



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 07:09 PM BST

PDB ID : 3BZ1
Title : Crystal Structure of cyanobacterial Photosystem II (part 1 of 2). This file contains first monomer of PSII dimer
Authors : Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on : 2008-01-17
Resolution : 2.90 Å(reported)

This is a wwPDB 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>

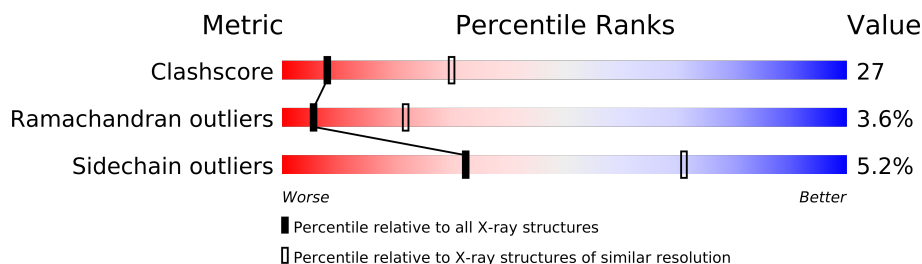
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	344	
2	B	510	
3	C	473	
4	D	352	
5	E	84	
6	F	45	
7	H	66	
8	I	38	
9	J	40	
10	K	37	
11	L	37	
12	M	36	
13	O	247	
14	T	32	
15	U	104	
16	V	137	
17	y	46	

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Mol	Chain	Length	Quality of chain
18	X	50	
19	Y	28	
20	Z	62	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 25117 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.

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	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

There are 12 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O		0	0	0
			666	434	108	124				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

- 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	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	S	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 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 PsbX protein.

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

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

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

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

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

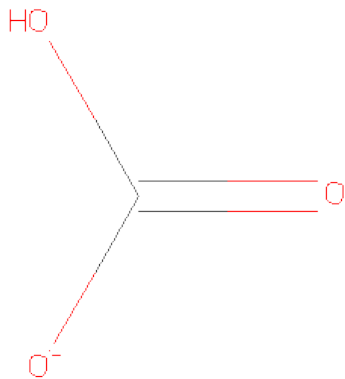
- Molecule 21 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

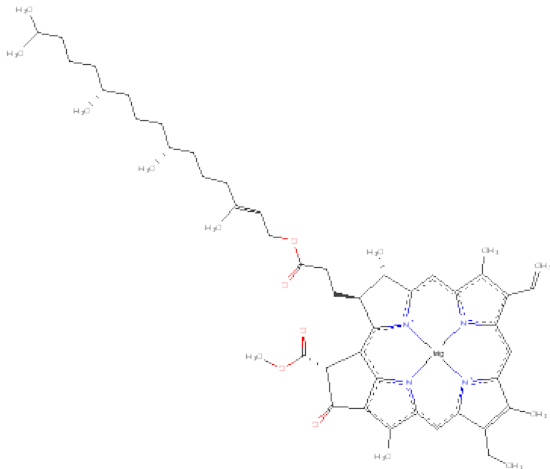
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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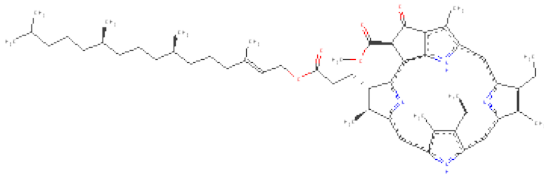
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N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

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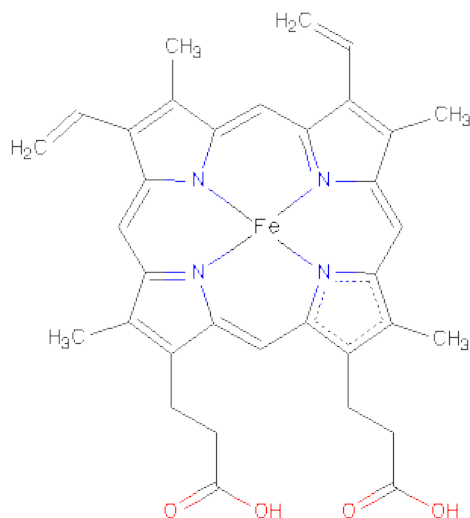
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



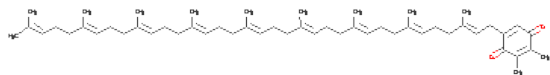
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



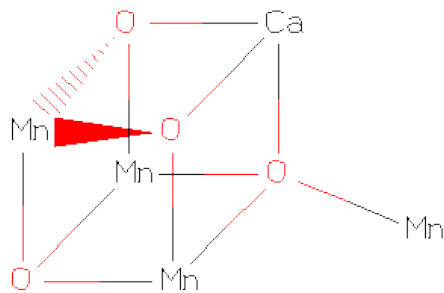
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
26	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 27 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: $C_{53}H_{80}O_2$).



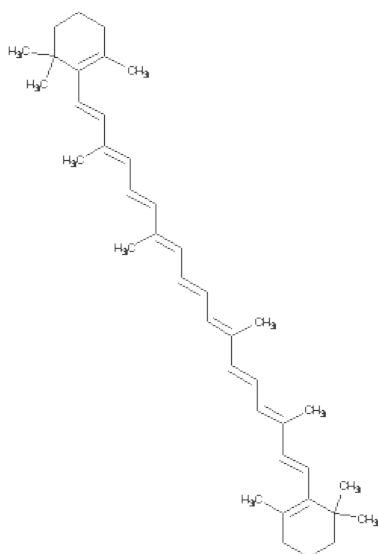
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	D	1	Total	C	O	0	0
			55	53	2		
27	A	1	Total	C	O	0	0
			45	43	2		
27	J	1	Total	C	O	0	0
			35	33	2		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



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

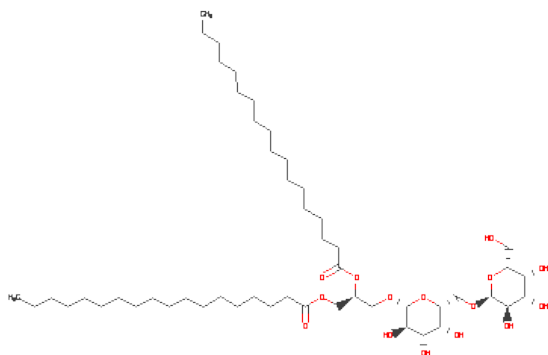
- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C 40 40	0	0
29	B	1	Total C 40 40	0	0
29	B	1	Total C 40 40	0	0
29	B	1	Total C 40 40	0	0
29	B	1	Total C 40 40	0	0
29	H	1	Total C 40 40	0	0
29	D	1	Total C 40 40	0	0
29	K	1	Total C 40 40	0	0
29	C	1	Total C 40 40	0	0
29	J	1	Total C 40 40	0	0
29	Z	1	Total C 40 40	0	0
29	C	1	Total C 40 40	0	0

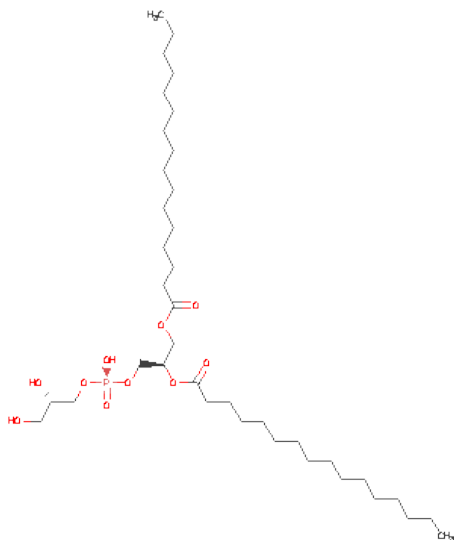
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: C₅₁H₉₆O₁₅).



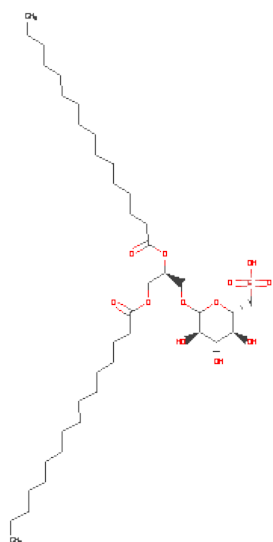
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			56	41	15		
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			62	47	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	H	1	Total	C	O	0	0
			58	43	15		
30	A	1	Total	C	O	0	0
			52	37	15		
30	D	1	Total	C	O	0	0
			63	48	15		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 32 is 1,2-di-O-acyl-3-O-[6-deoxy-6-sulfo-alpha-D-glucopyranosyl]-sn-glycerol (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



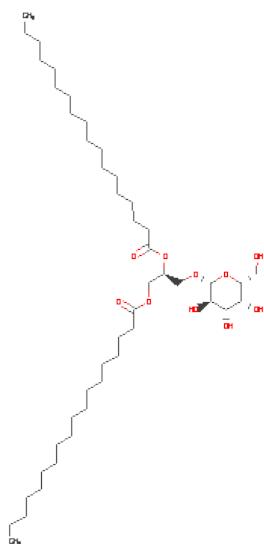
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	S	0	0
			51	38	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			54	41	12	1		
32	T	1	Total	C	O	S	0	0
			47	34	12	1		
32	D	1	Total	C	O	S	0	0
			43	30	12	1		
32	F	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



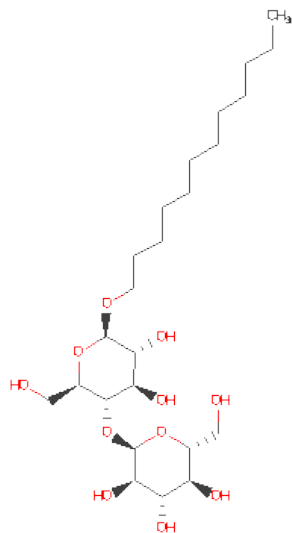
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			46	36	10		
33	B	1	Total	C	O	0	0
			49	39	10		
33	A	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			48	38	10		
33	B	1	Total	C	O	0	0
			49	39	10		
33	B	1	Total	C	O	0	0
			42	32	10		
33	M	1	Total	C	O	0	0
			42	32	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	E	1	Total	C	O	0	0
			44	34	10		
33	C	1	Total	C	O	0	0
			48	38	10		
33	I	1	Total	C	O	0	0
			43	33	10		
33	C	1	Total	C	O	0	0
			45	35	10		

- Molecule 34 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

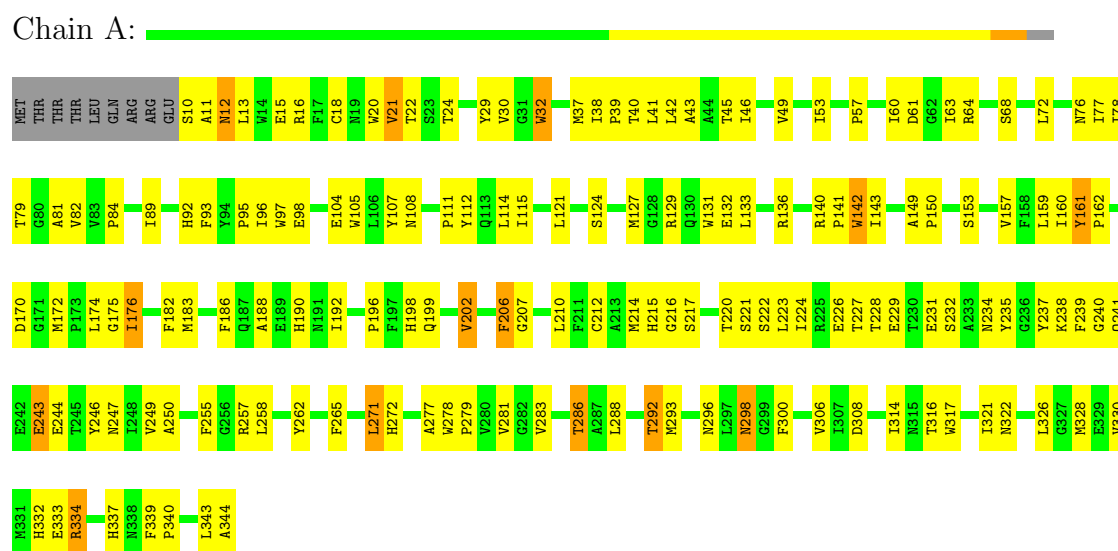
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

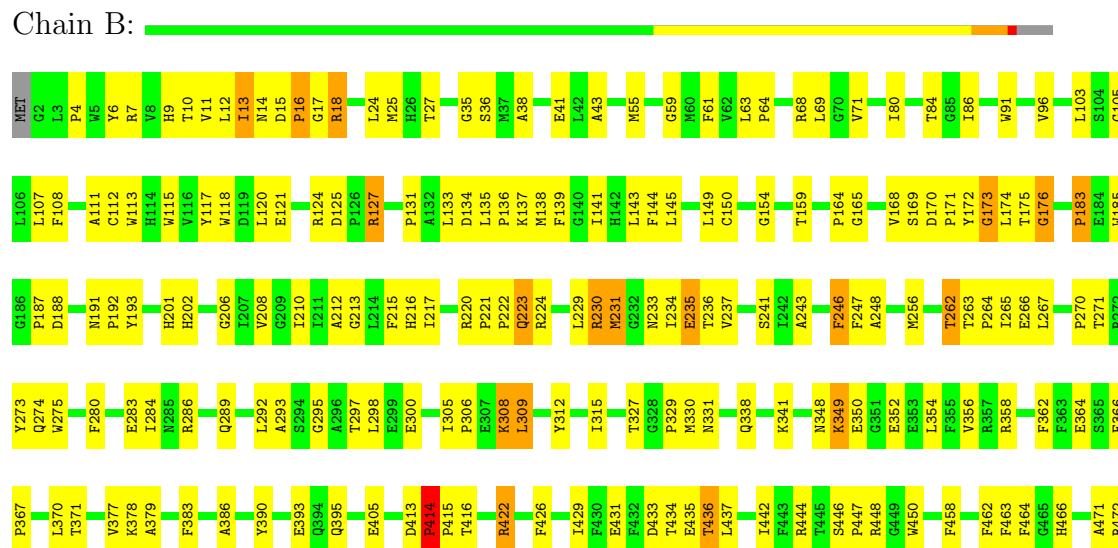
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: Photosystem Q(B) protein

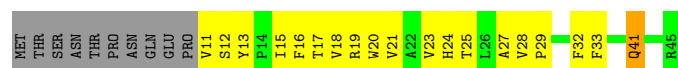


• Molecule 2: Photosystem II core light harvesting protein



- Molecule 6: Cytochrome b559 subunit beta

Chain F: 



- Molecule 7: Photosystem II reaction center protein H

Chain H: 



- Molecule 8: Photosystem II reaction center protein I

Chain I: 



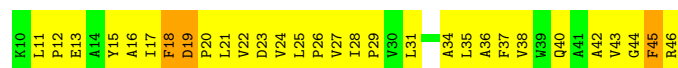
- Molecule 9: Photosystem II reaction center protein J

Chain J: 



- Molecule 10: Photosystem II reaction center protein K

Chain K: 



- Molecule 11: Photosystem II reaction center protein L

Chain L: 



- Molecule 12: Photosystem II reaction center protein M

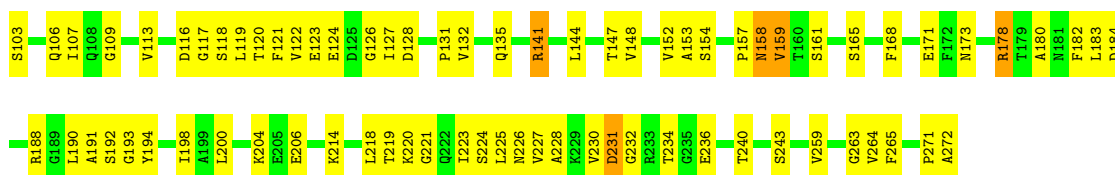
Chain M: 



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 





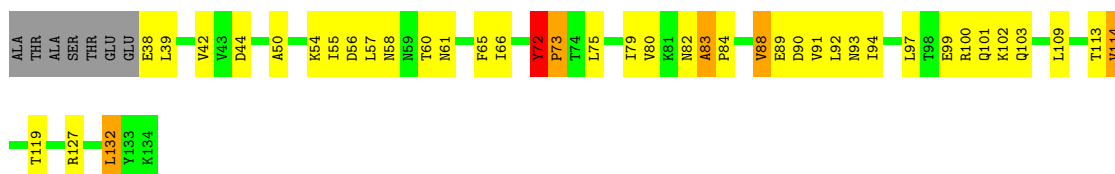
- Molecule 14: Photosystem II reaction center protein T

Chain T:



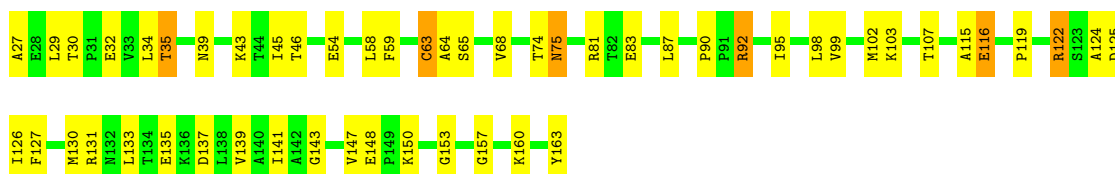
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



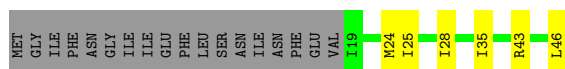
- Molecule 16: Cytochrome c-550

Chain V:



- Molecule 17: Protein ycf12

Chain y:



- Molecule 18: Photosystem II PsbX protein

Chain X:



- Molecule 19: Photosystem II protein Y

Chain Y:



- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 



4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	97.7 (10.00-2.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.292	Depositor
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.357	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 193457 reflections (0.001%)	Xtriage
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2713	0.66	0/3700
2	B	0.44	0/3986	0.67	3/5433 (0.1%)
3	C	0.41	0/3556	0.64	1/4842 (0.0%)
4	D	0.47	0/2801	0.65	0/3818
5	E	0.45	0/685	0.71	0/933
6	F	0.45	0/291	0.59	0/397
7	H	0.42	0/520	0.73	1/709 (0.1%)
8	I	0.51	0/293	0.68	0/395
9	J	0.43	0/255	0.69	0/346
10	K	0.43	0/303	0.63	0/416
11	L	0.39	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	0.50	0/284	0.62	0/381
15	U	0.42	0/785	0.73	1/1064 (0.1%)
16	V	0.38	0/1081	0.65	0/1468
17	y	0.46	0/202	0.73	0/272
18	X	0.43	0/273	0.63	0/370
20	Z	0.45	0/490	0.69	0/669
All	All	0.44	0/20975	0.67	6/28550 (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.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	LEU	CA-CB-CG	6.99	131.39	115.30
2	B	488	PRO	N-CA-C	5.86	127.33	112.10
2	B	489	GLU	N-CA-C	5.76	126.56	111.00
7	H	65	LEU	CA-CB-CG	5.72	128.45	115.30
3	C	32	GLY	N-CA-C	-5.54	99.24	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	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	A	2628	0	2524	175	0
2	B	3850	0	3718	224	0
3	C	3444	0	3365	258	0
4	D	2706	0	2608	177	0
5	E	666	0	651	71	0
6	F	282	0	291	28	0
7	H	507	0	521	52	0
8	I	286	0	308	15	0
9	J	249	0	262	28	0
10	K	293	0	305	42	0
11	L	304	0	316	15	0
12	M	267	0	289	15	0
13	O	1845	0	1801	113	0
14	T	275	0	288	18	0
15	U	774	0	773	46	0
16	V	1060	0	1068	42	0
17	y	201	0	226	0	0
18	X	270	0	299	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	140	0	32	4	0
20	Z	479	0	516	54	0
21	K	1	0	0	0	0
21	O	1	0	0	0	0
22	A	1	0	0	0	0
23	D	4	0	0	1	0
24	A	195	0	216	16	0
24	B	1040	0	1152	77	0
24	C	845	0	936	61	0
24	D	195	0	216	12	0
25	A	64	0	74	5	0
25	D	64	0	74	2	0
26	E	43	0	30	5	0
26	V	43	0	30	3	0
27	A	45	0	61	5	0
27	D	55	0	80	9	0
27	J	35	0	45	0	0
28	A	5	0	0	0	0
29	A	40	0	56	3	0
29	B	160	0	224	9	0
29	C	80	0	112	15	0
29	D	40	0	56	3	0
29	H	40	0	56	5	0
29	J	40	0	56	5	0
29	K	40	0	56	13	0
29	Z	40	0	56	5	0
30	A	108	0	132	3	0
30	C	181	0	245	19	0
30	D	63	0	87	0	0
30	H	58	0	74	1	0
31	A	76	0	95	8	0
32	A	51	0	68	5	0
32	B	54	0	77	1	0
32	D	43	0	49	2	0
32	F	45	0	53	2	0
32	T	47	0	60	2	0
33	A	51	0	72	1	0
33	B	140	0	190	3	0
33	C	93	0	126	6	0
33	D	94	0	128	8	0
33	E	44	0	58	4	0
33	I	43	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	M	42	0	54	4	0
34	B	70	0	92	3	0
34	D	31	0	35	2	0
34	I	35	0	46	4	0
34	M	35	0	46	0	0
34	O	35	0	46	3	0
34	T	35	0	46	3	0
35	A	1	0	0	0	0
All	All	25117	0	25682	1330	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 27.

The worst 5 of 1330 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:V:63:CYS:SG	26:V:164:HEM:HAB	1.85	1.16
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.23	1.16
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.22	1.09
2:B:68:ARG:HH22	24:B:514:CLA:HED1	1.12	1.07
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.19	1.06

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	11	39
2	B	488/510 (96%)	417 (86%)	57 (12%)	14 (3%)	7	28
3	C	445/473 (94%)	371 (83%)	58 (13%)	16 (4%)	5	22
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	8	30
5	E	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	3	11
6	F	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	1	2
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	7
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	6
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	3	8
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	241/247 (98%)	199 (83%)	30 (12%)	12 (5%)	3	11
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	6	24
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	4	16
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	30	72
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	1
18	X	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	1	1
20	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	11
All	All	2569/2740 (94%)	2133 (83%)	344 (13%)	92 (4%)	5	22

5 of 92 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 ⓘ

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%)	258 (95%)	13 (5%)	35	74
2	B	390/407 (96%)	374 (96%)	16 (4%)	41	80
3	C	347/374 (93%)	329 (95%)	18 (5%)	32	71
4	D	275/283 (97%)	256 (93%)	19 (7%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/73 (99%)	66 (92%)	6 (8%)	16	43
6	F	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	50 (94%)	3 (6%)	29	66
8	I	32/35 (91%)	31 (97%)	1 (3%)	52	88
9	J	24/28 (86%)	23 (96%)	1 (4%)	40	79
10	K	30/30 (100%)	28 (93%)	2 (7%)	23	56
11	L	35/35 (100%)	31 (89%)	4 (11%)	8	24
12	M	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	195 (96%)	7 (4%)	48	85
14	T	29/29 (100%)	28 (97%)	1 (3%)	49	86
15	U	84/89 (94%)	80 (95%)	4 (5%)	35	74
16	V	116/117 (99%)	111 (96%)	5 (4%)	40	78
17	y	20/37 (54%)	18 (90%)	2 (10%)	11	32
18	X	30/42 (71%)	26 (87%)	4 (13%)	6	16
20	Z	52/52 (100%)	47 (90%)	5 (10%)	12	35
All	All	2122/2246 (94%)	2011 (95%)	111 (5%)	32	71

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	60	THR
4	D	291	LEU
18	X	11	THR
4	D	84	SER
4	D	221	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	239	GLN
11	L	8	GLN
17	y	21	GLN
7	H	59	ASN
2	B	490	GLN

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 92 ligands modelled in this entry, 4 are monoatomic - leaving 88 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	$\# Z > 2$
24	CLA	A	362	1	73,73,73	1.48	13 (17%)	95,113,113	1.54	18 (18%)
24	CLA	A	363	-	73,73,73	1.43	12 (16%)	95,113,113	1.66	18 (18%)
25	PHO	A	365	-	69,69,69	1.86	6 (8%)	91,99,99	1.51	15 (16%)
24	CLA	A	366	1	73,73,73	1.44	10 (13%)	95,113,113	1.48	18 (18%)
27	PL9	A	367	-	45,45,55	1.00	2 (4%)	55,57,69	1.86	16 (29%)
28	OEC	A	368	1,3	0,0,13	0.00	-	0,0,27	0.00	-
29	BCR	A	369	-	41,41,41	1.61	7 (17%)	56,56,56	2.06	20 (35%)
30	DGD	A	370	-	57,57,67	2.09	14 (24%)	71,71,81	1.49	9 (12%)
31	LHG	A	371	-	38,38,48	1.93	6 (15%)	44,44,54	1.31	4 (9%)
32	SQD	A	372	-	51,51,54	6.80	25 (49%)	62,62,65	2.90	21 (33%)
33	LMG	A	373	-	51,51,55	1.41	4 (7%)	59,59,63	1.02	4 (6%)
31	LHG	A	374	-	36,36,48	1.72	4 (11%)	42,42,54	1.12	3 (7%)
30	DGD	A	375	-	53,53,67	2.50	19 (35%)	67,67,81	1.64	8 (11%)
24	CLA	B	511	-	73,73,73	1.70	12 (16%)	95,113,113	1.48	18 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	512	2	73,73,73	1.48	13 (17%)	95,113,113	1.49	19 (20%)
24	CLA	B	513	2	73,73,73	1.48	11 (15%)	95,113,113	1.54	19 (20%)
24	CLA	B	514	2	73,73,73	1.57	12 (16%)	95,113,113	1.49	18 (18%)
24	CLA	B	515	-	73,73,73	1.55	12 (16%)	95,113,113	1.48	17 (17%)
24	CLA	B	516	2	73,73,73	1.51	12 (16%)	95,113,113	1.45	18 (18%)
24	CLA	B	517	-	73,73,73	1.49	15 (20%)	95,113,113	1.55	18 (18%)
24	CLA	B	518	2	73,73,73	1.50	11 (15%)	95,113,113	1.54	19 (20%)
24	CLA	B	519	2	73,73,73	1.65	14 (19%)	95,113,113	1.48	18 (18%)
24	CLA	B	520	-	73,73,73	1.46	11 (15%)	95,113,113	1.53	21 (22%)
24	CLA	B	521	2	73,73,73	1.40	9 (12%)	95,113,113	1.49	19 (20%)
24	CLA	B	522	-	73,73,73	1.51	11 (15%)	95,113,113	1.51	18 (18%)
24	CLA	B	523	-	73,73,73	1.39	10 (13%)	95,113,113	1.49	20 (21%)
24	CLA	B	524	2	73,73,73	1.55	13 (17%)	95,113,113	1.59	25 (26%)
24	CLA	B	525	-	73,73,73	1.57	13 (17%)	95,113,113	1.55	20 (21%)
24	CLA	B	526	-	73,73,73	1.56	13 (17%)	95,113,113	1.57	21 (22%)
29	BCR	B	527	-	41,41,41	1.68	7 (17%)	56,56,56	1.96	14 (25%)
29	BCR	B	528	-	41,41,41	1.69	6 (14%)	56,56,56	2.17	27 (48%)
29	BCR	B	529	-	41,41,41	1.91	8 (19%)	56,56,56	2.05	15 (26%)
29	BCR	B	530	-	41,41,41	1.82	7 (17%)	56,56,56	2.03	17 (30%)
33	LMG	B	531	-	49,49,55	1.53	7 (14%)	57,57,63	1.05	4 (7%)
32	SQD	B	532	-	54,54,54	2.99	29 (53%)	65,65,65	2.70	20 (30%)
33	LMG	B	533	-	49,49,55	1.81	6 (12%)	57,57,63	1.07	5 (8%)
33	LMG	B	534	-	42,42,55	2.11	9 (21%)	50,50,63	1.05	3 (6%)
34	LMT	B	535	-	36,36,36	1.42	7 (19%)	47,47,47	1.20	3 (6%)
34	LMT	B	536	-	36,36,36	1.36	7 (19%)	47,47,47	0.96	3 (6%)
24	CLA	C	474	3	73,73,73	1.49	10 (13%)	95,113,113	1.50	20 (21%)
24	CLA	C	475	3	73,73,73	1.56	12 (16%)	95,113,113	1.46	17 (17%)
24	CLA	C	476	3	73,73,73	1.65	14 (19%)	95,113,113	1.48	17 (17%)
24	CLA	C	477	-	73,73,73	1.55	11 (15%)	95,113,113	1.53	18 (18%)
24	CLA	C	478	3	73,73,73	1.60	13 (17%)	95,113,113	1.56	20 (21%)
24	CLA	C	479	3	73,73,73	1.51	13 (17%)	95,113,113	1.50	19 (20%)
24	CLA	C	480	-	73,73,73	1.46	13 (17%)	95,113,113	1.53	22 (23%)
24	CLA	C	481	3	73,73,73	1.57	15 (20%)	95,113,113	1.55	20 (21%)
24	CLA	C	482	-	73,73,73	1.54	11 (15%)	95,113,113	1.55	19 (20%)
24	CLA	C	483	-	73,73,73	1.59	12 (16%)	95,113,113	1.51	17 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	484	3	73,73,73	1.66	11 (15%)	95,113,113	1.51	20 (21%)
24	CLA	C	485	-	73,73,73	1.66	13 (17%)	95,113,113	1.57	20 (21%)
24	CLA	C	486	3	73,73,73	1.64	13 (17%)	95,113,113	1.49	19 (20%)
29	BCR	C	487	-	41,41,41	1.73	6 (14%)	56,56,56	2.10	21 (37%)
29	BCR	C	488	-	41,41,41	1.66	6 (14%)	56,56,56	2.13	18 (32%)
30	DGD	C	489	-	54,54,67	1.57	10 (18%)	68,68,81	1.60	8 (11%)
30	DGD	C	490	-	63,63,67	1.28	6 (9%)	77,77,81	1.64	9 (11%)
30	DGD	C	491	-	67,67,67	1.02	6 (8%)	81,81,81	1.27	4 (4%)
33	LMG	C	492	-	48,48,55	1.90	7 (14%)	56,56,63	0.87	3 (5%)
33	LMG	C	493	-	45,45,55	2.01	10 (22%)	53,53,63	1.06	4 (7%)
23	BCT	D	353	22	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	D	354	4	73,73,73	1.57	13 (17%)	95,113,113	1.51	20 (21%)
25	PHO	D	355	-	69,69,69	1.95	6 (8%)	91,99,99	1.54	14 (15%)
24	CLA	D	356	-	73,73,73	1.57	12 (16%)	95,113,113	1.49	18 (18%)
27	PL9	D	357	-	55,55,55	0.54	0	69,69,69	1.81	18 (26%)
29	BCR	D	358	-	41,41,41	1.81	7 (17%)	56,56,56	2.27	19 (33%)
33	LMG	D	359	-	46,46,55	2.07	6 (13%)	54,54,63	0.95	2 (3%)
33	LMG	D	360	-	48,48,55	1.68	5 (10%)	56,56,63	1.06	3 (5%)
32	SQD	D	361	-	43,43,54	7.80	23 (53%)	54,54,65	3.30	18 (33%)
30	DGD	D	362	-	64,64,67	1.90	18 (28%)	78,78,81	1.42	7 (8%)
34	LMT	D	363	-	32,32,36	1.72	5 (15%)	43,43,47	1.03	2 (4%)
24	CLA	D	364	-	73,73,73	1.44	9 (12%)	95,113,113	1.47	16 (16%)
33	LMG	E	218	-	44,44,55	1.88	7 (15%)	52,52,63	1.12	5 (9%)
26	HEM	E	85	5,6	49,50,50	3.00	27 (55%)	46,82,82	2.53	11 (23%)
32	SQD	F	224	-	45,45,54	10.24	25 (55%)	56,56,65	3.17	20 (35%)
29	BCR	H	107	-	41,41,41	1.85	8 (19%)	56,56,56	2.22	21 (37%)
30	DGD	H	208	-	59,59,67	2.10	9 (15%)	73,73,81	1.48	7 (9%)
33	LMG	I	220	-	43,43,55	2.18	10 (23%)	51,51,63	1.11	4 (7%)
34	LMT	I	230	-	36,36,36	1.39	4 (11%)	47,47,47	0.95	1 (2%)
29	BCR	J	115	-	41,41,41	2.04	8 (19%)	56,56,56	3.23	22 (39%)
27	PL9	J	59	-	35,35,55	1.41	5 (14%)	43,45,69	1.88	14 (32%)
29	BCR	K	112	-	41,41,41	1.82	7 (17%)	56,56,56	2.50	25 (44%)
33	LMG	M	217	-	42,42,55	2.34	8 (19%)	50,50,63	1.24	6 (12%)
34	LMT	M	226	-	36,36,36	1.17	3 (8%)	47,47,47	0.95	2 (4%)
34	LMT	O	274	-	36,36,36	1.42	6 (16%)	47,47,47	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	SQD	T	213	-	47,47,54	3.29	24 (51%)	58,58,65	3.03	16 (27%)
34	LMT	T	227	-	36,36,36	1.34	5 (13%)	47,47,47	1.08	4 (8%)
26	HEM	V	164	16	49,50,50	3.53	26 (53%)	46,82,82	2.39	13 (28%)
29	BCR	Z	116	-	41,41,41	1.81	7 (17%)	56,56,56	2.06	18 (32%)

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
24	CLA	A	362	1	-	0/37/135/135	0/0/9/9
24	CLA	A	363	-	-	1/37/135/135	0/0/9/9
25	PHO	A	365	-	3/3/17/22	1/48/103/103	0/0/6/6
24	CLA	A	366	1	-	0/37/135/135	0/0/9/9
27	PL9	A	367	-	-	0/41/61/73	0/1/1/1
28	OEC	A	368	1,3	-	0/0/0/54	0/0/0/5
29	BCR	A	369	-	-	0/29/63/63	0/2/2/2
30	DGD	A	370	-	3/3/13/13	0/45/85/95	0/2/2/2
31	LHG	A	371	-	-	0/43/43/53	0/0/0/0
32	SQD	A	372	-	-	0/46/66/69	0/1/1/1
33	LMG	A	373	-	2/2/8/8	0/46/66/70	0/1/1/1
31	LHG	A	374	-	-	0/41/41/53	0/0/0/0
30	DGD	A	375	-	3/3/13/13	0/41/81/95	0/2/2/2
24	CLA	B	511	-	-	0/37/135/135	0/0/9/9
24	CLA	B	512	2	-	1/37/135/135	0/0/9/9
24	CLA	B	513	2	-	0/37/135/135	0/0/9/9
24	CLA	B	514	2	-	0/37/135/135	0/0/9/9
24	CLA	B	515	-	-	0/37/135/135	0/0/9/9
24	CLA	B	516	2	-	1/37/135/135	0/0/9/9
24	CLA	B	517	-	-	0/37/135/135	0/0/9/9
24	CLA	B	518	2	-	0/37/135/135	0/0/9/9
24	CLA	B	519	2	-	0/37/135/135	0/0/9/9
24	CLA	B	520	-	-	0/37/135/135	0/0/9/9
24	CLA	B	521	2	-	1/37/135/135	0/0/9/9
24	CLA	B	522	-	-	0/37/135/135	0/0/9/9
24	CLA	B	523	-	-	0/37/135/135	0/0/9/9
24	CLA	B	524	2	-	0/37/135/135	0/0/9/9
24	CLA	B	525	-	-	0/37/135/135	0/0/9/9
24	CLA	B	526	-	-	0/37/135/135	0/0/9/9
29	BCR	B	527	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	B	528	-	-	0/29/63/63	0/2/2/2
29	BCR	B	529	-	-	0/29/63/63	0/2/2/2
29	BCR	B	530	-	-	0/29/63/63	0/2/2/2
33	LMG	B	531	-	2/2/8/8	0/44/64/70	0/1/1/1
32	SQD	B	532	-	-	0/49/69/69	0/1/1/1
33	LMG	B	533	-	2/2/8/8	0/44/64/70	0/1/1/1
33	LMG	B	534	-	2/2/8/8	0/37/57/70	0/1/1/1
34	LMT	B	535	-	-	0/21/61/61	0/2/2/2
34	LMT	B	536	-	-	0/21/61/61	0/2/2/2
24	CLA	C	474	3	-	0/37/135/135	0/0/9/9
24	CLA	C	475	3	-	1/37/135/135	0/0/9/9
24	CLA	C	476	3	-	0/37/135/135	0/0/9/9
24	CLA	C	477	-	-	0/37/135/135	0/0/9/9
24	CLA	C	478	3	-	0/37/135/135	0/0/9/9
24	CLA	C	479	3	-	0/37/135/135	0/0/9/9
24	CLA	C	480	-	-	0/37/135/135	0/0/9/9
24	CLA	C	481	3	-	0/37/135/135	0/0/9/9
24	CLA	C	482	-	-	1/37/135/135	0/0/9/9
24	CLA	C	483	-	-	1/37/135/135	0/0/9/9
24	CLA	C	484	3	-	0/37/135/135	0/0/9/9
24	CLA	C	485	-	-	0/37/135/135	0/0/9/9
24	CLA	C	486	3	-	1/37/135/135	0/0/9/9
29	BCR	C	487	-	-	0/29/63/63	0/2/2/2
29	BCR	C	488	-	-	0/29/63/63	0/2/2/2
30	DGD	C	489	-	3/3/13/13	0/42/82/95	0/2/2/2
30	DGD	C	490	-	3/3/13/13	0/51/91/95	0/2/2/2
30	DGD	C	491	-	3/3/13/13	0/55/95/95	0/2/2/2
33	LMG	C	492	-	2/2/8/8	0/43/63/70	0/1/1/1
33	LMG	C	493	-	2/2/8/8	0/40/60/70	0/1/1/1
23	BCT	D	353	22	-	0/0/0/0	0/0/0/0
24	CLA	D	354	4	-	0/37/135/135	0/0/9/9
25	PHO	D	355	-	3/3/17/22	0/48/103/103	0/0/6/6
24	CLA	D	356	-	-	0/37/135/135	0/0/9/9
27	PL9	D	357	-	-	0/53/73/73	0/1/1/1
29	BCR	D	358	-	-	0/29/63/63	0/2/2/2
33	LMG	D	359	-	2/2/8/8	0/41/61/70	0/1/1/1
33	LMG	D	360	-	2/2/8/8	1/43/63/70	0/1/1/1
32	SQD	D	361	-	-	2/38/58/69	0/1/1/1
30	DGD	D	362	-	3/3/13/13	0/52/92/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	D	363	-	-	0/17/57/61	0/2/2/2
24	CLA	D	364	-	-	0/37/135/135	0/0/9/9
33	LMG	E	218	-	2/2/8/8	0/39/59/70	0/1/1/1
26	HEM	E	85	5,6	-	0/14/114/114	0/0/8/8
32	SQD	F	224	-	-	0/40/60/69	0/1/1/1
29	BCR	H	107	-	-	0/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	0/47/87/95	0/2/2/2
33	LMG	I	220	-	2/2/8/8	0/38/58/70	0/1/1/1
34	LMT	I	230	-	-	0/21/61/61	0/2/2/2
29	BCR	J	115	-	-	0/29/63/63	0/2/2/2
27	PL9	J	59	-	-	0/29/49/73	0/1/1/1
29	BCR	K	112	-	-	0/29/63/63	0/2/2/2
33	LMG	M	217	-	2/2/8/8	1/37/57/70	0/1/1/1
34	LMT	M	226	-	-	0/21/61/61	0/2/2/2
34	LMT	O	274	-	-	0/21/61/61	0/2/2/2
32	SQD	T	213	-	-	0/42/62/69	0/1/1/1
34	LMT	T	227	-	-	0/21/61/61	0/2/2/2
26	HEM	V	164	16	-	0/14/114/114	0/0/8/8
29	BCR	Z	116	-	-	0/29/63/63	0/2/2/2

The worst 5 of 912 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	224	SQD	C19-C18	-47.49	1.36	1.55
32	F	224	SQD	C32-C31	-45.64	1.37	1.55
32	D	361	SQD	C18-C17	-45.22	1.37	1.55
32	A	372	SQD	C35-C34	-43.95	1.37	1.55
26	V	164	HEM	C3D-C4D	13.41	1.47	1.44

The worst 5 of 1217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	J	115	BCR	C32-C1-C6	-9.81	94.07	110.33
32	D	361	SQD	O6-C1-C2	9.62	120.42	108.18
32	T	213	SQD	O6-C1-C2	9.45	120.21	108.18
32	F	224	SQD	O5-C1-O6	9.28	131.79	109.98
32	T	213	SQD	C5-C6-S	9.23	128.05	114.45

5 of 49 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	C	489	DGD	C2D
30	C	489	DGD	C5D
30	C	489	DGD	C5E
25	D	355	PHO	C2A
25	D	355	PHO	C13

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	D	361	SQD	C45-O47-C7-C8
32	D	361	SQD	C45-O47-C7-O49
33	M	217	LMG	C8-O7-C10-C11
24	C	475	CLA	C1-C2-C3-C4
33	D	360	LMG	C7-O1-C1-O6

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.