	1.60	13 (20%)	78,78,81	1.50	11 (14%)
36	HEM	AF	101	5,6	50,50,50	3.49	25 (50%)	46,82,82	3.17	18 (39%)
30	SQD	AF	102	-	45,45,54	10.56	25 (55%)	56,56,65	3.67	20 (35%)
28	DGD	AH	101	-	59,59,67	1.55	12 (20%)	73,73,81	2.13	18 (24%)
31	LMG	AI	101	-	43,43,55	1.67	4 (9%)	51,51,63	1.77	7 (13%)
32	LMT	AI	102	-	36,36,36	1.58	8 (22%)	47,47,47	1.00	1 (2%)
32	LMT	AI	103	-	36,36,36	1.41	6 (16%)	47,47,47	1.76	8 (17%)
27	BCR	AJ	101	-	41,41,41	2.46	12 (29%)	56,56,56	3.15	25 (44%)
31	LMG	AJ	102	-	46,46,55	1.21	5 (10%)	54,54,63	2.65	16 (29%)
27	BCR	AK	102	-	41,41,41	1.76	6 (14%)	56,56,56	2.45	26 (46%)
31	LMG	AM	101	-	42,42,55	1.18	5 (11%)	50,50,63	1.73	8 (16%)
32	LMT	AM	102	-	36,36,36	1.71	9 (25%)	47,47,47	0.91	2 (4%)
27	BCR	AT	101	-	41,41,41	1.62	6 (14%)	56,56,56	2.22	24 (42%)
33	DMS	AU	201	-	3,3,3	0.90	0	3,3,3	1.06	0
36	HEM	AV	201	16	50,50,50	3.38	26 (52%)	46,82,82	3.10	13 (28%)
33	DMS	AV	202	-	3,3,3	0.74	0	3,3,3	1.00	0
27	BCR	AX	101	-	41,41,41	1.84	8 (19%)	56,56,56	2.19	21 (37%)
30	SQD	BA	5401	-	54,54,54	2.69	29 (53%)	65,65,65	3.20	22 (33%)
31	LMG	BA	5402	-	42,42,55	1.50	5 (11%)	50,50,63	2.43	13 (26%)
22	BCT	BA	5403	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	BA	5405	-	73,73,73	2.51	23 (31%)	96,113,113	1.91	24 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	BA	5406	-	73,73,73	2.66	24 (32%)	96,113,113	2.32	27 (28%)
24	CLA	BA	5407	-	73,73,73	2.68	27 (36%)	96,113,113	2.15	24 (25%)
24	CLA	BA	5408	-	73,73,73	2.66	23 (31%)	96,113,113	2.02	25 (26%)
25	MST	BA	5409	-	16,16,16	0.48	0	22,22,22	3.78	8 (36%)
26	OEC	BA	5410	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	BA	5411	-	41,41,41	1.66	8 (19%)	56,56,56	2.06	21 (37%)
28	DGD	BA	5412	-	57,57,67	1.84	13 (22%)	71,71,81	3.81	24 (33%)
29	LHG	BA	5413	-	38,38,48	1.89	5 (13%)	44,44,54	1.38	4 (9%)
30	SQD	BA	5414	-	51,51,54	7.20	28 (54%)	62,62,65	3.39	24 (38%)
29	LHG	BA	5415	-	36,36,48	1.70	4 (11%)	42,42,54	1.10	3 (7%)
30	SQD	BB	5601	-	47,47,54	3.11	26 (55%)	58,58,65	3.29	17 (29%)
28	DGD	BB	5602	-	53,53,67	1.58	7 (13%)	67,67,81	2.17	14 (20%)
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	-	73,73,73	2.94	23 (31%)	96,113,113	1.79	17 (17%)
24	CLA	BB	5606	-	73,73,73	2.56	23 (31%)	96,113,113	1.91	21 (21%)
24	CLA	BB	5607	-	73,73,73	2.66	19 (26%)	96,113,113	2.23	29 (30%)
24	CLA	BB	5608	-	73,73,73	2.59	24 (32%)	96,113,113	1.94	26 (27%)
24	CLA	BB	5609	-	73,73,73	2.70	23 (31%)	96,113,113	1.99	27 (28%)
24	CLA	BB	5610	-	73,73,73	2.74	25 (34%)	96,113,113	1.98	26 (27%)
24	CLA	BB	5611	-	73,73,73	2.54	24 (32%)	96,113,113	2.24	30 (31%)
24	CLA	BB	5612	-	73,73,73	2.78	24 (32%)	96,113,113	2.24	27 (28%)
24	CLA	BB	5613	-	73,73,73	2.68	22 (30%)	96,113,113	1.92	26 (27%)
24	CLA	BB	5614	-	73,73,73	2.52	21 (28%)	96,113,113	1.82	20 (20%)
24	CLA	BB	5615	-	73,73,73	2.64	22 (30%)	96,113,113	2.09	31 (32%)
24	CLA	BB	5616	-	73,73,73	2.72	22 (30%)	96,113,113	1.97	24 (25%)
24	CLA	BB	5617	-	73,73,73	2.43	24 (32%)	96,113,113	1.87	20 (20%)
24	CLA	BB	5618	-	73,73,73	2.91	22 (30%)	96,113,113	2.08	23 (23%)
24	CLA	BB	5619	-	73,73,73	2.63	22 (30%)	96,113,113	1.92	23 (23%)
24	CLA	BB	5620	-	73,73,73	2.68	21 (28%)	96,113,113	1.81	20 (20%)
27	BCR	BB	5621	-	41,41,41	1.50	7 (17%)	56,56,56	2.08	19 (33%)
27	BCR	BB	5622	-	41,41,41	1.86	7 (17%)	56,56,56	2.04	17 (30%)
27	BCR	BB	5623	-	41,41,41	1.69	8 (19%)	56,56,56	1.92	17 (30%)
31	LMG	BB	5624	-	49,49,55	1.52	3 (6%)	57,57,63	1.90	14 (24%)
30	SQD	BB	5625	-	43,43,54	7.88	23 (53%)	54,54,65	3.52	18 (33%)

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	8 (22%)	47,47,47	1.01	2 (4%)
32	LMT	BB	5627	-	36,36,36	1.58	7 (19%)	47,47,47	0.92	2 (4%)
33	DMS	BB	5628	-	3,3,3	0.69	0	3,3,3	1.07	0
33	DMS	BB	5629	-	3,3,3	0.67	0	3,3,3	1.14	0
24	CLA	BC	5501	-	73,73,73	2.75	24 (32%)	96,113,113	2.03	24 (25%)
24	CLA	BC	5502	-	73,73,73	2.64	23 (31%)	96,113,113	1.96	22 (22%)
24	CLA	BC	5503	-	73,73,73	2.71	24 (32%)	96,113,113	2.02	27 (28%)
24	CLA	BC	5504	-	73,73,73	2.64	25 (34%)	96,113,113	2.08	24 (25%)
24	CLA	BC	5505	-	73,73,73	2.93	26 (35%)	96,113,113	2.06	21 (21%)
24	CLA	BC	5506	-	73,73,73	2.79	24 (32%)	96,113,113	1.97	25 (26%)
24	CLA	BC	5507	-	73,73,73	2.52	23 (31%)	96,113,113	1.83	21 (21%)
24	CLA	BC	5508	-	73,73,73	2.69	22 (30%)	96,113,113	2.10	28 (29%)
24	CLA	BC	5509	-	73,73,73	2.89	22 (30%)	96,113,113	1.90	20 (20%)
24	CLA	BC	5510	-	73,73,73	2.65	22 (30%)	96,113,113	1.85	20 (20%)
24	CLA	BC	5511	3	73,73,73	3.00	24 (32%)	96,113,113	2.04	21 (21%)
24	CLA	BC	5512	-	73,73,73	2.81	23 (31%)	96,113,113	1.87	21 (21%)
24	CLA	BC	5513	-	73,73,73	2.97	22 (30%)	96,113,113	1.88	21 (21%)
27	BCR	BC	5514	-	41,41,41	1.78	6 (14%)	56,56,56	2.09	24 (42%)
27	BCR	BC	5515	-	41,41,41	1.88	7 (17%)	56,56,56	2.21	22 (39%)
27	BCR	BC	5516	-	41,41,41	1.77	7 (17%)	56,56,56	2.19	20 (35%)
28	DGD	BC	5517	-	54,54,67	1.66	10 (18%)	68,68,81	2.88	22 (32%)
28	DGD	BC	5518	-	63,63,67	1.38	7 (11%)	77,77,81	2.93	24 (31%)
28	DGD	BC	5519	-	67,67,67	1.49	11 (16%)	81,81,81	3.46	30 (37%)
31	LMG	BC	5520	-	48,48,55	1.93	5 (10%)	56,56,63	1.92	17 (30%)
31	LMG	BC	5521	-	45,45,55	1.32	4 (8%)	53,53,63	2.04	14 (26%)
32	LMT	BC	5522	-	36,36,36	1.48	7 (19%)	47,47,47	1.76	8 (17%)
24	CLA	BD	5402	-	73,73,73	2.59	24 (32%)	96,113,113	1.96	24 (25%)
34	PHO	BD	5403	-	69,69,69	2.99	18 (26%)	92,99,99	1.77	21 (22%)
34	PHO	BD	5404	-	69,69,69	3.17	21 (30%)	92,99,99	1.82	22 (23%)
24	CLA	BD	5405	-	73,73,73	2.67	24 (32%)	96,113,113	1.95	23 (23%)
35	PL9	BD	5406	-	55,55,55	4.43	20 (36%)	69,69,69	3.00	24 (34%)
27	BCR	BD	5407	-	41,41,41	1.81	9 (21%)	56,56,56	2.31	24 (42%)
31	LMG	BD	5408	-	46,46,55	1.16	5 (10%)	54,54,63	2.64	17 (31%)
31	LMG	BD	5409	-	49,49,55	5.79	2 (4%)	57,57,63	2.73	22 (38%)
31	LMG	BD	5410	-	48,48,55	5.79	3 (6%)	56,56,63	2.17	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	BD	5411	-	32,32,36	1.71	7 (21%)	43,43,47	1.31	3 (6%)
31	LMG	BE	5101	-	44,44,55	1.45	4 (9%)	52,52,63	1.69	8 (15%)
28	DGD	BE	5102	-	64,64,67	1.58	12 (18%)	78,78,81	1.49	9 (11%)
36	HEM	BF	5101	5,6	50,50,50	3.62	26 (52%)	46,82,82	3.19	18 (39%)
30	SQD	BF	5102	-	45,45,54	10.56	26 (57%)	56,56,65	3.68	21 (37%)
28	DGD	BH	5101	-	59,59,67	1.50	10 (16%)	73,73,81	2.13	19 (26%)
31	LMG	BI	5101	-	43,43,55	1.77	4 (9%)	51,51,63	1.76	7 (13%)
32	LMT	BI	5102	-	36,36,36	1.62	7 (19%)	47,47,47	0.99	2 (4%)
27	BCR	BJ	5101	-	41,41,41	2.40	13 (31%)	56,56,56	3.13	25 (44%)
27	BCR	BK	5102	-	41,41,41	1.90	8 (19%)	56,56,56	2.41	24 (42%)
31	LMG	BL	5101	-	51,51,55	5.70	5 (9%)	59,59,63	2.02	14 (23%)
32	LMT	BM	5101	-	36,36,36	1.72	8 (22%)	47,47,47	0.90	2 (4%)
31	LMG	BM	5102	-	42,42,55	1.26	5 (11%)	50,50,63	1.73	8 (16%)
27	BCR	BT	5101	-	41,41,41	1.76	6 (14%)	56,56,56	2.22	24 (42%)
36	HEM	BV	5201	16	50,50,50	3.41	27 (54%)	46,82,82	3.13	13 (28%)
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	1.87	9 (21%)	56,56,56	2.22	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	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	405	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	406	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AA	407	-	1/1/20/25	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
30	SQD	AA	416	-	-	0/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	AA	417	-	-	0/37/57/70	0/1/1/1
24	CLA	AB	601	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	602	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	603	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	604	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	605	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	606	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	608	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	610	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	611	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	612	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	613	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	614	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	615	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AB	616	-	1/1/20/25	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	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	503	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	504	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	505	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	506	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	507	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	508	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	509	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	510	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	511	3	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AC	512	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	AC	513	-	1/1/20/25	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	-	1/1/20/25	0/37/135/135	0/0/9/9
34	PHO	AD	402	-	2/2/17/22	0/49/103/103	0/1/6/6
34	PHO	AD	403	-	2/2/17/22	0/49/103/103	0/1/6/6
24	CLA	AD	404	-	1/1/20/25	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	-	0/14/114/114	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	-	0/14/114/114	0/0/8/8
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	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5406	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BA	5407	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BA	5408	-	1/1/20/25	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	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5606	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5608	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5610	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5611	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5612	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5613	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5614	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5615	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5616	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5617	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5618	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5619	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BB	5620	-	1/1/20/25	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
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	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5503	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5504	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5505	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BC	5506	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5507	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5508	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5509	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5510	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5511	3	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5512	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	BC	5513	-	1/1/20/25	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	-	1/1/20/25	0/37/135/135	0/0/9/9
34	PHO	BD	5403	-	2/2/17/22	0/49/103/103	0/1/6/6
34	PHO	BD	5404	-	2/2/17/22	0/49/103/103	0/1/6/6
24	CLA	BD	5405	-	1/1/20/25	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
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	-	0/14/114/114	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	-	0/14/114/114	0/0/8/8
33	DMS	BV	5202	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 2655 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BF	5102	SQD	C19-C18	-48.56	1.35	1.55
30	AF	102	SQD	C32-C31	-48.38	1.35	1.55
30	AF	102	SQD	C19-C18	-48.33	1.35	1.55
30	BF	5102	SQD	C32-C31	-48.02	1.36	1.55
30	AA	413	SQD	C35-C34	-47.92	1.36	1.55

The worst 5 of 3253 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	AC	518	DGD	O5D-C1E-C2E	13.73	125.75	108.15
28	BC	5518	DGD	O5D-C1E-C2E	13.49	125.43	108.15
28	AC	519	DGD	O5D-C6D-C5D	12.96	131.44	108.96
28	BC	5519	DGD	O5D-C6D-C5D	12.87	131.30	108.96
30	BF	5102	SQD	O7-S-C6	12.72	118.07	106.83

5 of 82 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	BC	5502	CLA	C8
24	BC	5511	CLA	C8
24	AC	507	CLA	C8
24	BB	5617	CLA	C8
34	BD	5403	PHO	C2A

All (3) torsion outliers are listed below:

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

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	335/344 (97%)	-0.09	1 (0%) 91 58	82, 104, 147, 160	0
1	BA	335/344 (97%)	-0.06	2 (0%) 86 41	86, 106, 148, 160	0
2	AB	490/510 (96%)	-0.11	1 (0%) 93 66	81, 103, 136, 152	0
2	BB	490/510 (96%)	-0.02	5 (1%) 79 29	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.10	2 (0%) 90 51	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.09	6 (1%) 74 24	91, 124, 149, 159	0
4	AD	341/352 (96%)	-0.09	1 (0%) 91 58	81, 105, 139, 153	0
4	BD	341/352 (96%)	-0.09	3 (0%) 81 32	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.13	1 (1%) 75 26	104, 126, 151, 155	0
5	BE	82/84 (97%)	0.59	4 (4%) 28 6	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.06	2 (5%) 23 5	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.04	0 100 100	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.19	0 100 100	113, 124, 140, 147	0
7	BH	65/66 (98%)	0.16	2 (3%) 47 10	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.13	1 (2%) 49 10	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.16	3 (8%) 11 3	108, 116, 142, 147	0
9	AJ	38/40 (95%)	-0.08	0 100 100	109, 122, 157, 159	0
9	BJ	38/40 (95%)	0.08	1 (2%) 53 11	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.16	1 (2%) 52 11	121, 135, 145, 147	0
10	BK	37/37 (100%)	0.18	1 (2%) 52 11	123, 136, 147, 148	0
11	AL	37/37 (100%)	0.07	1 (2%) 52 11	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.18	2 (5%) 25 5	90, 104, 158, 160	0
12	AM	34/36 (94%)	-0.04	0 100 100	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.20	1 (2%) 49 10	90, 99, 140, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.08	2 (0%) 83 35	83, 116, 148, 160	0
13	BO	243/247 (98%)	0.09	3 (1%) 75 26	85, 117, 147, 160	0
14	AT	32/32 (100%)	0.23	2 (6%) 19 4	92, 106, 158, 160	0
14	BT	32/32 (100%)	0.10	2 (6%) 19 4	93, 106, 158, 160	0
15	AU	97/104 (93%)	0.08	0 100 100	93, 105, 116, 125	0
15	BU	97/104 (93%)	-0.03	0 100 100	94, 106, 116, 127	0
16	AV	137/137 (100%)	-0.01	1 (0%) 84 38	96, 112, 128, 132	0
16	BV	137/137 (100%)	0.21	0 100 100	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.18	1 (3%) 41 8	141, 154, 160, 160	0
17	By	28/46 (60%)	0.44	1 (3%) 41 8	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.12	2 (5%) 25 5	121, 129, 147, 150	0
18	BX	37/41 (90%)	0.13	0 100 100	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.23	5 (8%) 12 3	134, 148, 160, 160	0
20	BZ	62/62 (100%)	0.85	6 (9%) 8 2	135, 150, 160, 160	0
All	All	5224/5494 (95%)	0.04	66 (1%) 74 24	81, 113, 149, 160	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BZ	5062	VAL	6.0
20	BZ	5001	MET	5.0
20	BZ	5061	VAL	4.7
17	By	5046	LEU	4.5
11	BL	5001	MET	3.6

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	BCR	AJ	101	40/40	0.74	17.34	158,160,160,160	0
28	DGD	AE	101	63/66	0.70	12.39	146,160,160,160	0
32	LMT	BB	5626	35/35	0.54	12.12	131,160,160,160	0
28	DGD	BB	5602	52/66	0.45	7.76	152,160,160,160	0
31	LMG	BA	5402	42/55	0.48	7.11	144,157,160,160	0
27	BCR	BJ	5101	40/40	0.58	6.70	160,160,160,160	0
28	DGD	AC	518	62/66	0.44	5.55	146,155,160,160	0
28	DGD	AB	628	52/66	0.57	5.53	154,160,160,160	0
33	DMS	BB	5628	4/4	0.46	5.45	156,157,157,157	0
31	LMG	AA	417	42/55	0.40	5.22	145,157,160,160	0
33	DMS	AV	202	4/4	0.50	5.01	148,148,148,149	0
28	DGD	BC	5518	62/66	0.45	4.88	147,156,160,160	0
32	LMT	AB	624	35/35	0.54	4.81	156,160,160,160	0
31	LMG	BD	5410	48/55	0.48	4.69	126,131,141,141	0
32	LMT	AB	629	35/35	0.45	4.49	133,160,160,160	0
31	LMG	AJ	102	46/55	0.39	4.39	139,144,160,160	0
32	LMT	BB	5603	35/35	0.40	4.15	132,160,160,160	0
33	DMS	AB	625	4/4	0.54	4.14	156,157,157,157	0
28	DGD	AC	519	66/66	0.38	4.12	110,120,157,158	0
27	BCR	BB	5621	40/40	0.35	4.10	112,120,124,125	0
28	DGD	BE	5102	63/66	0.68	4.10	145,160,160,160	0
31	LMG	AB	621	49/55	0.44	4.09	145,150,157,160	0
30	SQD	BA	5401	54/54	0.53	3.95	136,160,160,160	0
32	LMT	BI	5102	35/35	0.73	3.92	151,160,160,160	0
31	LMG	BB	5624	49/55	0.37	3.73	145,150,157,160	0
33	DMS	BV	5203	4/4	0.38	3.40	160,160,160,160	0
31	LMG	AD	408	48/55	0.43	3.37	121,130,139,139	0
31	LMG	AD	407	49/55	0.37	3.33	126,133,143,145	0
28	DGD	BC	5519	66/66	0.37	3.32	112,121,158,159	0
31	LMG	AA	414	44/55	0.44	3.31	140,160,160,160	0
31	LMG	AI	101	43/55	0.81	3.27	159,160,160,160	0
31	LMG	AC	520	48/55	0.49	3.22	136,157,160,160	0
31	LMG	AB	620	51/55	0.45	3.20	125,139,150,151	0
32	LMT	AM	102	35/35	0.44	3.13	126,149,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	LMT	BB	5604	35/35	0.47	3.10	131,160,160,160	0
29	LHG	BA	5415	37/49	0.61	3.03	151,160,160,160	0
24	CLA	BA	5408	65/65	0.34	3.03	95,103,150,150	0
24	CLA	AD	404	65/65	0.36	3.03	126,130,148,149	0
27	BCR	AK	102	40/40	0.38	3.00	133,139,151,152	0
27	BCR	AB	617	40/40	0.32	2.98	112,121,125,125	0
31	LMG	BI	5101	43/55	0.67	2.95	160,160,160,160	0
30	SQD	AB	622	43/54	0.40	2.95	133,149,160,160	0
37	CA	BO	5301	1/1	0.43	2.91	160,160,160,160	0
32	LMT	BB	5627	35/35	0.42	2.90	156,160,160,160	0
27	BCR	AT	101	40/40	0.36	2.89	126,140,146,147	0
31	LMG	BD	5408	46/55	0.39	2.82	139,145,160,160	0
33	DMS	AB	626	4/4	0.28	2.81	129,130,130,130	0
24	CLA	AB	601	65/65	0.50	2.79	146,159,160,160	0
27	BCR	BT	5101	40/40	0.32	2.78	124,143,147,147	0
30	SQD	BB	5625	43/54	0.39	2.75	132,148,160,160	0
24	CLA	AA	407	65/65	0.35	2.74	93,101,150,151	0
28	DGD	AC	517	53/66	0.35	2.73	121,128,135,140	0
27	BCR	AX	101	40/40	0.58	2.71	135,143,158,159	0
32	LMT	BC	5522	35/35	0.63	2.67	157,160,160,160	0
35	PL9	AD	405	55/55	0.34	2.66	99,109,113,113	0
24	CLA	BB	5605	65/65	0.60	2.64	146,159,160,160	0
27	BCR	BD	5407	40/40	0.28	2.64	112,127,132,132	0
24	CLA	AA	406	65/65	0.32	2.63	105,112,138,139	0
24	CLA	BB	5609	65/65	0.33	2.56	103,110,124,124	0
28	DGD	BA	5412	56/66	0.46	2.55	150,160,160,160	0
31	LMG	BC	5520	48/55	0.46	2.51	138,159,160,160	0
30	SQD	AF	102	45/54	0.51	2.45	154,160,160,160	0
28	DGD	AA	411	56/66	0.51	2.44	148,158,160,160	0
27	BCR	AD	406	40/40	0.32	2.44	110,126,131,131	0
24	CLA	BC	5504	65/65	0.31	2.43	132,135,160,160	0
27	BCR	BB	5623	40/40	0.39	2.42	111,116,131,131	0
32	LMT	AD	409	31/35	0.39	2.40	139,154,160,160	0
32	LMT	BM	5101	35/35	0.42	2.40	126,149,154,155	0
27	BCR	AC	516	40/40	0.45	2.35	135,138,143,143	0
31	LMG	BE	5101	44/55	0.44	2.35	140,160,160,160	0
32	LMT	AI	102	35/35	0.66	2.34	149,158,160,160	0
24	CLA	AC	504	65/65	0.34	2.29	129,134,160,160	0
32	LMT	AI	103	35/35	0.43	2.24	156,158,160,160	0
24	CLA	AB	605	65/65	0.26	2.22	105,113,122,124	0
27	BCR	BX	5101	40/40	0.55	2.18	136,143,157,158	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	LMG	BL	5101	51/55	0.41	2.17	122,138,151,152	0
32	LMT	AB	623	35/35	0.56	2.16	135,160,160,160	0
24	CLA	AB	616	65/65	0.43	2.15	143,147,160,160	0
24	CLA	BB	5612	65/65	0.37	2.12	122,127,136,139	0
24	CLA	AB	615	65/65	0.39	2.11	134,139,155,157	0
24	CLA	BD	5405	65/65	0.37	2.10	125,131,148,149	0
24	CLA	AB	608	65/65	0.35	2.09	123,127,135,140	0
27	BCR	AC	515	40/40	0.42	2.02	149,152,155,155	0
24	CLA	BB	5617	65/65	0.30	1.99	98,102,138,141	0
32	LMT	AB	630	35/35	0.50	1.95	132,160,160,160	0
27	BCR	BC	5515	40/40	0.53	1.92	150,152,155,156	0
24	CLA	AC	505	65/65	0.38	1.86	121,146,150,151	0
31	LMG	AC	521	45/55	0.59	1.85	154,160,160,160	0
34	PHO	BD	5403	64/64	0.32	1.79	102,109,118,118	0
28	DGD	BH	5101	58/66	0.30	1.77	107,118,156,160	0
24	CLA	AC	503	65/65	0.44	1.76	137,144,147,152	0
24	CLA	AB	610	65/65	0.34	1.66	117,121,123,127	0
24	CLA	BA	5407	65/65	0.28	1.66	110,114,138,139	0
30	SQD	AA	416	54/54	0.32	1.63	136,160,160,160	0
24	CLA	AB	603	65/65	0.33	1.61	107,109,119,121	0
24	CLA	BB	5614	65/65	0.32	1.59	117,123,124,128	0
24	CLA	AC	507	65/65	0.38	1.59	137,149,152,153	0
35	PL9	BD	5406	55/55	0.32	1.55	103,110,115,116	0
27	BCR	AB	619	40/40	0.30	1.53	111,117,131,131	0
24	CLA	AB	609	65/65	0.35	1.51	126,136,141,143	0
24	CLA	BC	5502	65/65	0.30	1.50	108,111,143,144	0
31	LMG	BD	5409	49/55	0.36	1.50	128,133,144,146	0
27	BCR	BK	5102	40/40	0.36	1.50	136,140,152,152	0
27	BCR	BA	5411	40/40	0.30	1.47	94,122,132,132	0
24	CLA	BC	5513	65/65	0.57	1.45	158,160,160,160	0
27	BCR	BC	5514	40/40	0.44	1.44	123,126,129,129	0
24	CLA	AC	508	65/65	0.36	1.42	140,144,157,158	0
30	SQD	AA	413	51/54	0.37	1.42	143,150,160,160	0
29	LHG	AA	415	37/49	0.40	1.40	149,160,160,160	0
32	LMT	BD	5411	31/35	0.49	1.40	140,152,160,160	0
24	CLA	BC	5505	65/65	0.35	1.38	123,148,152,153	0
34	PHO	AD	402	64/64	0.29	1.36	99,109,116,117	0
24	CLA	BA	5406	65/65	0.25	1.36	89,94,108,112	0
24	CLA	AC	502	65/65	0.35	1.31	103,109,142,143	0
27	BCR	AA	410	40/40	0.29	1.30	91,122,130,130	0
24	CLA	BB	5611	65/65	0.25	1.25	95,102,132,136	0
34	PHO	AD	403	64/64	0.26	1.22	119,123,128,129	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	SQD	BF	5102	45/54	0.47	1.21	154,160,160,160	0
24	CLA	BB	5607	65/65	0.28	1.16	108,111,120,123	0
24	CLA	AB	606	65/65	0.32	1.15	120,133,140,141	0
24	CLA	BB	5613	65/65	0.30	1.12	127,135,140,142	0
28	DGD	AH	101	58/66	0.27	1.11	108,120,155,157	0
24	CLA	AC	501	65/65	0.34	1.10	133,136,139,143	0
27	BCR	AB	618	40/40	0.24	1.08	109,117,122,122	0
33	DMS	BB	5629	4/4	0.22	1.08	125,126,127,127	0
24	CLA	BB	5616	65/65	0.31	1.07	108,110,120,122	0
24	CLA	AC	506	65/65	0.32	1.05	136,143,160,160	0
24	CLA	BC	5507	65/65	0.36	1.04	136,150,153,154	0
24	CLA	AB	614	65/65	0.34	1.03	129,133,160,160	0
24	CLA	BB	5608	65/65	0.31	1.01	96,103,124,125	0
31	LMG	AM	101	42/55	0.42	1.01	136,158,160,160	0
24	CLA	AB	612	65/65	0.29	0.99	107,111,120,121	0
34	PHO	BD	5404	64/64	0.29	0.99	123,125,129,130	0
24	CLA	AB	602	65/65	0.28	0.98	124,127,129,132	0
24	CLA	AB	604	65/65	0.29	0.86	96,104,125,127	0
24	CLA	AD	401	65/65	0.25	0.84	93,100,115,119	0
29	LHG	AA	412	39/49	0.28	0.83	110,118,128,132	0
24	CLA	AB	607	65/65	0.24	0.83	94,100,132,135	0
24	CLA	AC	509	65/65	0.38	0.83	115,128,135,137	0
24	CLA	BD	5402	65/65	0.25	0.82	97,101,117,119	0
36	HEM	AF	101	43/43	0.33	0.81	148,152,159,160	0
27	BCR	BB	5622	40/40	0.26	0.81	110,117,120,121	0
28	DGD	BC	5517	53/66	0.27	0.80	124,130,136,139	0
30	SQD	BB	5601	47/54	0.35	0.80	137,156,160,160	0
24	CLA	BA	5405	65/65	0.27	0.78	90,101,105,109	0
30	SQD	AB	627	47/54	0.33	0.77	138,157,160,160	0
37	CA	AO	301	1/1	0.31	0.75	152,152,152,152	0
24	CLA	AB	611	65/65	0.29	0.74	99,113,116,122	0
24	CLA	BC	5511	65/65	0.44	0.73	154,158,159,160	0
27	BCR	AC	514	40/40	0.31	0.72	120,123,127,128	0
24	CLA	BC	5510	65/65	0.35	0.71	113,116,130,131	0
24	CLA	AC	513	65/65	0.47	0.71	158,160,160,160	0
24	CLA	BC	5503	65/65	0.32	0.69	137,147,148,152	0
24	CLA	AA	404	65/65	0.24	0.68	89,99,106,108	0
24	CLA	BC	5506	65/65	0.35	0.68	136,143,160,160	0
24	CLA	BB	5618	65/65	0.30	0.68	128,133,160,160	0
37	CA	BK	5101	1/1	0.21	0.67	145,145,145,145	0
27	BCR	BC	5516	40/40	0.39	0.65	136,140,145,145	0
31	LMG	BM	5102	42/55	0.40	0.63	136,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	CL	BA	5404[A]	1/1	0.22	0.60	29,29,29,29	1
24	CLA	AC	510	65/65	0.34	0.58	110,113,129,130	0
24	CLA	AC	512	65/65	0.38	0.56	154,158,160,160	0
24	CLA	BB	5606	65/65	0.28	0.54	124,127,130,131	0
24	CLA	BC	5501	65/65	0.29	0.51	134,137,141,144	0
24	CLA	BC	5508	65/65	0.29	0.51	142,146,157,159	0
24	CLA	BB	5610	65/65	0.30	0.50	121,132,140,141	0
23	CL	AA	403[B]	1/1	0.27	0.50	108,108,108,108	1
23	CL	AA	403[A]	1/1	0.27	0.49	33,33,33,33	1
30	SQD	BA	5414	51/54	0.36	0.47	145,150,160,160	0
24	CLA	BC	5509	65/65	0.30	0.42	116,128,138,138	0
24	CLA	BC	5512	65/65	0.35	0.40	157,160,160,160	0
36	HEM	BV	5201	43/43	0.25	0.39	97,102,106,109	0
24	CLA	BB	5619	65/65	0.31	0.37	135,137,155,157	0
26	OEC	AA	409	5/9	0.28	0.36	82,83,90,110	0
36	HEM	AV	201	43/43	0.26	0.35	94,100,102,103	0
29	LHG	BA	5413	39/49	0.27	0.35	113,122,128,129	0
31	LMG	BC	5521	45/55	0.49	0.35	154,160,160,160	0
25	MST	AA	408	16/16	0.25	0.33	123,126,129,130	0
24	CLA	AA	405	65/65	0.24	0.32	88,93,108,111	0
33	DMS	AU	201	4/4	0.28	0.29	160,160,160,160	0
24	CLA	AC	511	65/65	0.31	0.27	152,155,157,158	0
24	CLA	AB	613	65/65	0.23	0.26	99,102,136,140	0
36	HEM	BF	5101	43/43	0.42	0.25	148,152,160,160	0
24	CLA	BB	5615	65/65	0.24	0.22	101,113,117,120	0
24	CLA	BB	5620	65/65	0.30	0.11	143,147,160,160	0
23	CL	BA	5404[B]	1/1	0.22	-0.14	115,115,115,115	1
37	CA	AK	101	1/1	0.12	-0.23	146,146,146,146	0
25	MST	BA	5409	16/16	0.20	-0.25	124,129,131,132	0
26	OEC	BA	5410	5/9	0.22	-0.41	23,88,99,134	0
33	DMS	BV	5202	4/4	0.19	-0.59	148,149,149,150	0
22	BCT	AA	402	4/4	0.19	-0.93	135,136,137,137	0
21	FE2	AA	401	1/1	0.15	-1.32	115,115,115,115	0
22	BCT	BA	5403	4/4	0.14	-1.32	135,136,136,137	0
21	FE2	BD	5401	1/1	0.08	-2.97	119,119,119,119	0
37	CA	AF	103	1/1	0.20	-5.12	150,150,150,150	0
37	CA	BF	5103	1/1	0.17	-9.15	146,146,146,146	0

6.5 Other polymers ⓘ

There are no such residues in this entry.