wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:12 AM GMT

PDB ID	:	3KZI
Title	:	Crystal Structure of Monomeric Form of Cyanobacterial Photosystem II
Authors	:	Gabdulkhakov, A.; Guskov, A.; Broser, M.; Kern, J.; Zouni, A.; Saenger, W.
Deposited on	:	2009-12-08
Resolution	:	3.60 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

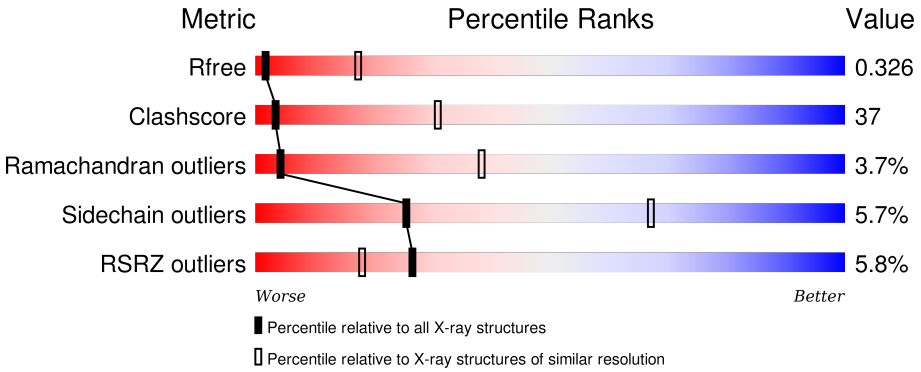
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	6% 47% 46% 5%
2	B	510	3% 53% 38% 5%
3	C	461	5% 41% 50% 6%
4	D	352	7% 51% 39% 7%
5	E	83	2% 28% 57% 7% 7%

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Mol	Chain	Length	Quality of chain
6	F	44	14% 25% 50% 11% 14%
7	H	65	5% 38% 49% 11%
8	I	38	13% 47% 45% 8%
9	J	40	20% 58% 8% 15%
10	K	37	3% 11% 78% 11%
11	L	37	8% 54% 32% 14%
12	M	36	22% 39% 56% 6%
13	O	246	8% 50% 45%
14	T	32	6% 56% 34% 6%
15	U	104	3% 55% 34% 7%
16	V	137	4% 60% 36%
17	y	46	4% 48% 13% 39%
18	X	40	10% 48% 25% 13% 13%
19	Z	62	6% 37% 53% 10%

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
21	CLA	A	362	X	-	-	-
21	CLA	A	363	X	-	-	X
21	CLA	A	364	X	-	-	-
21	CLA	A	366	X	-	-	X
21	CLA	B	511	X	-	-	X
21	CLA	B	512	X	-	-	-
21	CLA	B	513	X	-	X	-
21	CLA	B	514	X	-	-	-
21	CLA	B	515	X	-	-	-
21	CLA	B	516	X	-	-	-
21	CLA	B	517	X	-	-	-
21	CLA	B	518	X	-	-	-
21	CLA	B	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	520	X	-	-	-
21	CLA	B	521	X	-	-	-
21	CLA	B	522	X	-	-	-
21	CLA	B	523	X	-	-	-
21	CLA	B	524	X	-	-	X
21	CLA	B	525	X	-	-	-
21	CLA	B	526	X	-	-	X
21	CLA	C	477	X	-	-	-
21	CLA	C	478	X	-	-	-
21	CLA	C	479	X	-	-	-
21	CLA	C	480	X	-	-	-
21	CLA	C	481	X	-	-	-
21	CLA	C	482	X	-	-	X
21	CLA	C	483	X	-	-	-
21	CLA	C	484	X	-	-	-
21	CLA	C	485	X	-	-	-
21	CLA	C	486	X	-	X	-
21	CLA	C	487	X	-	-	-
21	CLA	C	488	X	-	-	-
21	CLA	D	354	X	-	-	X
21	CLA	D	356	X	-	-	-
21	CLA	K	483	X	-	-	-
22	PHO	A	365	X	-	-	-
22	PHO	D	355	X	-	-	-
23	MES	A	367	-	-	X	-
25	BCR	A	369	-	-	-	X
25	BCR	B	527	-	-	-	X
25	BCR	B	529	-	-	-	X
25	BCR	B	530	-	-	-	X
25	BCR	C	490	-	-	-	X
25	BCR	J	115	-	-	-	X
25	BCR	X	107	-	-	-	X
25	BCR	Z	116	-	-	-	X
26	DGD	B	528	-	-	X	-
26	DGD	C	474	-	-	-	X
26	DGD	C	492	X	-	-	-
26	DGD	C	493	X	-	X	-
26	DGD	D	362	-	-	-	X
28	SQD	C	475	-	-	-	X
28	SQD	F	224	-	-	-	X
28	SQD	L	213	-	-	-	X
29	LMG	A	373	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	LMG	C	494	-	-	-	X
29	LMG	D	360	-	-	X	X
29	LMG	J	492	-	-	-	X
29	LMG	M	217	-	-	-	X
30	LMT	A	376	-	-	-	X
30	LMT	D	363	-	-	-	X
30	LMT	I	274	-	-	-	X
32	PL9	D	357	-	-	X	X

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 24678 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	485	Total	C	N	O	S	0	0	0
			3812	2505	635	659	13			

- Molecule 3 is a protein called Photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3455	2262	580	600	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	0	0	0
			635	417	103	115			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	38	Total	C	N	O	S	0	0	0
			307	207	50	49	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

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

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	35	Total	C	N	O	0	0	0
			254	172	38	44			

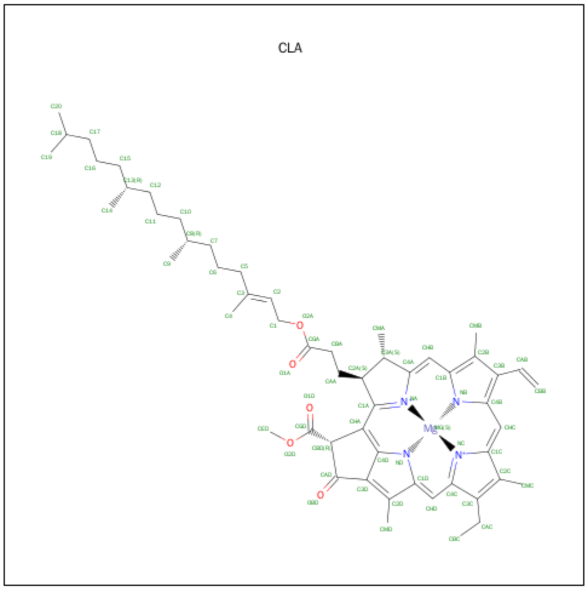
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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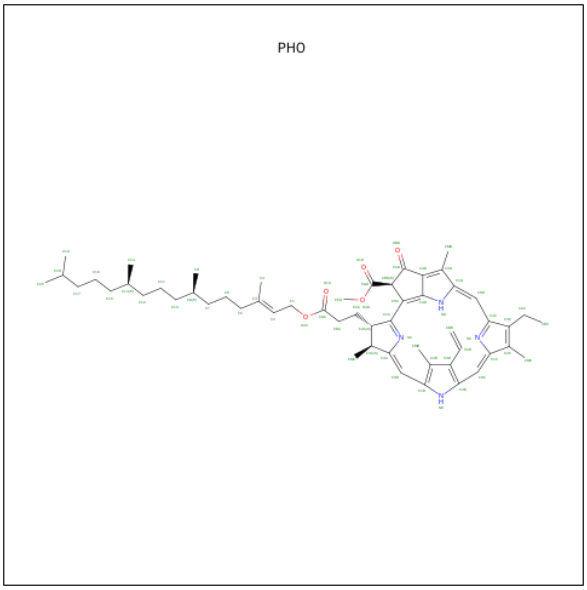
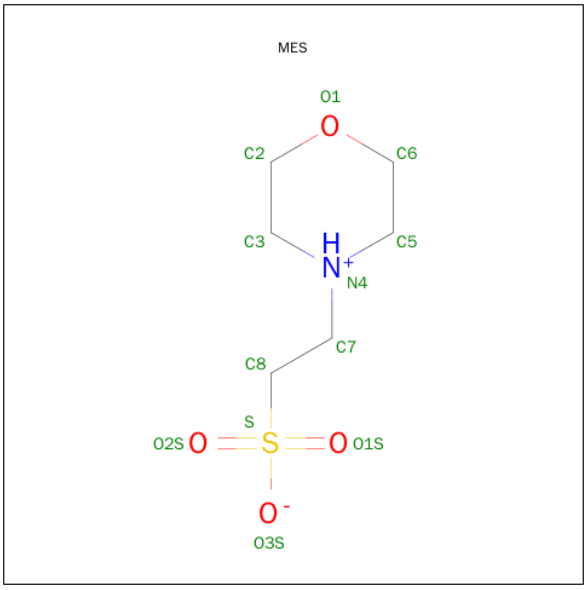
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C Mg N O 65 55 1 4 5	0	0
21	B	1	Total C Mg N O 65 55 1 4 5	0	0
21	B	1	Total C Mg N O 65 55 1 4 5	0	0
21	B	1	Total C Mg N O 65 55 1 4 5	0	0
21	B	1	Total C Mg N O 65 55 1 4 5	0	0
21	C	1	Total C Mg N O 65 55 1 4 5	0	0
21	C	1	Total C Mg N O 65 55 1 4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

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



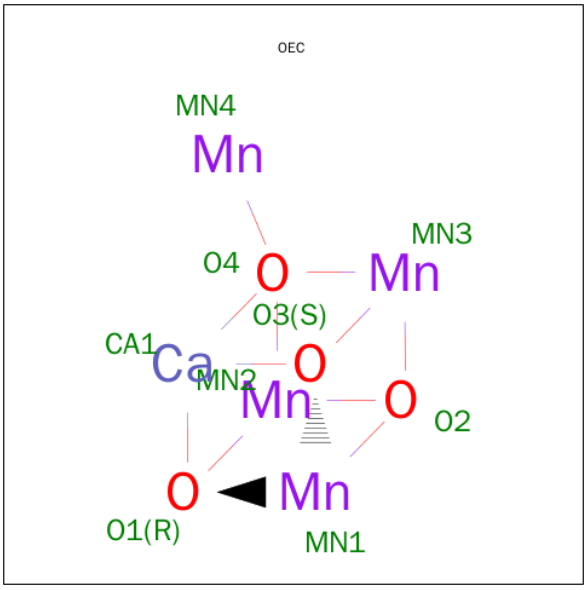
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C N O 64 55 4 5	0	0
22	D	1	Total C N O 64 55 4 5	0	0

- Molecule 23 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



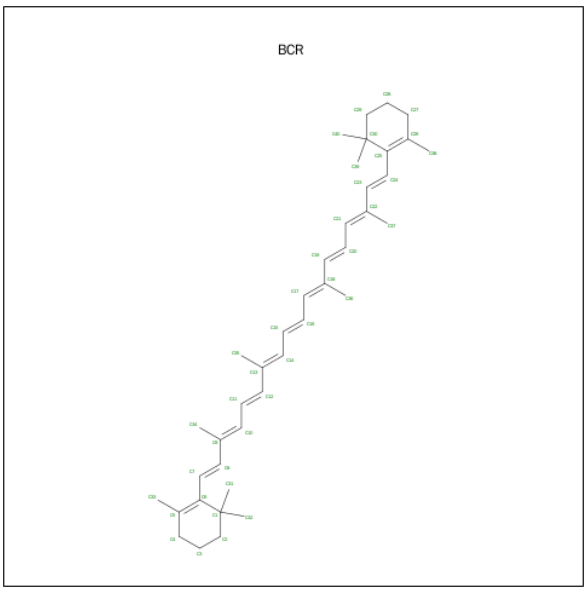
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 24 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



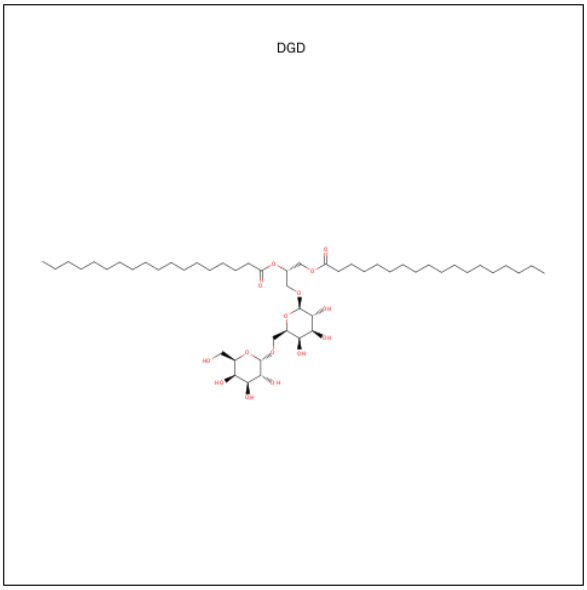
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	Ca	Mn		0	0
			5	1	4			

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



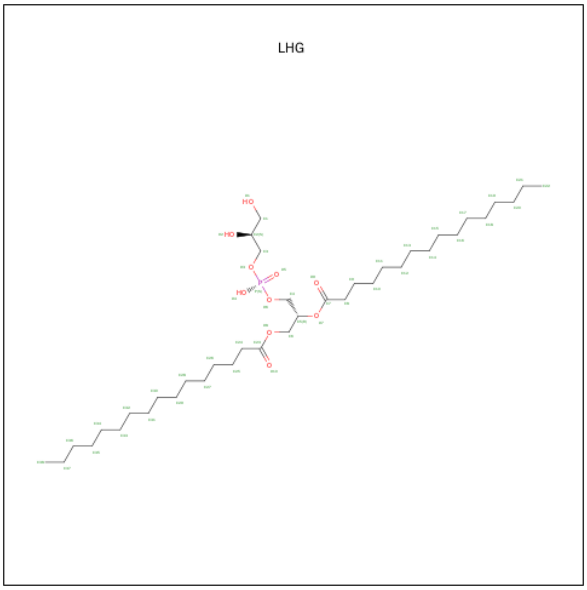
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	X	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	Z	1	Total C 40 40	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



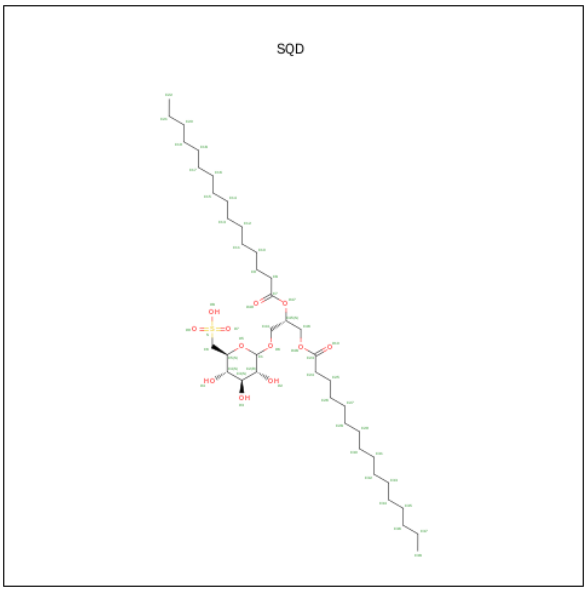
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O 56 41 15	0	0
26	A	1	Total C O 52 37 15	0	0
26	B	1	Total C O 66 51 15	0	0
26	C	1	Total C O 53 38 15	0	0
26	C	1	Total C O 62 47 15	0	0
26	C	1	Total C O 66 51 15	0	0
26	D	1	Total C O 63 48 15	0	0
26	B	1	Total C O 58 43 15	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



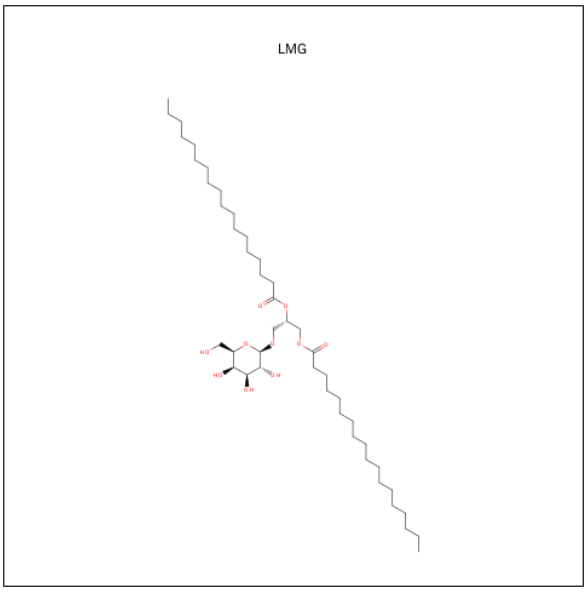
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O P 39 28 10 1	0	0
27	C	1	Total C O P 37 26 10 1	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



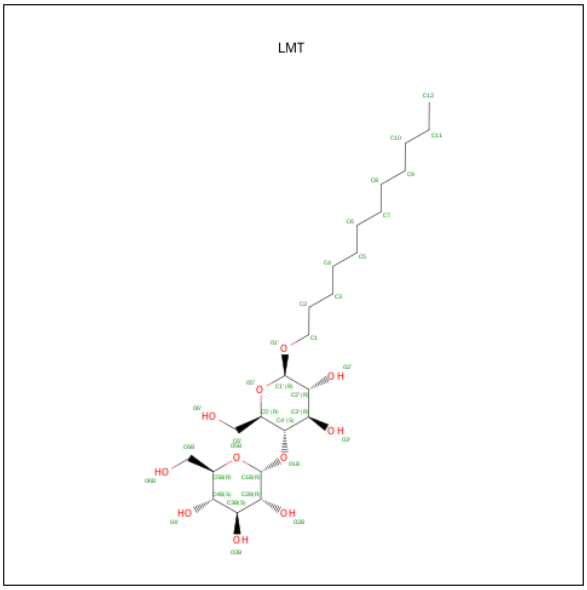
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total	C	O	S	0	0
			51	38	12	1		
28	D	1	Total	C	O	S	0	0
			43	30	12	1		
28	F	1	Total	C	O	S	0	0
			45	32	12	1		
28	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	B	1	Total C O 49 39 10	0	0
29	J	1	Total C O 48 38 10	0	0
29	C	1	Total C O 45 35 10	0	0
29	D	1	Total C O 46 36 10	0	0
29	D	1	Total C O 48 38 10	0	0
29	I	1	Total C O 43 33 10	0	0
29	M	1	Total C O 42 32 10	0	0

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

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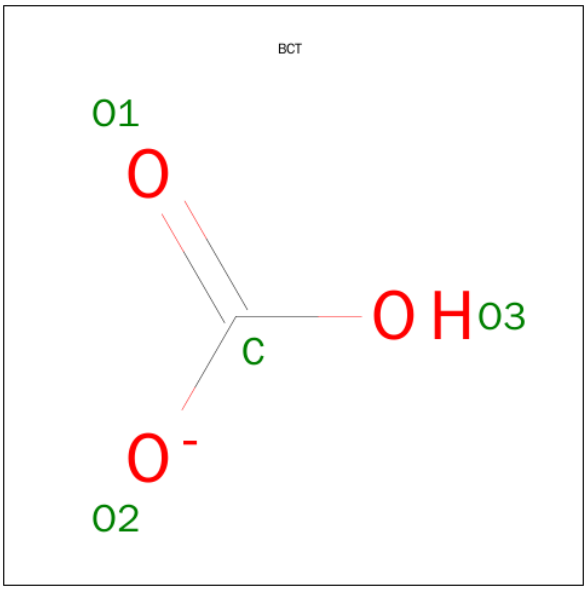
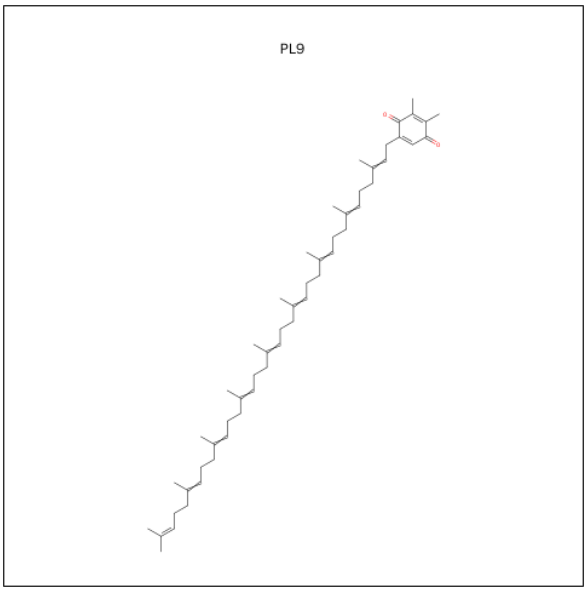
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	D	1	Total C O 31 20 11	0	0
30	T	1	Total C O 35 24 11	0	0
30	I	1	Total C O 35 24 11	0	0
30	O	1	Total C O 35 24 11	0	0

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



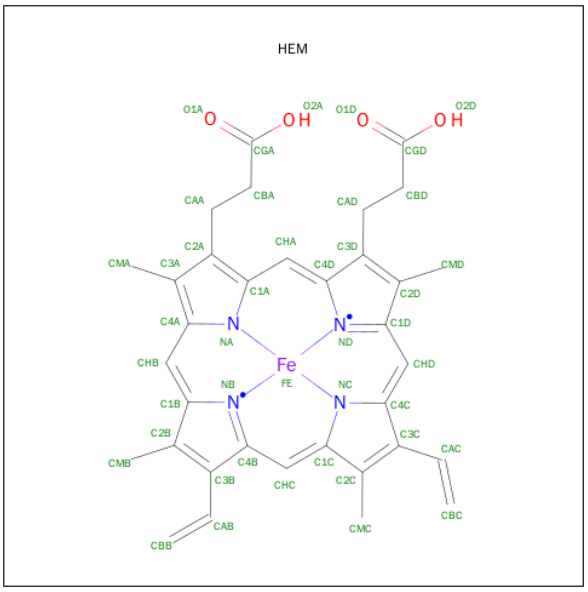
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	D	1	Total C O 4 1 3	0	0

- Molecule 32 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
32	D	1	Total	C	O	0	0
			55	53	2		

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

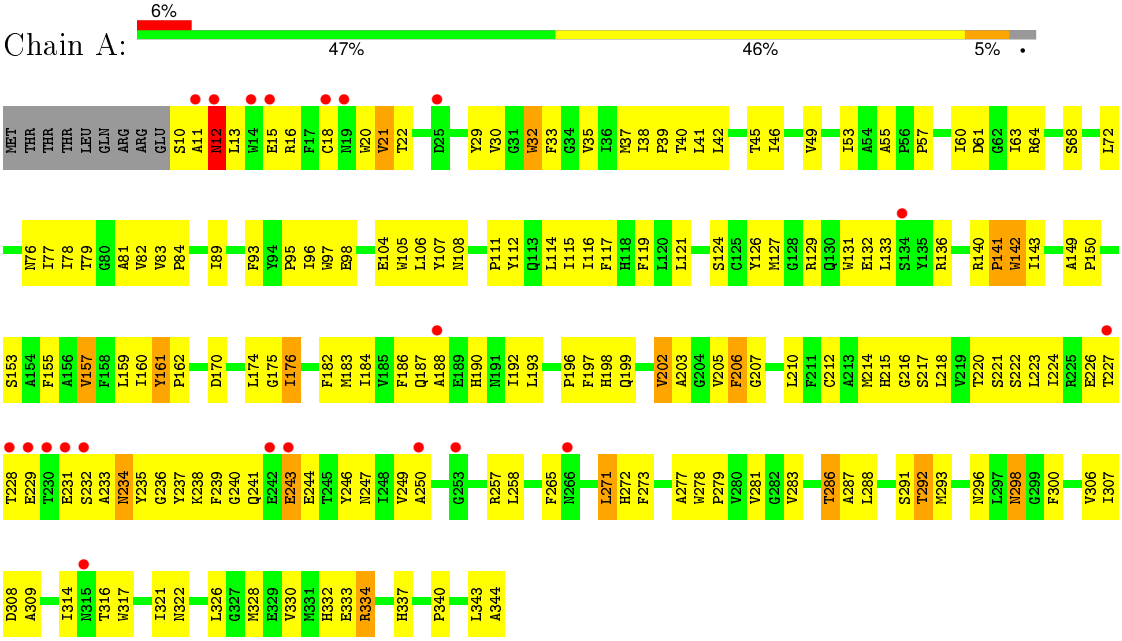
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	O	1	Total Ca 1 1	0	0
34	K	1	Total Ca 1 1	0	0
34	F	1	Total Ca 1 1	0	0

3 Residue-property plots (i)

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.

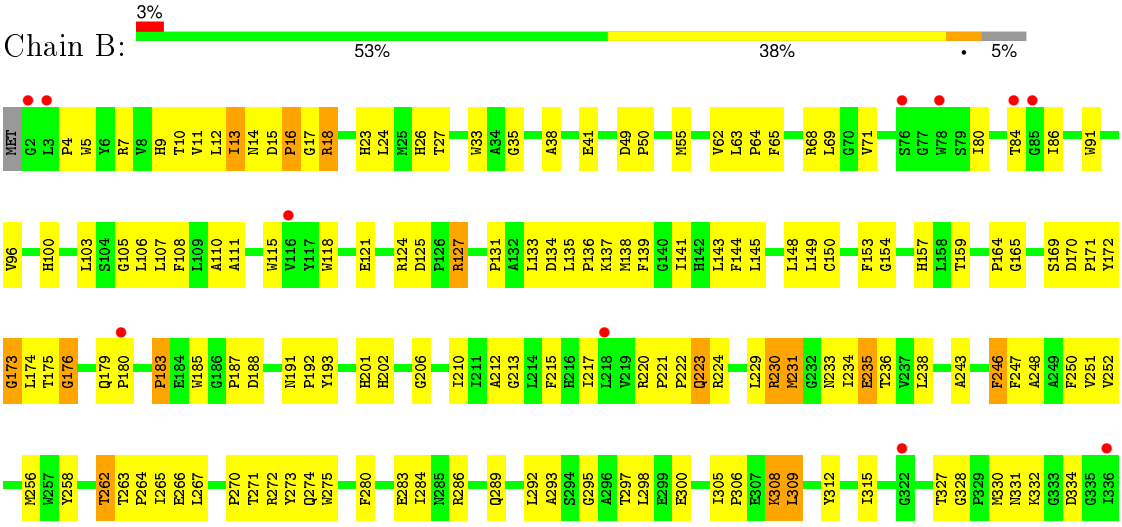
- Molecule 1: Photosystem Q(B) protein 1

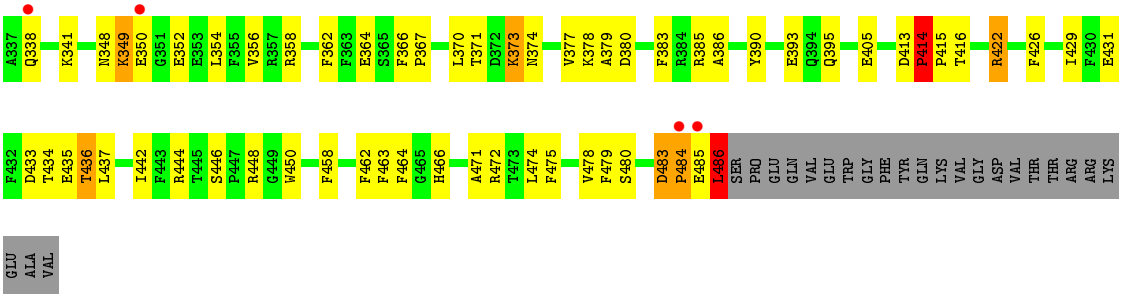
Chain A:



- Molecule 2: Photosystem II core light harvesting protein

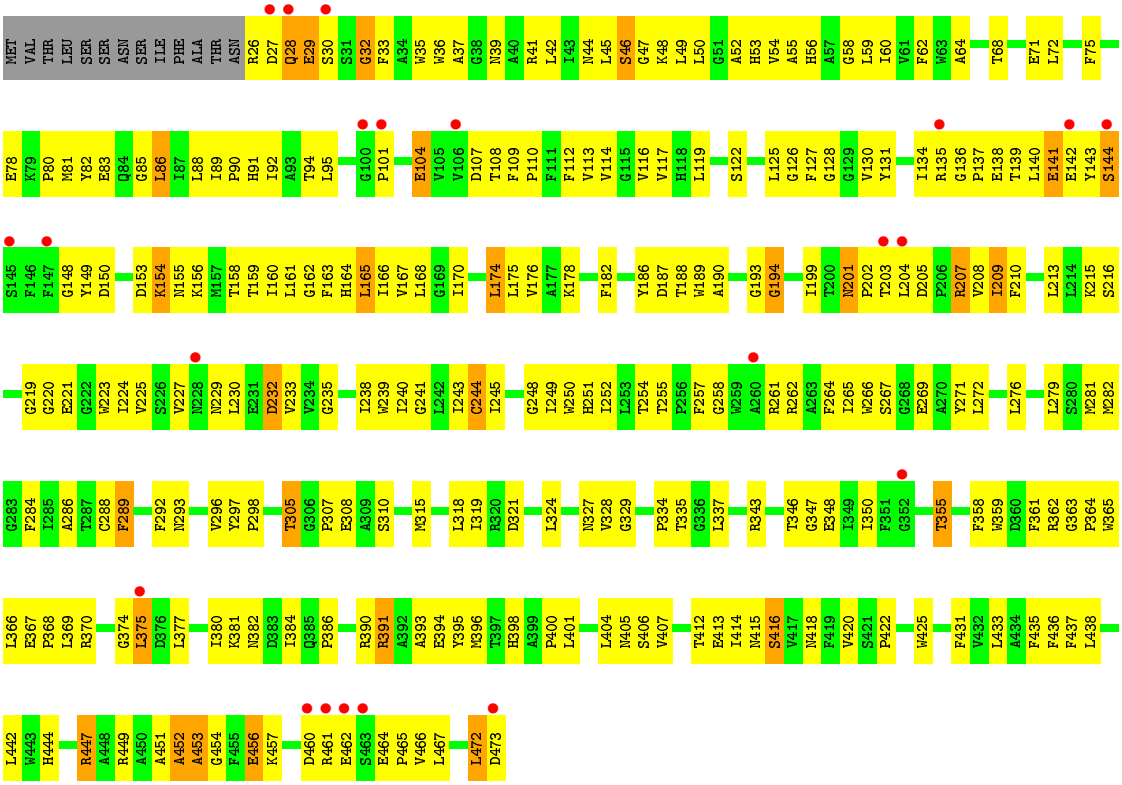
Chain B:





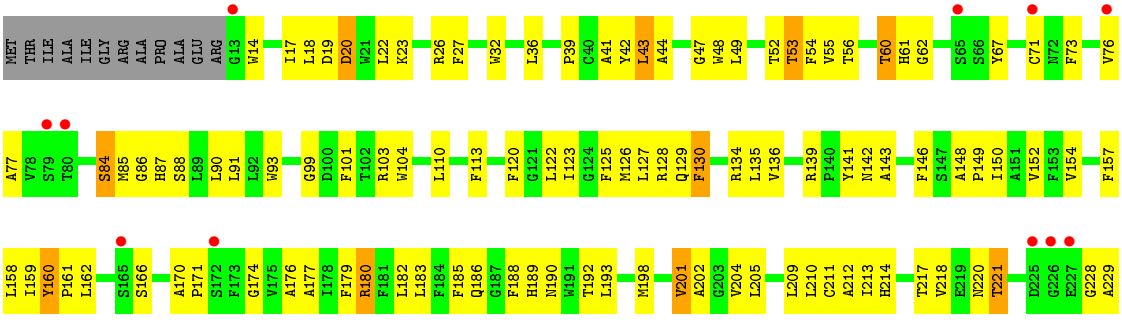
• Molecule 3: Photosystem II CP43 protein

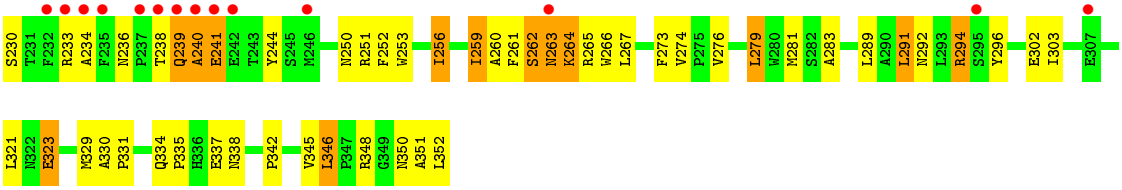
Chain C:



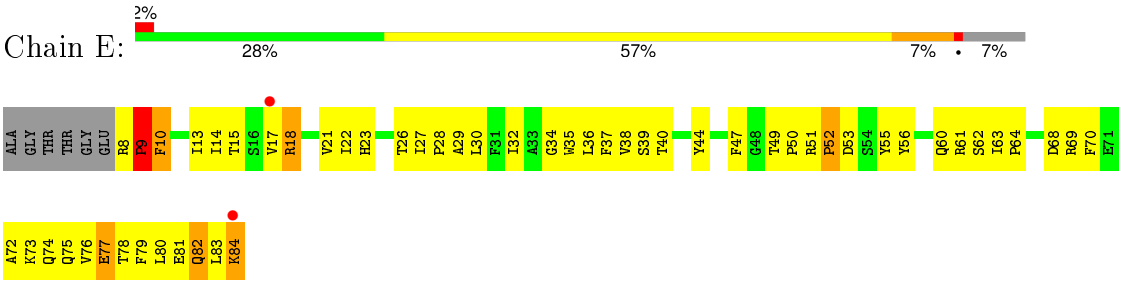
• Molecule 4: Photosystem II D2 protein

Chain D:

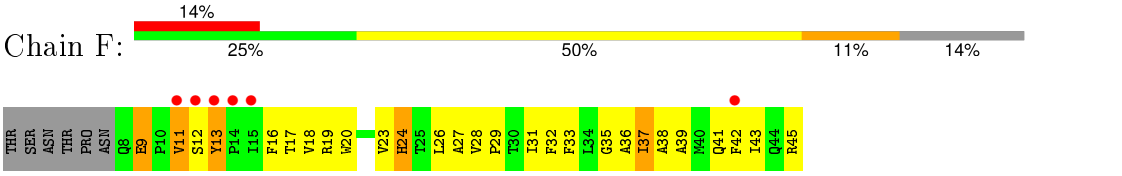




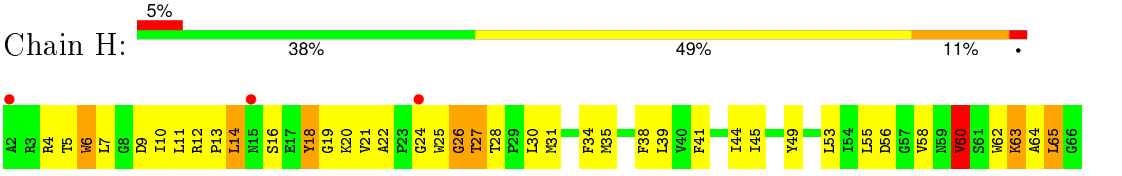
- Molecule 5: Cytochrome b559 subunit alpha



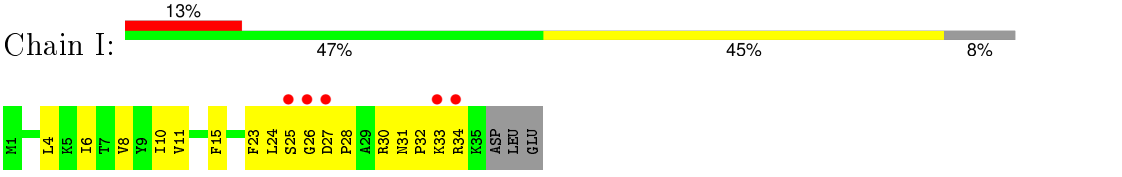
- Molecule 6: Cytochrome b559 subunit beta



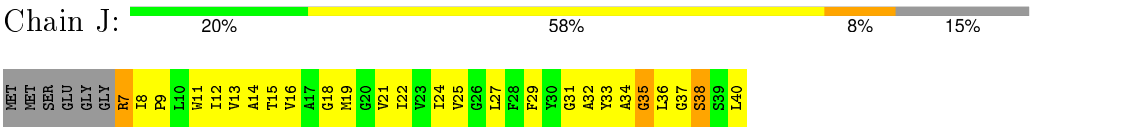
- Molecule 7: Photosystem II reaction center protein H



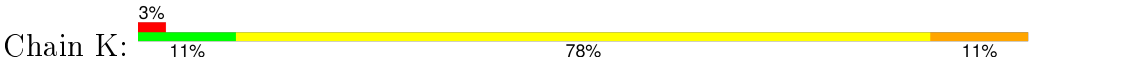
- Molecule 8: Photosystem II reaction center protein I

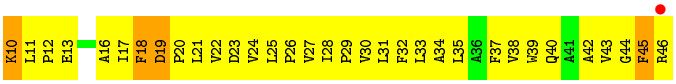


- Molecule 9: Photosystem II reaction center protein J



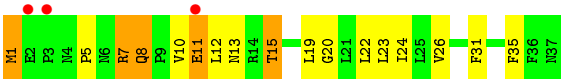
- Molecule 10: Photosystem II reaction center protein K





• Molecule 11: Photosystem II reaction center protein L

Chain L:

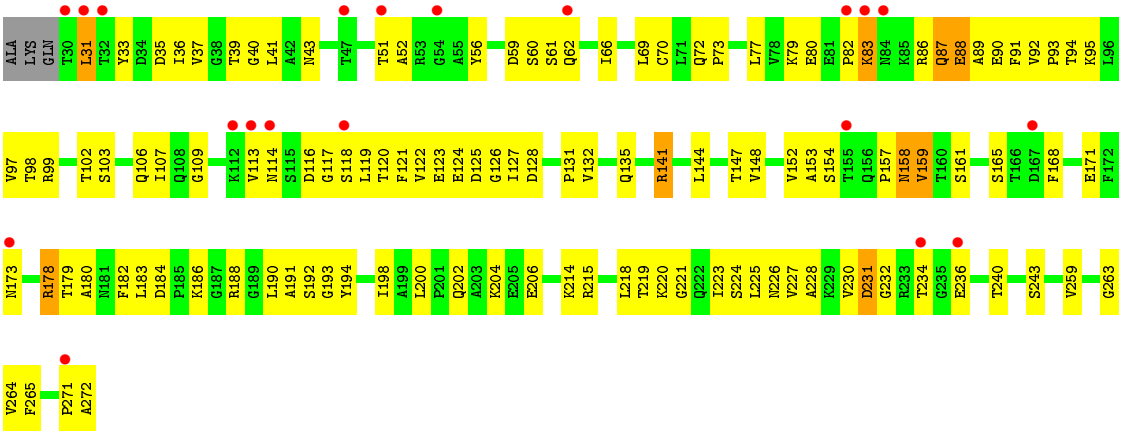


• Molecule 12: Photosystem II reaction center protein M

Chain M:

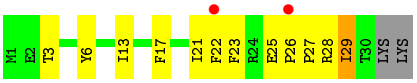
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



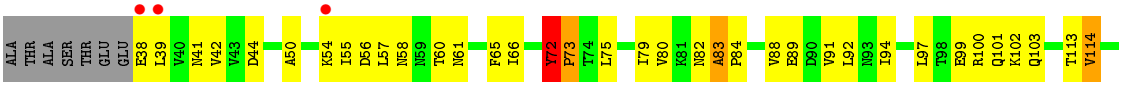
• Molecule 14: Photosystem II reaction center protein T

Chain T:

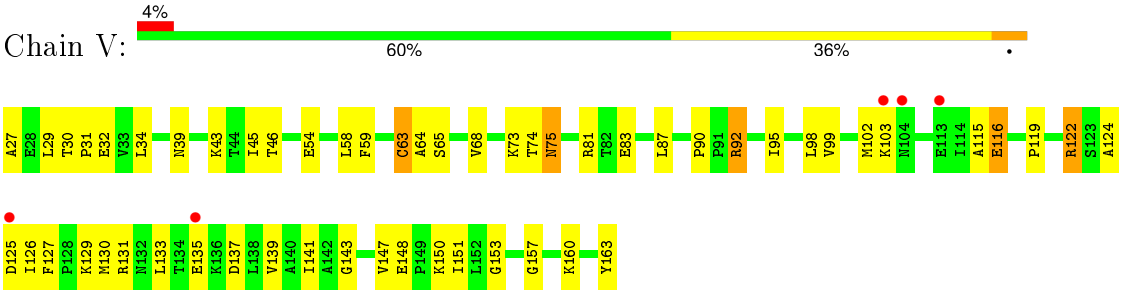


• Molecule 15: Photosystem II 12 kDa extrinsic protein

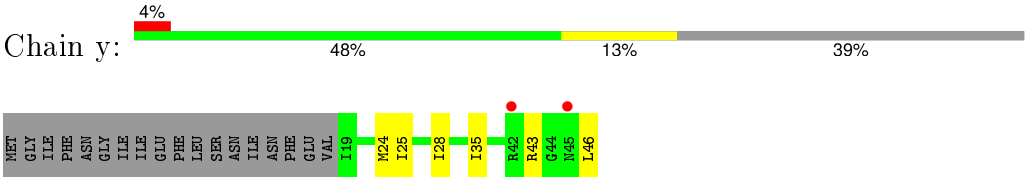
Chain U:



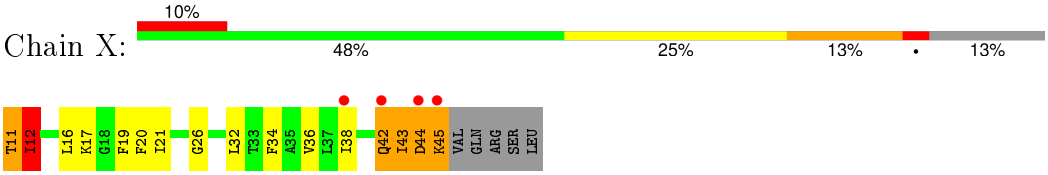
• Molecule 16: Cytochrome c-550



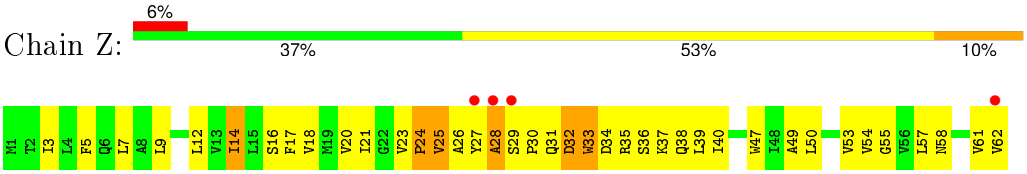
• Molecule 17: Photosystem II reaction center protein ycf12



• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.89Å 224.69Å 337.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 29.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.87-3.60) 99.3 (29.87-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.297 , 0.308 0.303 , 0.326	Depositor DCC
R_{free} test set	1054 reflections (2.04%)	DCC
Wilson B-factor (Å^2)	153.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 83.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 52688 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24678	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CA, LMT, CLA, PL9, BCT, FE2, MES, OEC, HEM, LMG, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/2713	0.66	0/3700
2	B	0.43	0/3947	0.66	1/5379 (0.0%)
3	C	0.41	0/3567	0.64	1/4856 (0.0%)
4	D	0.47	0/2801	0.65	0/3818
5	E	0.43	0/654	0.69	0/891
6	F	0.62	0/317	0.71	0/433
7	H	0.38	0/520	0.67	0/709
8	I	0.51	0/293	0.68	0/395
9	J	0.41	0/255	0.68	0/346
10	K	0.41	0/303	0.62	0/416
11	L	0.37	0/311	0.65	0/422
12	M	0.44	0/270	0.70	0/367
13	O	0.44	0/1876	0.70	0/2548
14	T	0.49	0/265	0.63	0/359
15	U	0.42	0/785	0.73	1/1064 (0.1%)
16	V	0.39	0/1081	0.65	0/1468
17	y	0.46	0/202	0.73	0/272
18	X	0.42	0/257	0.59	0/348
19	Z	0.45	0/490	0.69	0/669
All	All	0.43	0/20907	0.66	3/28460 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	486	LEU	CA-CB-CG	6.98	131.36	115.30
3	C	32	GLY	N-CA-C	-5.55	99.23	113.10
15	U	72	TYR	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	244	0
2	B	3812	0	3683	272	0
3	C	3455	0	3378	373	0
4	D	2706	0	2608	238	0
5	E	635	0	625	82	0
6	F	307	0	312	49	0
7	H	507	0	521	67	0
8	I	286	0	308	18	0
9	J	249	0	262	50	0
10	K	293	0	305	56	0
11	L	304	0	316	28	0
12	M	267	0	289	34	0
13	O	1845	0	1801	119	0
14	T	256	0	262	24	0
15	U	774	0	773	47	0
16	V	1060	0	1068	49	0
17	y	201	0	226	0	0
18	X	254	0	282	28	0
19	Z	479	0	516	64	0
20	A	1	0	0	0	0
21	A	260	0	288	49	0
21	B	1040	0	1152	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	780	0	864	143	0
21	D	130	0	144	20	0
21	K	65	0	72	15	0
22	A	64	0	74	8	0
22	D	64	0	74	12	0
23	A	12	0	13	13	0
24	A	5	0	0	0	0
25	A	40	0	56	8	0
25	B	120	0	168	7	0
25	C	80	0	112	26	0
25	D	40	0	56	8	0
25	J	80	0	112	19	0
25	X	40	0	56	6	0
25	Z	40	0	56	4	0
26	A	52	0	62	1	0
26	B	124	0	170	42	0
26	C	237	0	311	76	0
26	D	63	0	87	0	0
27	A	39	0	51	7	0
27	C	37	0	44	5	0
28	C	51	0	68	5	0
28	D	43	0	49	9	0
28	F	45	0	53	0	0
28	L	47	0	60	2	0
29	A	51	0	72	40	0
29	B	49	0	68	6	0
29	C	45	0	60	6	0
29	D	94	0	127	36	0
29	I	43	0	56	0	0
29	J	48	0	66	4	0
29	M	42	0	54	3	0
30	A	35	0	46	0	0
30	B	35	0	46	2	0
30	D	66	0	81	3	0
30	I	35	0	46	2	0
30	O	35	0	46	1	0
30	T	35	0	46	1	0
31	D	4	0	0	0	0
32	D	55	0	80	31	0
33	F	43	0	30	6	0
33	V	43	0	30	5	0
34	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	K	1	0	0	0	0
34	O	1	0	0	0	0
All	All	24678	0	25265	1799	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 1799 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)
28:C:475:SQD:C4	28:C:475:SQD:C3	1.74	1.58
16:V:63:CYS:SG	33:V:164:HEM:HAB	1.65	1.35
29:A:373:LMG:H112	4:D:266:TRP:CH2	1.77	1.19
1:A:271:LEU:HD11	23:A:367:MES:C8	1.73	1.17
26:B:533:DGD:HAH1	12:M:17:VAL:HG21	1.21	1.14

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	9 52
2	B	483/510 (95%)	416 (86%)	54 (11%)	13 (3%)	6 46
3	C	446/461 (97%)	370 (83%)	60 (14%)	16 (4%)	4 39
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	6 46
5	E	75/83 (90%)	66 (88%)	5 (7%)	4 (5%)	2 27
6	F	36/44 (82%)	22 (61%)	9 (25%)	5 (14%)	0 6
7	H	63/65 (97%)	45 (71%)	9 (14%)	9 (14%)	0 5
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2 23
10	K	35/37 (95%)	26 (74%)	7 (20%)	2 (6%)	2 25
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100 100
13	O	241/246 (98%)	201 (83%)	29 (12%)	11 (5%)	3 31
14	T	28/32 (88%)	25 (89%)	3 (11%)	0	100 100
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3 33
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	26 72
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0 4
18	X	33/40 (82%)	25 (76%)	5 (15%)	3 (9%)	1 13
19	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3 29
All	All	2559/2714 (94%)	2121 (83%)	343 (13%)	95 (4%)	4 38

5 of 95 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/280 (97%)	257 (95%)	14 (5%)	29 69
2	B	385/407 (95%)	369 (96%)	16 (4%)	36 75
3	C	348/362 (96%)	327 (94%)	21 (6%)	24 65
4	D	275/283 (97%)	256 (93%)	19 (7%)	19 60
5	E	69/72 (96%)	64 (93%)	5 (7%)	18 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	32/38 (84%)	31 (97%)	1 (3%)	47 81
7	H	53/54 (98%)	49 (92%)	4 (8%)	17 57
8	I	32/35 (91%)	31 (97%)	1 (3%)	47 81
9	J	24/28 (86%)	23 (96%)	1 (4%)	36 75
10	K	30/30 (100%)	27 (90%)	3 (10%)	9 43
11	L	35/35 (100%)	30 (86%)	5 (14%)	4 27
12	M	31/33 (94%)	31 (100%)	0	100 100
13	O	202/208 (97%)	193 (96%)	9 (4%)	34 74
14	T	27/29 (93%)	26 (96%)	1 (4%)	41 77
15	U	84/89 (94%)	80 (95%)	4 (5%)	31 72
16	V	116/117 (99%)	111 (96%)	5 (4%)	35 75
17	y	20/37 (54%)	18 (90%)	2 (10%)	9 43
18	X	28/33 (85%)	24 (86%)	4 (14%)	4 27
19	Z	52/52 (100%)	47 (90%)	5 (10%)	10 45
All	All	2114/2222 (95%)	1994 (94%)	120 (6%)	25 67

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	60	THR
4	D	294	ARG
17	y	46	LEU
4	D	84	SER
4	D	221	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	142	ASN
5	E	74	GLN
15	U	82	ASN
4	D	250	ASN
6	F	44	GLN

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 87 ligands modelled in this entry, 4 are monoatomic - leaving 83 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	$\#\|Z\| > 2$
21	CLA	A	362	-	55,73,73	2.30	12 (21%)	61,113,113	1.51	11 (18%)
21	CLA	A	363	-	55,73,73	2.50	14 (25%)	61,113,113	1.76	13 (21%)
21	CLA	A	364	-	55,73,73	2.61	13 (23%)	61,113,113	1.60	12 (19%)
22	PHO	A	365	-	67,69,69	2.36	14 (20%)	84,99,99	1.48	13 (15%)
21	CLA	A	366	-	55,73,73	2.63	12 (21%)	61,113,113	1.46	9 (14%)
23	MES	A	367	-	11,12,12	0.92	0	14,16,16	1.33	2 (14%)
24	OEC	A	368	1,3	0,0,13	0.00	-	0,0,27	0.00	-
25	BCR	A	369	-	41,41,41	1.90	6 (14%)	56,56,56	2.15	18 (32%)
27	LHG	A	371	-	38,38,48	2.10	6 (15%)	39,44,54	1.37	4 (10%)
29	LMG	A	373	-	51,51,55	0.54	1 (1%)	59,59,63	1.12	6 (10%)
26	DGD	A	375	-	53,53,67	2.02	13 (24%)	67,67,81	2.57	22 (32%)
30	LMT	A	376	-	36,36,36	1.96	10 (27%)	47,47,47	1.48	8 (17%)
21	CLA	B	511	-	55,73,73	3.19	18 (32%)	61,113,113	1.58	10 (16%)
21	CLA	B	512	-	55,73,73	2.43	11 (20%)	61,113,113	1.42	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	513	-	55,73,73	2.48	13 (23%)	61,113,113	1.66	16 (26%)
21	CLA	B	514	-	55,73,73	2.71	12 (21%)	61,113,113	1.48	13 (21%)
21	CLA	B	515	-	55,73,73	2.72	14 (25%)	61,113,113	1.64	11 (18%)
21	CLA	B	516	-	55,73,73	2.88	14 (25%)	61,113,113	1.73	17 (27%)
21	CLA	B	517	-	55,73,73	2.84	15 (27%)	61,113,113	1.97	17 (27%)
21	CLA	B	518	-	55,73,73	2.89	15 (27%)	61,113,113	1.96	20 (32%)
21	CLA	B	519	-	55,73,73	2.70	11 (20%)	61,113,113	1.60	13 (21%)
21	CLA	B	520	-	55,73,73	2.61	12 (21%)	61,113,113	1.51	9 (14%)
21	CLA	B	521	-	55,73,73	2.77	13 (23%)	61,113,113	1.79	16 (26%)
21	CLA	B	522	-	55,73,73	2.49	13 (23%)	61,113,113	1.50	13 (21%)
21	CLA	B	523	-	55,73,73	2.48	12 (21%)	61,113,113	1.37	10 (16%)
21	CLA	B	524	-	55,73,73	2.87	15 (27%)	61,113,113	1.79	12 (19%)
21	CLA	B	525	-	55,73,73	2.75	14 (25%)	61,113,113	1.49	10 (16%)
21	CLA	B	526	-	55,73,73	2.81	13 (23%)	61,113,113	1.48	10 (16%)
25	BCR	B	527	-	41,41,41	1.79	7 (17%)	56,56,56	2.39	20 (35%)
26	DGD	B	528	-	59,59,67	0.58	2 (3%)	73,73,81	1.09	8 (10%)
25	BCR	B	529	-	41,41,41	2.18	9 (21%)	56,56,56	2.24	19 (33%)
25	BCR	B	530	-	41,41,41	2.48	11 (26%)	56,56,56	2.27	23 (41%)
29	LMG	B	531	-	49,49,55	1.59	6 (12%)	57,57,63	2.79	18 (31%)
26	DGD	B	533	-	67,67,67	1.45	13 (19%)	81,81,81	1.85	19 (23%)
30	LMT	B	535	-	36,36,36	1.84	9 (25%)	47,47,47	1.16	2 (4%)
26	DGD	C	474	-	57,57,67	2.03	15 (26%)	71,71,81	3.74	25 (35%)
28	SQD	C	475	-	50,51,54	2.61	27 (54%)	58,62,65	2.99	17 (29%)
27	LHG	C	476	-	36,36,48	2.26	7 (19%)	37,42,54	1.46	4 (10%)
21	CLA	C	477	-	55,73,73	2.68	12 (21%)	61,113,113	1.68	10 (16%)
21	CLA	C	478	-	55,73,73	2.58	13 (23%)	61,113,113	1.55	10 (16%)
21	CLA	C	479	-	55,73,73	2.78	14 (25%)	61,113,113	1.70	10 (16%)
21	CLA	C	480	-	55,73,73	2.71	14 (25%)	61,113,113	1.93	12 (19%)
21	CLA	C	481	-	55,73,73	2.89	13 (23%)	61,113,113	2.03	15 (24%)
21	CLA	C	482	-	55,73,73	3.17	17 (30%)	61,113,113	1.57	15 (24%)
21	CLA	C	483	-	55,73,73	2.80	16 (29%)	61,113,113	1.51	11 (18%)
21	CLA	C	484	-	55,73,73	2.71	13 (23%)	61,113,113	1.63	12 (19%)
21	CLA	C	485	-	55,73,73	2.61	12 (21%)	61,113,113	1.42	8 (13%)
21	CLA	C	486	3	55,73,73	2.88	17 (30%)	61,113,113	1.65	14 (22%)
21	CLA	C	487	-	55,73,73	3.08	16 (29%)	61,113,113	1.49	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	C	488	-	55,73,73	2.72	14 (25%)	61,113,113	1.63	13 (21%)
25	BCR	C	489	-	41,41,41	1.87	9 (21%)	56,56,56	2.13	17 (30%)
25	BCR	C	490	-	41,41,41	1.96	8 (19%)	56,56,56	2.26	22 (39%)
26	DGD	C	491	-	54,54,67	1.59	9 (16%)	68,68,81	3.18	23 (33%)
26	DGD	C	492	-	63,63,67	1.33	9 (14%)	77,77,81	2.90	21 (27%)
26	DGD	C	493	-	67,67,67	1.42	16 (23%)	81,81,81	3.14	27 (33%)
29	LMG	C	494	-	45,45,55	1.85	8 (17%)	53,53,63	2.27	15 (28%)
31	BCT	D	353	20	0,3,3	0.00	-	0,3,3	0.00	-
21	CLA	D	354	-	55,73,73	2.60	13 (23%)	61,113,113	1.59	13 (21%)
22	PHO	D	355	-	67,69,69	2.24	14 (20%)	84,99,99	1.40	12 (14%)
21	CLA	D	356	-	55,73,73	2.63	15 (27%)	61,113,113	1.63	11 (18%)
32	PL9	D	357	-	55,55,55	3.48	22 (40%)	68,69,69	3.18	26 (38%)
25	BCR	D	358	-	41,41,41	1.71	7 (17%)	56,56,56	2.36	20 (35%)
29	LMG	D	359	-	46,46,55	1.65	6 (13%)	54,54,63	2.58	16 (29%)
29	LMG	D	360	-	48,48,55	0.55	1 (2%)	56,56,63	1.14	6 (10%)
28	SQD	D	361	-	42,43,54	2.65	20 (47%)	50,54,65	3.26	16 (32%)
26	DGD	D	362	-	64,64,67	2.04	22 (34%)	78,78,81	2.70	20 (25%)
30	LMT	D	363	-	32,32,36	1.77	7 (21%)	43,43,47	1.47	6 (13%)
30	LMT	D	536	-	36,36,36	1.66	9 (25%)	47,47,47	1.56	8 (17%)
28	SQD	F	224	-	44,45,54	2.69	21 (47%)	52,56,65	3.04	16 (30%)
33	HEM	F	85	5	30,50,50	2.37	12 (40%)	24,82,82	4.02	12 (50%)
29	LMG	I	220	-	43,43,55	1.95	11 (25%)	51,51,63	2.18	14 (27%)
30	LMT	I	274	-	36,36,36	1.82	11 (30%)	47,47,47	1.33	7 (14%)
25	BCR	J	112	-	41,41,41	1.88	7 (17%)	56,56,56	2.46	25 (44%)
25	BCR	J	115	-	41,41,41	2.26	11 (26%)	56,56,56	3.28	18 (32%)
29	LMG	J	492	-	48,48,55	1.88	9 (18%)	56,56,63	1.87	16 (28%)
21	CLA	K	483	-	55,73,73	2.50	12 (21%)	61,113,113	1.48	9 (14%)
28	SQD	L	213	-	46,47,54	2.66	24 (52%)	54,58,65	3.11	17 (31%)
29	LMG	M	217	-	42,42,55	1.87	8 (19%)	50,50,63	1.53	7 (14%)
30	LMT	O	274	-	36,36,36	1.97	11 (30%)	47,47,47	1.39	8 (17%)
30	LMT	T	226	-	36,36,36	1.75	9 (25%)	47,47,47	0.99	2 (4%)
33	HEM	V	164	16	30,50,50	2.41	8 (26%)	24,82,82	3.99	12 (50%)
25	BCR	X	107	-	41,41,41	1.55	6 (14%)	56,56,56	2.44	20 (35%)
25	BCR	Z	116	-	41,41,41	1.93	8 (19%)	56,56,56	2.14	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
21	CLA	A	362	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	A	363	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	A	364	-	4/4/20/25	0/37/135/135	0/0/9/9
22	PHO	A	365	-	1/1/17/22	0/53/103/103	0/1/6/6
21	CLA	A	366	-	4/4/20/25	0/37/135/135	0/0/9/9
23	MES	A	367	-	-	0/6/14/14	0/1/1/1
24	OEC	A	368	1,3	-	0/0/0/54	0/0/0/5
25	BCR	A	369	-	-	0/29/63/63	0/2/2/2
27	LHG	A	371	-	-	0/43/43/53	0/0/0/0
29	LMG	A	373	-	-	0/46/66/70	0/1/1/1
26	DGD	A	375	-	-	0/41/81/95	0/2/2/2
30	LMT	A	376	-	-	0/21/61/61	0/2/2/2
21	CLA	B	511	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	512	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	513	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	514	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	515	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	516	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	517	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	518	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	519	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	520	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	521	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	522	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	523	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	524	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	525	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	B	526	-	4/4/20/25	0/37/135/135	0/0/9/9
25	BCR	B	527	-	-	0/29/63/63	0/2/2/2
26	DGD	B	528	-	-	0/47/87/95	0/2/2/2
25	BCR	B	529	-	-	0/29/63/63	0/2/2/2
25	BCR	B	530	-	-	0/29/63/63	0/2/2/2
29	LMG	B	531	-	-	0/44/64/70	0/1/1/1
26	DGD	B	533	-	-	0/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	B	535	-	-	0/21/61/61	0/2/2/2
26	DGD	C	474	-	-	0/45/85/95	0/2/2/2
28	SQD	C	475	-	-	0/46/66/69	0/1/1/1
27	LHG	C	476	-	-	0/41/41/53	0/0/0/0
21	CLA	C	477	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	478	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	479	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	480	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	481	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	482	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	483	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	484	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	485	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	486	3	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	487	-	4/4/20/25	0/37/135/135	0/0/9/9
21	CLA	C	488	-	4/4/20/25	0/37/135/135	0/0/9/9
25	BCR	C	489	-	-	0/29/63/63	0/2/2/2
25	BCR	C	490	-	-	0/29/63/63	0/2/2/2
26	DGD	C	491	-	-	0/42/82/95	0/2/2/2
26	DGD	C	492	-	1/1/13/13	0/51/91/95	0/2/2/2
26	DGD	C	493	-	1/1/13/13	0/55/95/95	0/2/2/2
29	LMG	C	494	-	-	0/40/60/70	0/1/1/1
31	BCT	D	353	20	-	0/0/0/0	0/0/0/0
21	CLA	D	354	-	4/4/20/25	0/37/135/135	0/0/9/9
22	PHO	D	355	-	1/1/17/22	0/53/103/103	0/1/6/6
21	CLA	D	356	-	4/4/20/25	0/37/135/135	0/0/9/9
32	PL9	D	357	-	-	2/53/73/73	0/1/1/1
25	BCR	D	358	-	-	0/29/63/63	0/2/2/2
29	LMG	D	359	-	-	0/41/61/70	0/1/1/1
29	LMG	D	360	-	-	0/43/63/70	0/1/1/1
28	SQD	D	361	-	-	2/38/58/69	0/1/1/1
26	DGD	D	362	-	-	0/52/92/95	0/2/2/2
30	LMT	D	363	-	-	0/17/57/61	0/2/2/2
30	LMT	D	536	-	-	0/21/61/61	0/2/2/2
28	SQD	F	224	-	-	0/40/60/69	0/1/1/1
33	HEM	F	85	5	-	0/10/54/54	0/0/8/8
29	LMG	I	220	-	-	0/38/58/70	0/1/1/1
30	LMT	I	274	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	J	112	-	-	0/29/63/63	0/2/2/2
25	BCR	J	115	-	-	0/29/63/63	0/2/2/2
29	LMG	J	492	-	-	0/43/63/70	0/1/1/1
21	CLA	K	483	-	4/4/20/25	0/37/135/135	0/0/9/9
28	SQD	L	213	-	-	0/42/62/69	0/1/1/1
29	LMG	M	217	-	-	0/37/57/70	0/1/1/1
30	LMT	O	274	-	-	0/21/61/61	0/2/2/2
30	LMT	T	226	-	-	0/21/61/61	0/2/2/2
33	HEM	V	164	16	-	0/10/54/54	0/0/8/8
25	BCR	X	107	-	-	0/29/63/63	0/2/2/2
25	BCR	Z	116	-	-	0/29/63/63	0/2/2/2

The worst 5 of 956 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	531	LMG	O1-C1	-9.18	1.23	1.40
29	M	217	LMG	O1-C1	-9.15	1.23	1.40
29	I	220	LMG	O1-C1	-9.10	1.23	1.40
29	C	494	LMG	O1-C1	-9.08	1.23	1.40
29	J	492	LMG	O1-C1	-9.07	1.23	1.40

The worst 5 of 1100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	J	115	BCR	C32-C1-C6	-10.95	93.14	110.30
25	J	115	BCR	C32-C1-C31	-8.91	79.83	108.37
32	D	357	PL9	C7-C8-C9	-8.84	111.71	126.70
33	F	85	HEM	C3C-CAC-CBC	-8.71	111.09	124.46
33	F	85	HEM	CMA-C3A-C2A	-8.68	107.09	125.24

5 of 144 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	C	479	CLA	C8
21	C	479	CLA	NC
21	C	479	CLA	ND
21	C	479	CLA	NA
21	C	480	CLA	C8

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	D	357	PL9	C29-C28-C27-C26
32	D	357	PL9	C49-C48-C47-C46
28	D	361	SQD	C45-O47-C7-O49
28	D	361	SQD	C45-O47-C7-C8

There are no ring outliers.

76 monomers are involved in 704 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	362	CLA	20	0
21	A	363	CLA	14	0
21	A	364	CLA	6	0
22	A	365	PHO	8	0
21	A	366	CLA	10	0
23	A	367	MES	13	0
25	A	369	BCR	8	0
27	A	371	LHG	7	0
29	A	373	LMG	40	0
26	A	375	DGD	1	0
21	B	511	CLA	6	0
21	B	512	CLA	9	0
21	B	513	CLA	24	0
21	B	514	CLA	10	0
21	B	515	CLA	10	0
21	B	516	CLA	6	0
21	B	517	CLA	20	0
21	B	518	CLA	15	0
21	B	519	CLA	8	0
21	B	520	CLA	7	0
21	B	521	CLA	12	0
21	B	522	CLA	13	0
21	B	523	CLA	7	0
21	B	524	CLA	5	0
21	B	525	CLA	7	0
21	B	526	CLA	6	0
26	B	528	DGD	23	0
25	B	529	BCR	5	0
25	B	530	BCR	2	0
29	B	531	LMG	6	0
26	B	533	DGD	19	0
30	B	535	LMT	2	0
26	C	474	DGD	8	0
28	C	475	SQD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	476	LHG	5	0
21	C	477	CLA	12	0
21	C	478	CLA	16	0
21	C	479	CLA	18	0
21	C	480	CLA	11	0
21	C	481	CLA	17	0
21	C	482	CLA	6	0
21	C	483	CLA	13	0
21	C	484	CLA	15	0
21	C	485	CLA	5	0
21	C	486	CLA	24	0
21	C	487	CLA	15	0
21	C	488	CLA	7	0
25	C	489	BCR	18	0
25	C	490	BCR	8	0
26	C	491	DGD	17	0
26	C	492	DGD	14	0
26	C	493	DGD	39	0
29	C	494	LMG	6	0
21	D	354	CLA	15	0
22	D	355	PHO	12	0
21	D	356	CLA	5	0
32	D	357	PL9	31	0
25	D	358	BCR	8	0
29	D	359	LMG	6	0
29	D	360	LMG	30	0
28	D	361	SQD	9	0
30	D	363	LMT	2	0
30	D	536	LMT	1	0
33	F	85	HEM	6	0
30	I	274	LMT	2	0
25	J	112	BCR	12	0
25	J	115	BCR	7	0
29	J	492	LMG	4	0
21	K	483	CLA	15	0
28	L	213	SQD	2	0
29	M	217	LMG	3	0
30	O	274	LMT	1	0
30	T	226	LMT	1	0
33	V	164	HEM	5	0
25	X	107	BCR	6	0
25	Z	116	BCR	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/344 (97%)	0.11	21 (6%) 23 15	134, 163, 180, 180	0
2	B	485/510 (95%)	-0.02	15 (3%) 52 38	129, 158, 178, 180	0
3	C	448/461 (97%)	0.07	22 (4%) 33 23	136, 168, 180, 180	0
4	D	340/352 (96%)	0.23	25 (7%) 17 12	126, 154, 179, 180	0
5	E	77/83 (92%)	0.17	2 (2%) 59 44	138, 157, 179, 180	0
6	F	38/44 (86%)	0.23	6 (15%) 3 2	138, 157, 169, 177	0
7	H	65/65 (100%)	0.08	3 (4%) 36 26	139, 164, 177, 180	0
8	I	35/38 (92%)	0.29	5 (14%) 4 3	163, 172, 180, 180	0
9	J	34/40 (85%)	-0.38	0 100 100	141, 155, 169, 171	0
10	K	37/37 (100%)	-0.06	1 (2%) 58 43	156, 166, 179, 180	0
11	L	37/37 (100%)	0.29	3 (8%) 15 10	152, 168, 180, 180	0
12	M	34/36 (94%)	0.76	8 (23%) 1 1	153, 165, 180, 180	0
13	O	243/246 (98%)	0.41	20 (8%) 14 10	143, 174, 180, 180	0
14	T	30/32 (93%)	0.17	2 (6%) 21 13	152, 169, 180, 180	0
15	U	97/104 (93%)	0.20	3 (3%) 52 38	141, 160, 171, 179	0
16	V	137/137 (100%)	0.12	5 (3%) 46 33	136, 160, 171, 174	0
17	y	28/46 (60%)	-0.05	2 (7%) 19 12	158, 175, 180, 180	0
18	X	35/40 (87%)	-0.11	4 (11%) 7 6	144, 156, 174, 178	0
19	Z	62/62 (100%)	0.10	4 (6%) 22 14	166, 178, 180, 180	0
All	All	2597/2714 (95%)	0.13	151 (5%) 26 18	126, 164, 180, 180	0

The worst 5 of 151 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	M	1	MET	7.7

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Mol	Chain	Res	Type	RSRZ
10	K	46	ARG	5.1
7	H	2	ALA	5.0
1	A	18	CYS	4.9
12	M	2	GLU	4.8

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
25	BCR	X	107	40/40	0.81	0.55	6.82	154,158,161,163	0
25	BCR	B	529	40/40	0.74	0.53	5.70	166,169,173,174	0
25	BCR	J	115	40/40	0.66	0.73	4.61	171,180,180,180	0
21	CLA	B	526	65/65	0.67	0.51	4.23	167,177,180,180	0
25	BCR	B	527	40/40	0.78	0.71	4.07	161,169,176,178	0
25	BCR	B	530	40/40	0.42	0.85	3.56	173,180,180,180	0
30	LMT	I	274	35/35	0.73	0.64	3.28	170,180,180,180	0
21	CLA	B	511	65/65	0.73	0.55	3.25	148,179,180,180	0
29	LMG	J	492	48/55	0.73	0.51	3.20	155,175,180,180	0
21	CLA	A	363	65/65	0.78	0.43	3.12	154,161,175,177	0
30	LMT	A	376	35/35	0.72	0.46	2.92	162,180,180,180	0
26	DGD	D	362	63/66	0.70	0.54	2.80	177,180,180,180	0
28	SQD	F	224	45/54	0.55	0.79	2.63	152,179,180,180	0
30	LMT	D	363	31/35	0.69	0.72	2.53	170,180,180,180	0
26	DGD	C	474	56/66	0.69	0.43	2.35	158,180,180,180	0
21	CLA	D	354	65/65	0.86	0.37	2.25	135,154,164,168	0
29	LMG	D	360	48/55	0.67	0.51	2.16	140,169,176,177	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
21	CLA	A	366	65/65	0.76	0.39	2.05	152,162,164,166	0
21	CLA	B	518	65/65	0.90	0.33	1.98	150,164,167,169	0
26	DGD	C	493	66/66	0.81	0.34	1.88	159,174,180,180	0
21	CLA	B	522	65/65	0.92	0.29	1.87	134,144,163,165	0
28	SQD	L	213	47/54	0.71	0.62	1.82	155,178,180,180	0
30	LMT	D	536	35/35	0.74	0.37	1.82	168,173,180,180	0
25	BCR	J	112	40/40	0.83	0.31	1.67	157,160,172,173	0
26	DGD	B	528	58/66	0.82	0.36	1.59	126,136,172,173	0
32	PL9	D	357	55/55	0.65	0.44	1.56	146,153,161,162	0
26	DGD	C	492	62/66	0.77	0.36	1.48	153,171,180,180	0
25	BCR	C	490	40/40	0.79	0.49	1.46	164,169,180,180	0
21	CLA	C	484	65/65	0.88	0.29	1.42	168,177,180,180	0
21	CLA	B	524	65/65	0.80	0.53	1.42	157,180,180,180	0
21	CLA	D	356	65/65	0.83	0.34	1.41	149,154,162,164	0
25	BCR	A	369	40/40	0.82	0.40	1.37	164,171,178,178	0
22	PHO	D	355	64/64	0.91	0.39	1.37	140,162,169,171	0
29	LMG	C	494	45/55	0.69	0.59	1.35	168,180,180,180	0
21	CLA	B	520	65/65	0.93	0.38	1.34	150,162,165,167	0
21	CLA	C	477	65/65	0.88	0.30	1.28	163,169,179,180	0
26	DGD	B	533	66/66	0.78	0.35	1.18	166,179,180,180	0
21	CLA	C	478	65/65	0.87	0.33	1.15	153,155,166,170	0
28	SQD	D	361	43/54	0.86	0.30	1.10	160,173,180,180	0
21	CLA	A	362	65/65	0.90	0.28	0.98	149,154,159,163	0
21	CLA	B	515	65/65	0.93	0.32	0.94	142,162,168,170	0
22	PHO	A	365	64/64	0.92	0.29	0.90	143,154,162,164	0
21	CLA	B	525	65/65	0.84	0.37	0.88	148,167,180,180	0
25	BCR	Z	116	40/40	0.79	0.45	0.85	163,165,170,171	0
21	CLA	C	483	65/65	0.88	0.37	0.84	164,180,180,180	0
29	LMG	M	217	42/55	0.65	0.77	0.79	166,180,180,180	0
21	CLA	C	482	65/65	0.73	0.46	0.74	148,179,180,180	0
25	BCR	D	358	40/40	0.88	0.28	0.70	135,151,162,162	0
29	LMG	D	359	46/55	0.84	0.33	0.68	142,163,180,180	0
21	CLA	K	483	65/65	0.92	0.38	0.65	155,160,174,176	0
29	LMG	A	373	51/55	0.71	0.44	0.63	169,174,180,180	0
21	CLA	B	519	65/65	0.85	0.31	0.61	152,157,158,159	0
21	CLA	C	480	65/65	0.89	0.27	0.58	151,159,180,180	0
26	DGD	C	491	53/66	0.87	0.29	0.58	155,160,166,168	0
21	CLA	B	521	65/65	0.93	0.26	0.54	149,169,175,179	0
25	BCR	C	489	40/40	0.77	0.33	0.53	152,169,171,171	0
21	CLA	C	485	65/65	0.88	0.30	0.53	170,176,178,180	0
21	CLA	B	513	65/65	0.94	0.26	0.52	133,170,171,172	0
28	SQD	C	475	51/54	0.74	0.43	0.52	156,172,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
21	CLA	A	364	65/65	0.88	0.31	0.48	126,141,175,177	0
29	LMG	B	531	49/55	0.80	0.35	0.47	160,167,175,176	0
21	CLA	B	514	65/65	0.91	0.30	0.45	139,146,168,169	0
21	CLA	B	523	65/65	0.94	0.23	0.36	134,142,169,170	0
33	HEM	F	85	43/43	0.94	0.39	0.36	154,159,162,163	0
21	CLA	C	481	65/65	0.86	0.28	0.28	152,180,180,180	0
21	CLA	C	487	65/65	0.85	0.34	0.22	176,180,180,180	0
21	CLA	B	516	65/65	0.89	0.27	0.22	152,155,180,180	0
27	LHG	A	371	39/49	0.87	0.31	0.20	156,175,179,180	0
33	HEM	V	164	43/43	0.95	0.29	0.14	89,102,122,129	0
21	CLA	B	512	65/65	0.93	0.25	0.12	142,165,172,173	0
21	CLA	C	486	65/65	0.83	0.31	-0.13	143,180,180,180	0
21	CLA	C	488	65/65	0.79	0.34	-0.14	169,176,179,180	0
21	CLA	C	479	65/65	0.89	0.25	-0.29	162,180,180,180	0
21	CLA	B	517	65/65	0.87	0.26	-0.42	144,160,164,167	0
31	BCT	D	353	4/4	0.96	0.27	-0.53	169,170,170,171	0
24	OEC	A	368	5/9	0.89	0.24	-0.73	118,138,151,154	0
23	MES	A	367	12/12	0.93	0.20	-0.90	136,144,152,153	0
20	FE2	A	361	1/1	0.96	0.18	-1.08	160,160,160,160	0
34	CA	O	273	1/1	0.34	0.67	-	180,180,180,180	0
30	LMT	O	274	35/35	0.70	0.39	-	180,180,180,180	0
30	LMT	T	226	35/35	0.65	0.96	-	156,180,180,180	0
27	LHG	C	476	37/49	0.53	0.45	-	143,176,180,180	0
26	DGD	A	375	52/66	0.78	0.64	-	164,180,180,180	0
30	LMT	B	535	35/35	0.77	0.73	-	163,180,180,180	0
34	CA	K	56	1/1	0.81	0.42	-	180,180,180,180	0
34	CA	F	225	1/1	0.88	0.43	-	142,142,142,142	0
29	LMG	I	220	43/55	0.63	0.84	-	158,180,180,180	0

6.5 Other polymers (i)

There are no such residues in this entry.