



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:12 PM GMT

PDB ID : 1IZL
Title : Crystal Structure of Photosystem II
Authors : Kamiya, N.; Shen, J.-R.
Deposited on : 2002-10-04
Resolution : 3.70 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

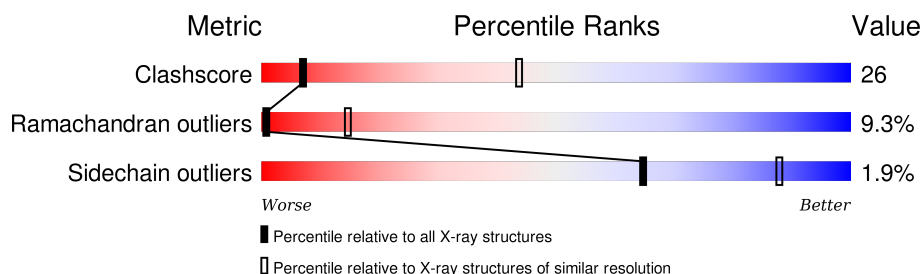
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)






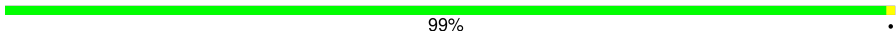
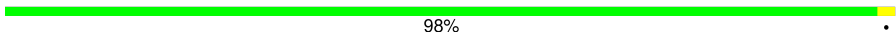
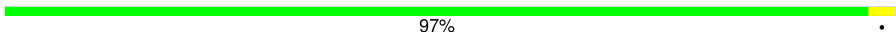







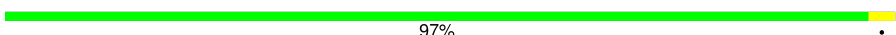
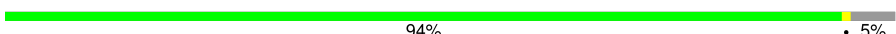




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	
1	J	360	
2	B	472	
2	L	472	
3	C	473	
3	M	473	
4	D	352	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	N	352	
5	E	83	
5	P	83	
6	F	44	
6	Q	44	
7	G	220	
7	R	220	
8	H	33	
8	S	33	
9	I	26	
9	T	26	
10	K	37	
10	W	37	
11	O	205	
11	Y	205	
12	U	97	
12	Z	97	
13	0	137	
13	V	137	
14	1	25	
14	X	25	

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
17	CLA	A	365	X	-	-	-
17	CLA	A	366	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	368	X	-	X	-
17	CLA	A	369	X	-	-	-
17	CLA	B	1107	X	-	-	-
17	CLA	B	1108	X	-	-	-
17	CLA	B	1109	X	-	-	-
17	CLA	B	1110	X	-	-	-
17	CLA	B	1111	X	-	-	-
17	CLA	B	1112	X	-	-	-
17	CLA	B	1113	X	-	-	-
17	CLA	B	1114	X	-	-	-
17	CLA	B	1115	X	-	-	-
17	CLA	B	1116	X	-	-	-
17	CLA	B	1117	X	-	-	-
17	CLA	B	1118	X	-	-	-
17	CLA	B	1119	X	-	-	-
17	CLA	B	1120	X	-	-	-
17	CLA	B	1121	X	-	-	-
17	CLA	B	1122	X	-	-	-
17	CLA	C	1078	X	-	-	-
17	CLA	C	1079	X	-	-	-
17	CLA	C	1080	X	-	-	-
17	CLA	C	1081	X	-	-	-
17	CLA	C	1082	X	-	-	-
17	CLA	C	1083	X	-	-	-
17	CLA	C	1084	X	-	-	-
17	CLA	C	1085	X	-	-	-
17	CLA	C	1086	X	-	-	-
17	CLA	C	1087	X	-	-	-
17	CLA	C	1088	X	-	-	-
17	CLA	C	1089	X	-	X	-
17	CLA	D	354	X	-	-	-
17	CLA	D	355	X	-	-	-
17	CLA	D	357	X	-	-	-
17	CLA	G	221	X	-	-	-
17	CLA	J	365	X	-	-	-
17	CLA	J	367	X	-	X	-
17	CLA	J	368	X	-	-	-
17	CLA	L	1107	X	-	-	-
17	CLA	L	1108	X	-	-	-
17	CLA	L	1109	X	-	-	-
17	CLA	L	1110	X	-	-	-
17	CLA	L	1111	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	L	1112	X	-	-	-
17	CLA	L	1113	X	-	-	-
17	CLA	L	1114	X	-	-	-
17	CLA	L	1115	X	-	-	-
17	CLA	L	1116	X	-	-	-
17	CLA	L	1117	X	-	-	-
17	CLA	L	1118	X	-	-	-
17	CLA	L	1119	X	-	X	-
17	CLA	L	1120	X	-	X	-
17	CLA	L	1121	X	-	-	-
17	CLA	L	1122	X	-	-	-
17	CLA	M	1078	X	-	-	-
17	CLA	M	1079	X	-	-	-
17	CLA	M	1080	X	-	-	-
17	CLA	M	1081	X	-	-	-
17	CLA	M	1082	X	-	-	-
17	CLA	M	1083	X	-	-	-
17	CLA	M	1084	X	-	-	-
17	CLA	M	1085	X	-	-	-
17	CLA	M	1086	X	-	-	-
17	CLA	M	1087	X	-	-	-
17	CLA	M	1088	X	-	-	-
17	CLA	N	354	X	-	-	-
17	CLA	N	355	X	-	-	-
17	CLA	N	356	X	-	-	-
17	CLA	N	358	X	-	-	-
17	CLA	R	221	X	-	-	-
17	CLA	W	64	X	-	-	-
18	PHO	N	357	-	-	X	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 22804 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 II: Subunit PsbA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	0	0	0
			1595	975	310	310			
1	J	299	Total	C	N	O	0	0	0
			1602	984	308	310			

- Molecule 2 is a protein called Photosystem II: Subunit PsbB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	48
			2004	1238	386	379	1			
2	L	424	Total	C	N	O		0	0	48
			2001	1242	383	376				

- Molecule 3 is a protein called Photosystem II: Subunit PsbC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	349	Total	C	N	O	0	0	0
			1792	1082	358	352			
3	M	347	Total	C	N	O	0	0	0
			1759	1057	354	348			

- Molecule 4 is a protein called Photosystem II: Subunit PsbD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	277	Total	C	N	O	0	0	0
			1460	899	282	279			
4	N	277	Total	C	N	O	0	0	0
			1451	888	284	279			

- Molecule 5 is a protein called Photosystem II: Subunit PsbE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	35	Total	C	N	O	0	0	0
			175	105	35	35			
5	P	17	Total	C	N	O	0	0	0
			83	49	17	17			

- Molecule 6 is a protein called Photosystem II: Subunit PsbF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	30	Total	C	N	O	0	0	0
			166	105	31	30			
6	Q	26	Total	C	N	O	0	0	0
			129	77	26	26			

- Molecule 7 is a protein called Photosystem II: Subunit PsbG.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
7	G	220	Total	C	0	0	220
			220	220			
7	R	220	Total	C	0	0	220
			220	220			

- Molecule 8 is a protein called Photosystem II: Subunit PsbH.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	33	Total	C	N	O	0	0	0
			165	99	33	33			
8	S	32	Total	C	N	O	0	0	0
			160	96	32	32			

- Molecule 9 is a protein called Photosystem II: Subunit PsbI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	26	Total	C	N	O	0	0	0
			130	78	26	26			
9	T	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 10 is a protein called Photosystem II: Subunit PsbK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	27	Total	C	N	O	0	0	0
			137	83	27	27			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	W	27	Total	C	N	O	0	0	0
			137	83	27	27			

- Molecule 11 is a protein called Photosystem II: Subunit PsbO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	O	205	Total	C	N	O	0	0	0
			1025	615	205	205			
11	Y	192	Total	C	N	O	0	0	0
			960	576	192	192			

- Molecule 12 is a protein called Photosystem II: Subunit PsbU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	U	97	Total	C	N	O	0	0	0
			485	291	97	97			
12	Z	92	Total	C	N	O	0	0	0
			460	276	92	92			

- Molecule 13 is a protein called Photosystem II: Subunit PsbV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	V	129	Total	C	N	O	0	0	0
			676	410	136	130			
13	0	115	Total	C	N	O	0	0	0
			597	360	121	116			

- Molecule 14 is a protein called Photosystem II: Subunit PsbX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	X	25	Total	C	N	O	0	0	0
			125	75	25	25			
14	1	25	Total	C	N	O	0	0	0
			125	75	25	25			

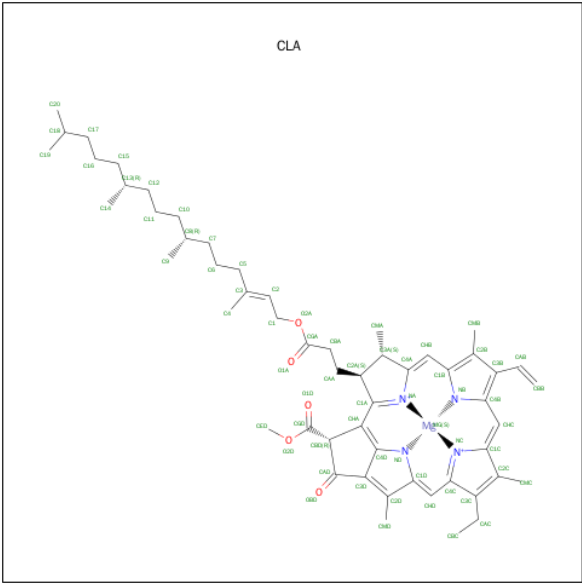
- Molecule 15 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	4	Total	Mn	0	0
			4	4		
15	A	4	Total	Mn	0	0
			4	4		

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	D	1	Total	Fe	0	0
			1	1		
16	N	1	Total	Fe	0	0
			1	1		

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	D	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	D	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	D	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	A	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	C	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

Continued on next page...

Continued from previous page...

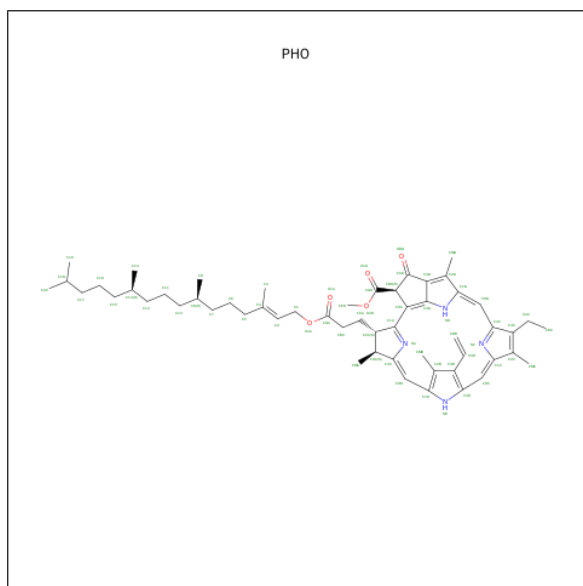
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	G	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	B	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	N	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	W	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

Continued on next page...

Continued from previous page...

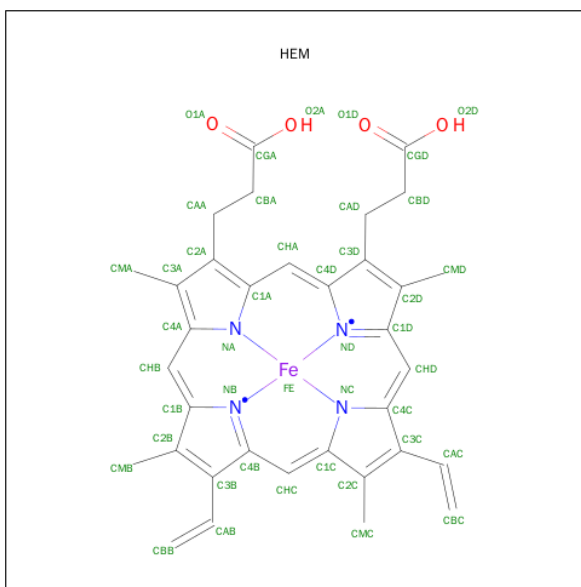
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	J	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	M	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	R	1	Total 35	C 29	Mg 1	N 4	O 1	0	0
17	L	1	Total 35	C 29	Mg 1	N 4	O 1	0	0

- Molecule 18 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



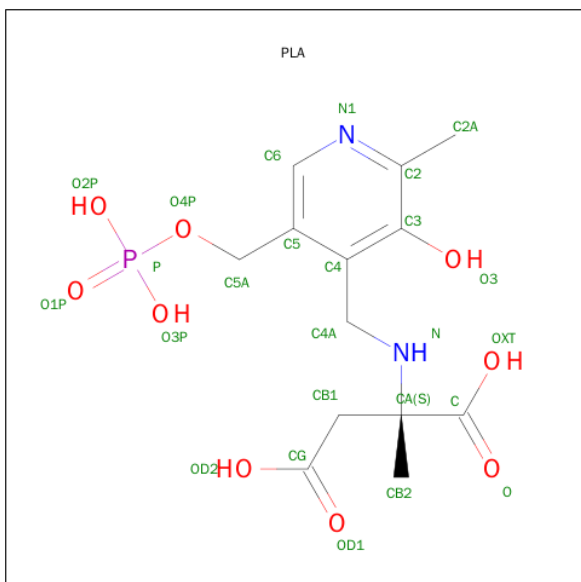
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	N	O	0	0
			34	29	4	1		
18	A	1	Total	C	N	O	0	0
			34	29	4	1		
18	N	1	Total	C	N	O	0	0
			34	29	4	1		
18	J	1	Total	C	N	O	0	0
			34	29	4	1		

- Molecule 19 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



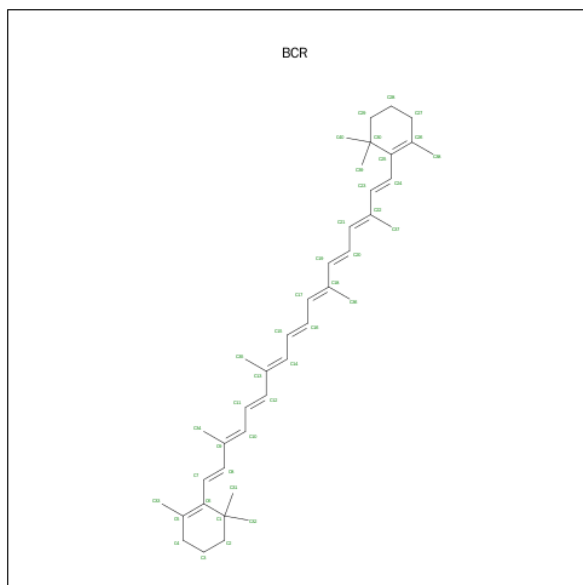
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	E	1	Total	C	Fe	N	0	0
			25	20	1	4		
19	V	1	Total	C	Fe	N	0	0
			25	20	1	4		
19	P	1	Total	C	Fe	N	0	0
			25	20	1	4		
19	0	1	Total	C	Fe	N	0	0
			25	20	1	4		

- Molecule 20 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (three-letter code: PLA) (formula: $C_{13}H_{19}N_2O_9P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C N 6 5 1	0	0
20	N	1	Total C N 6 5 1	0	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



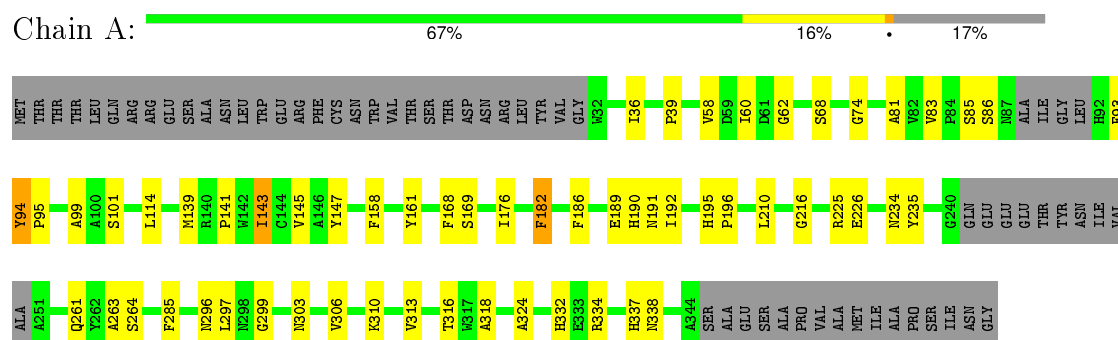
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	1	Total C 22 22	0	0
21	D	1	Total C 40 40	0	0

3 Residue-property plots

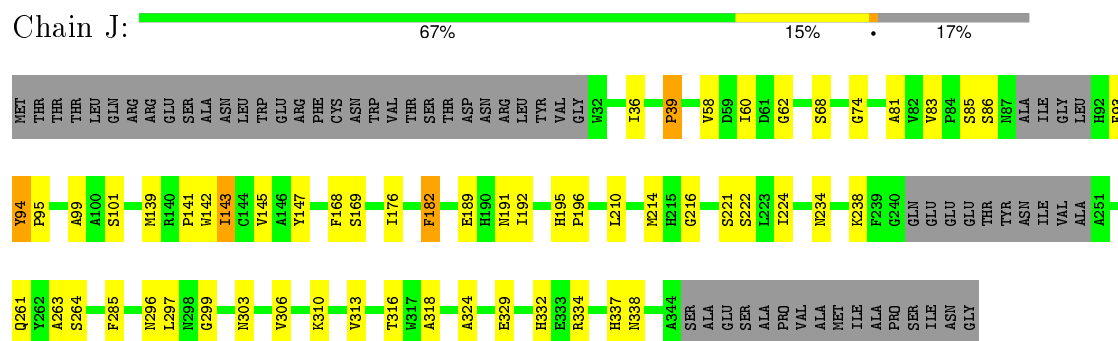
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

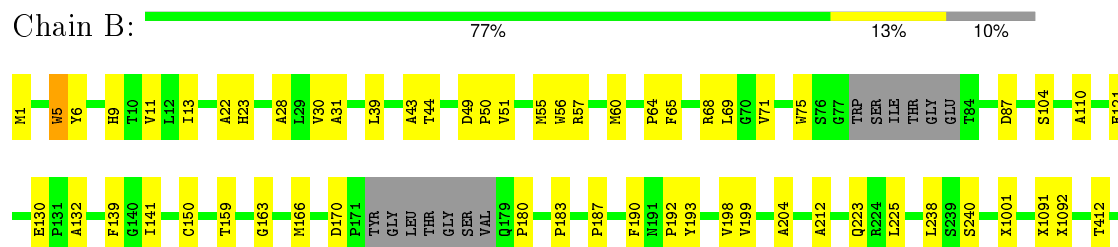
• Molecule 1: Photosystem II: Subunit PsbA

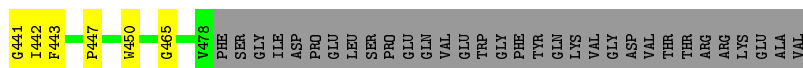


• Molecule 1: Photosystem II: Subunit PsbA



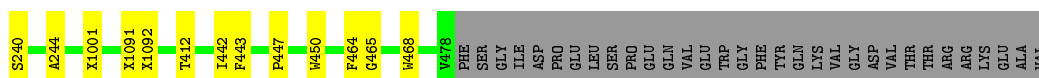
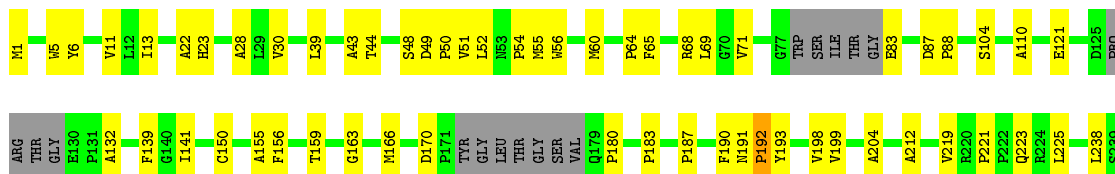
• Molecule 2: Photosystem II: Subunit PsbB





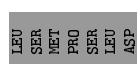
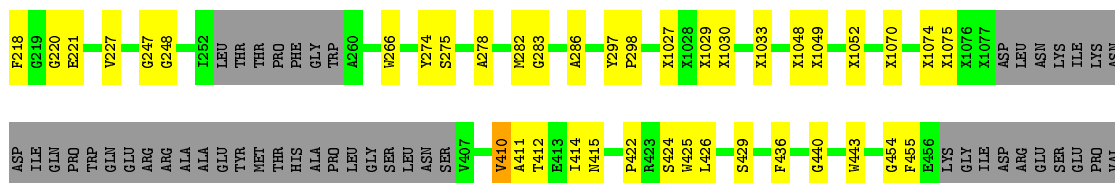
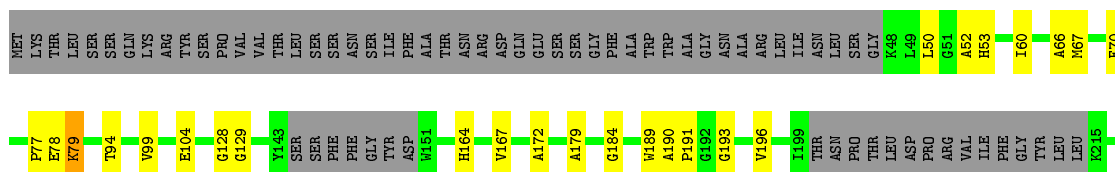
• Molecule 2: Photosystem II: Subunit PsbB

Chain L: 75% 15% 10%



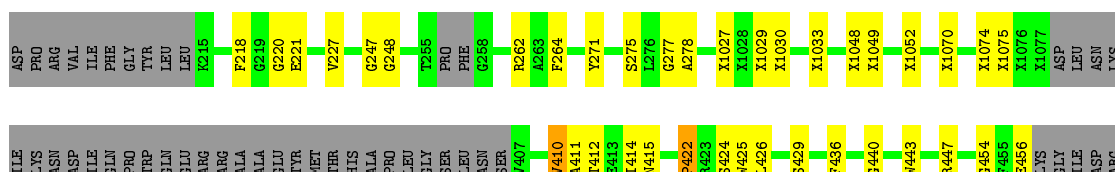
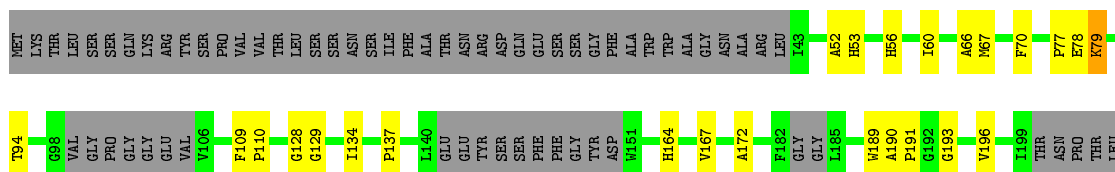
• Molecule 3: Photosystem II: Subunit PsbC

Chain C: 60% 13% 26%



• Molecule 3: Photosystem II: Subunit PsbC

Chain M: 60% 13% 27%



GLU
SER
GLU
PRO
VAL
LEU
SER
MET
SER
PRO
SER
LEU
ASP

• Molecule 4: Photosystem II: Subunit PsbD

Chain D: 63% 14% 21%

MET THR ILE ALA ALA GLY ARG ALA PRO GLU GLU ARG GLY TRP PHE PHE ASP ILE LEU LEU ASP ASP TRP TRP LYS LEU LEU ASP ARG ARG PHE VAL PHE VAL GLY TRP SER G34 Y42 W48 T53 F54 V55 T56 S57 G62 T75 V76 A77 V78 S79 T80 PRO ALA ASN SER MET GLY HIS
SER LEU LEU LEU LEU TRP GLY PRO E96 G99 H111 T112 F113 L122 I123 I124 G124 V138 R139 P140 A145 F146 S147 A148 P149 Y160 G163 GLN SER TRP PHE F169 A170 P171 S172 F184 V345 L346 G200 L209 A212 A216 N220 T221 LEU PHE GLN ASP GLY
GLU GLY ALA SER THR PHE ARG ALA PHE PRO ASN GLN ALA Y244 A249 G258 S262 H268 M271 F298 D308 P309 T313 A330 F339 V340 T56 P341 P342 V345 L346 P347 R348 G349 N350 A351 L352

• Molecule 4: Photosystem II: Subunit PsbD

Chain N: 65% 13% 21%

MET THR ILE ALA ALA GLY ARG ALA PRO GLU GLU ARG GLY TRP PHE PHE ASP ILE LEU LEU ASP ASP TRP TRP LYS LEU LEU ASP ARG ARG PHE VAL PHE VAL GLY TRP SER G34 Y42 T53 F54 V55 T56 S57 G62 T75 V76 T80 PRO ALA ASN SER MET GLY HIS SER LEU LEU
LEU TRP GLY PRO E96 H111 H117 I123 G124 V138 R139 P140 A145 F146 S147 A148 P149 G163 GLN SER TRP PHE F169 A170 A176 F184 P195 G200 A208 L209 A212 I213 A216 N220 T221 LEU PHE GLN ASP GLY
ALA PHE ASN PRO GLN ALA GLU THR Y244 V247 F248 A249 G258 S262 M271 D308 P309 E310 T313 R326 A330 F339 V340 P341 P342 V345 L346 P347 R348 G349 N350 A351 L352

• Molecule 5: Photosystem II: Subunit PsbE

Chain E: 35% 6% 58%

ALA GLY THR GLY GLU P8 E7 I13 T14 V20 G33 G40 I41 ALA TYR ASP VAL PHE GLY THR PRO ARG PRO ASP TYR TYR ALA GLN GLU GLN ARG SER ILE PRO LEU VAL VAL THR PHE LEU GLU LYS GLN GLN VAL VAL THR PHE LEU GLU LYS

• Molecule 5: Photosystem II: Subunit PsbE

Chain P: 19% 80%

ALA GLY THR THR GLY ARG PRO PHE SER ASP ILE ILE THR SER VAL TYR TRP VAL ILE HIS SER HIS T25 G33 L41 TYR TYR ASP VAL PHE GLY THR PRO ARG PRO ASP PRO SER TYR TYR ALA GLN GLN GLN GLN ARG SER ILE PRO VAL VAL THR ASP PHE GLU LYS
GLN GLN VAL GLU THR PHE LEU GLN GLN LYS

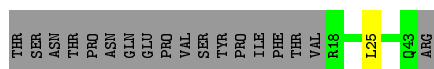
• Molecule 6: Photosystem II: Subunit PsbF

Chain F: 57% 11% 32%

THR SER ASN THR PRO ASN GLN GLU VAL SER TYR P13 I14 V17 R18 L25 Q40 F41 I42 GLN ARG

- Molecule 6: Photosystem II: Subunit PsbF

Chain Q:  57% 41%



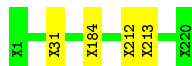
- Molecule 7: Photosystem II: Subunit PsbG

Chain G:  99%



- Molecule 7: Photosystem II: Subunit PsbG

Chain R:  98%



- Molecule 8: Photosystem II: Subunit PsbH

Chain H:  97%




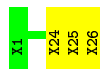
- Molecule 8: Photosystem II: Subunit PsbH

Chain S:  94%




- Molecule 9: Photosystem II: Subunit PsbI

Chain I:  88% 12%



- Molecule 9: Photosystem II: Subunit PsbI

Chain T:  88% 8%



- Molecule 10: Photosystem II: Subunit PsbK

Chain K:  62% 8% 27%



- Molecule 10: Photosystem II: Subunit PsbK

Chain W:  62% 8% 27%




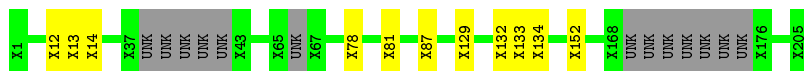
- Molecule 11: Photosystem II: Subunit PsbO

Chain O:  93% 7%



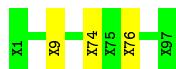
- Molecule 11: Photosystem II: Subunit PsbO

Chain Y:  88% 5% 6%



- Molecule 12: Photosystem II: Subunit PsbU

Chain U:  97%




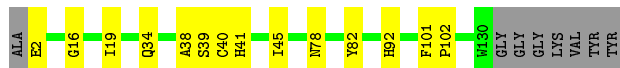
- Molecule 12: Photosystem II: Subunit PsbU

Chain Z:  94% 5%



- Molecule 13: Photosystem II: Subunit PsbV

Chain V:  84% 10% 6%



- Molecule 13: Photosystem II: Subunit PsbV

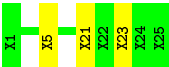
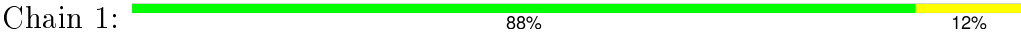
Chain 0:  75% 9% 16%



- Molecule 14: Photosystem II: Subunit PsbX



- Molecule 14: Photosystem II: Subunit PsbX



4 Data and refinement statistics

Xtriage (Phenix) and EDS were 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	129.38Å 225.19Å 308.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.70	Depositor
% Data completeness (in resolution range)	100.0 (25.00-3.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	?	Depositor
R, R_{free}	0.530 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22804	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, MN, CLA, FE, PLA, HEM, BCR

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	0.25	0/1613	0.40	0/2229
1	J	0.26	0/1621	0.40	0/2239
2	B	0.24	0/1685	0.41	0/2331
2	L	0.26	0/1682	0.40	0/2323
3	C	0.24	0/1421	0.40	0/1961
3	M	0.25	0/1379	0.40	0/1898
4	D	0.27	0/1475	0.40	0/2037
4	N	0.27	0/1464	0.39	0/2022
5	E	0.24	0/175	0.46	0/243
5	P	0.31	0/82	0.42	0/112
6	F	0.28	0/169	0.47	0/234
6	Q	0.26	0/128	0.40	0/177
10	K	0.25	0/137	0.45	0/191
10	W	0.25	0/137	0.45	0/191
13	O	0.24	0/600	0.37	0/831
13	V	0.23	0/683	0.38	0/949
All	All	0.25	0/14451	0.40	0/19968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1595	0	834	94	0
1	J	1602	0	843	80	0
2	B	2004	0	968	141	0
2	L	2001	0	961	139	0
3	C	1792	0	842	122	0
3	M	1759	0	793	112	0
4	D	1460	0	761	69	0
4	N	1451	0	746	67	0
5	E	175	0	81	6	0
5	P	83	0	40	2	0
6	F	166	0	95	4	0
6	Q	129	0	66	4	0
7	G	220	0	0	8	0
7	R	220	0	0	10	0
8	H	165	0	36	1	0
8	S	160	0	35	2	0
9	I	130	0	30	2	0
9	T	125	0	29	1	0
10	K	137	0	68	11	0
10	W	137	0	68	11	0
11	O	1025	0	279	37	0
11	Y	960	0	265	34	0
12	U	485	0	112	5	0
12	Z	460	0	106	1	0
13	0	597	0	278	15	0
13	V	676	0	323	16	0
14	1	125	0	28	3	0
14	X	125	0	29	6	0
15	A	4	0	0	0	0
15	J	4	0	0	0	0
16	D	1	0	0	0	0
16	N	1	0	0	0	0
17	A	140	0	68	36	0
17	B	560	0	272	113	0
17	C	420	0	204	95	0
17	D	105	0	48	12	0
17	G	35	0	17	0	0
17	J	105	0	50	23	0
17	L	560	0	272	126	0
17	M	385	0	187	75	0
17	N	140	0	68	10	0
17	R	35	0	17	0	0
17	W	35	0	17	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	A	34	0	19	20	0
18	D	34	0	19	8	0
18	J	34	0	19	19	0
18	N	34	0	19	28	0
19	O	25	0	4	8	0
19	E	25	0	4	0	0
19	P	25	0	4	0	0
19	V	25	0	4	8	0
20	D	6	0	1	0	0
20	N	6	0	1	0	0
21	D	40	0	56	9	0
21	K	22	0	24	1	0
All	All	22804	0	10110	848	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 26.

The worst 5 of 848 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)
2:B:450:TRP:HB3	17:B:1110:CLA:CMB	1.26	1.64
3:M:52:ALA:HB1	17:M:1081:CLA:CAB	1.27	1.62
2:B:465:GLY:CA	17:B:1119:CLA:HMA1	1.22	1.60
2:B:1:MET:HA	7:G:31:UNK:CA	1.20	1.60
1:A:95:PRO:HA	17:A:368:CLA:C3A	1.32	1.59

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	293/360 (81%)	195 (67%)	66 (22%)	32 (11%)	0	10
1	J	293/360 (81%)	199 (68%)	59 (20%)	35 (12%)	0	8
2	B	314/472 (66%)	219 (70%)	62 (20%)	33 (10%)	1	11
2	L	309/472 (66%)	215 (70%)	60 (19%)	34 (11%)	0	10
3	C	263/473 (56%)	198 (75%)	47 (18%)	18 (7%)	1	23
3	M	257/473 (54%)	189 (74%)	47 (18%)	21 (8%)	1	17
4	D	269/352 (76%)	187 (70%)	56 (21%)	26 (10%)	1	13
4	N	269/352 (76%)	184 (68%)	59 (22%)	26 (10%)	1	13
5	E	33/83 (40%)	23 (70%)	5 (15%)	5 (15%)	0	5
5	P	15/83 (18%)	11 (73%)	4 (27%)	0	100	100
6	F	28/44 (64%)	22 (79%)	3 (11%)	3 (11%)	0	10
6	Q	24/44 (54%)	22 (92%)	2 (8%)	0	100	100
10	K	25/37 (68%)	14 (56%)	9 (36%)	2 (8%)	1	18
10	W	25/37 (68%)	15 (60%)	8 (32%)	2 (8%)	1	18
13	O	111/137 (81%)	90 (81%)	17 (15%)	4 (4%)	4	41
13	V	127/137 (93%)	102 (80%)	19 (15%)	6 (5%)	3	33
All	All	2655/3916 (68%)	1885 (71%)	523 (20%)	247 (9%)	1	15

5 of 247 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	101	SER
1	A	168	PHE
1	A	191	ASN
1	A	192	ILE

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	21/290 (7%)	20 (95%)	1 (5%)	31	72
1	J	22/290 (8%)	21 (96%)	1 (4%)	34	74
2	B	21/290 (7%)	21 (100%)	0	100	100
2	L	21/290 (7%)	21 (100%)	0	100	100
3	C	16/315 (5%)	16 (100%)	0	100	100
3	M	10/315 (3%)	9 (90%)	1 (10%)	9	44
4	D	16/283 (6%)	16 (100%)	0	100	100
4	N	14/283 (5%)	14 (100%)	0	100	100
5	E	1/72 (1%)	1 (100%)	0	100	100
6	F	3/38 (8%)	3 (100%)	0	100	100
10	K	1/30 (3%)	1 (100%)	0	100	100
10	W	1/30 (3%)	1 (100%)	0	100	100
13	O	5/117 (4%)	5 (100%)	0	100	100
13	V	7/117 (6%)	7 (100%)	0	100	100
All	All	159/2760 (6%)	156 (98%)	3 (2%)	65	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	J	182	PHE
3	M	422	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	164	HIS
4	N	117	HIS
1	J	332	HIS
2	B	9	HIS
3	M	164	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 94 ligands modelled in this entry, 10 are monoatomic - leaving 84 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$
19	HEM	0	138	13	25,32,50	3.98	11 (44%)	22,54,82	2.96	10 (45%)
17	CLA	A	365	-	25,43,73	1.61	4 (16%)	28,76,113	2.55	10 (35%)
17	CLA	A	366	-	25,43,73	1.10	3 (12%)	28,76,113	2.15	10 (35%)
18	PHO	A	367	-	37,39,69	1.19	4 (10%)	52,62,99	1.67	5 (9%)
17	CLA	A	368	1	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	A	369	-	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	B	1107	-	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	B	1108	2	25,43,73	1.30	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1109	2	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1110	-	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	B	1111	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	B	1112	-	25,43,73	1.32	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	B	1113	2	25,43,73	1.31	3 (12%)	28,76,113	2.07	9 (32%)
17	CLA	B	1114	2	25,43,73	1.33	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	B	1115	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	B	1116	2	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1117	2	25,43,73	1.33	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	B	1118	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	1119	2	25,43,73	1.33	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	B	1120	-	25,43,73	1.34	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	B	1121	-	25,43,73	1.31	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	B	1122	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1078	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1079	3	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	C	1080	3	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	C	1081	-	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	C	1082	3	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	C	1083	-	25,43,73	1.32	4 (16%)	28,76,113	2.04	9 (32%)
17	CLA	C	1084	-	25,43,73	1.33	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	C	1085	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1086	3	25,43,73	1.34	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	C	1087	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	C	1088	3	25,43,73	1.33	4 (16%)	28,76,113	2.04	9 (32%)
17	CLA	C	1089	3	25,43,73	1.32	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	D	354	4	25,43,73	1.27	3 (12%)	28,76,113	2.03	8 (28%)
17	CLA	D	355	-	25,43,73	1.09	1 (4%)	28,76,113	2.06	10 (35%)
18	PHO	D	356	4	37,39,69	1.17	4 (10%)	52,62,99	1.69	5 (9%)
17	CLA	D	357	4	25,43,73	1.35	4 (16%)	28,76,113	2.07	9 (32%)
20	PLA	D	358	-	6,6,25	2.91	5 (83%)	6,6,37	0.88	0
21	BCR	D	359	-	41,41,41	1.25	5 (12%)	56,56,56	1.77	17 (30%)
19	HEM	E	84	-	25,32,50	3.98	11 (44%)	22,54,82	2.95	10 (45%)
17	CLA	G	221	-	25,43,73	1.34	4 (16%)	28,76,113	1.92	8 (28%)
17	CLA	J	365	-	25,43,73	1.59	3 (12%)	28,76,113	2.66	10 (35%)
18	PHO	J	366	-	37,39,69	1.19	4 (10%)	52,62,99	1.69	5 (9%)
17	CLA	J	367	1	25,43,73	1.32	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	J	368	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
21	BCR	K	47	-	19,21,41	0.83	0	20,24,56	1.21	2 (10%)
17	CLA	L	1107	-	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	L	1108	-	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	L	1109	2	25,43,73	1.31	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	L	1110	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1111	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1112	-	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	L	1113	2	25,43,73	1.30	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1114	-	25,43,73	1.34	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	L	1115	-	25,43,73	1.32	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1116	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1117	2	25,43,73	1.33	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1118	-	25,43,73	1.32	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	L	1119	-	25,43,73	1.34	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	L	1120	-	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	L	1121	2	25,43,73	1.31	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	L	1122	-	25,43,73	1.32	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	M	1078	-	25,43,73	1.33	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	M	1079	3	25,43,73	1.32	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	M	1080	-	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	M	1081	-	25,43,73	1.32	3 (12%)	28,76,113	2.03	9 (32%)
17	CLA	M	1082	-	25,43,73	1.32	4 (16%)	28,76,113	2.04	9 (32%)
17	CLA	M	1083	-	25,43,73	1.31	4 (16%)	28,76,113	2.07	9 (32%)
17	CLA	M	1084	-	25,43,73	1.31	3 (12%)	28,76,113	2.05	9 (32%)
17	CLA	M	1085	3	25,43,73	1.33	4 (16%)	28,76,113	2.06	9 (32%)
17	CLA	M	1086	-	25,43,73	1.32	3 (12%)	28,76,113	2.04	9 (32%)
17	CLA	M	1087	3	25,43,73	1.34	4 (16%)	28,76,113	2.05	9 (32%)
17	CLA	M	1088	-	25,43,73	1.33	3 (12%)	28,76,113	2.06	9 (32%)
17	CLA	N	354	4	25,43,73	1.27	2 (8%)	28,76,113	2.03	8 (28%)
17	CLA	N	355	-	25,43,73	1.11	3 (12%)	28,76,113	2.15	10 (35%)
17	CLA	N	356	-	25,43,73	1.08	1 (4%)	28,76,113	2.06	10 (35%)
18	PHO	N	357	-	37,39,69	1.16	4 (10%)	52,62,99	1.70	5 (9%)
17	CLA	N	358	4	25,43,73	1.32	4 (16%)	28,76,113	2.07	9 (32%)
20	PLA	N	359	-	6,6,25	2.91	5 (83%)	6,6,37	0.88	0
19	HEM	P	92	-	25,32,50	3.98	11 (44%)	22,54,82	2.97	10 (45%)
17	CLA	R	221	-	25,43,73	1.34	4 (16%)	28,76,113	1.92	8 (28%)
19	HEM	V	138	13	25,32,50	3.98	11 (44%)	22,54,82	2.95	10 (45%)
17	CLA	W	64	-	25,43,73	1.33	4 (16%)	28,76,113	2.05	9 (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
19	HEM	0	138	13	-	0/0/40/54	0/0/8/8
17	CLA	A	365	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	A	366	-	2/2/13/25	0/0/92/135	0/0/9/9
18	PHO	A	367	-	-	0/15/60/103	0/1/6/6
17	CLA	A	368	1	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	A	369	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1107	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1108	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1109	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1110	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1111	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1112	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1113	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1114	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1115	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1116	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1117	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1118	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1119	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1120	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1121	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	B	1122	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1078	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1079	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1080	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1081	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1082	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1083	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1084	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1085	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1086	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1087	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1088	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	C	1089	3	4/4/13/25	0/0/92/135	0/0/9/9
17	CLA	D	354	4	1/1/13/25	0/0/92/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	D	355	-	2/2/13/25	0/0/92/135	0/0/9/9
18	PHO	D	356	4	-	0/15/60/103	0/1/6/6
17	CLA	D	357	4	3/3/13/25	0/0/92/135	0/0/9/9
20	PLA	D	358	-	-	0/0/0/23	0/1/1/1
21	BCR	D	359	-	-	0/29/63/63	0/2/2/2
19	HEM	E	84	-	-	0/0/40/54	0/0/8/8
17	CLA	G	221	-	2/2/13/25	0/0/92/135	0/0/9/9
17	CLA	J	365	-	3/3/13/25	0/0/92/135	0/0/9/9
18	PHO	J	366	-	-	0/15/60/103	0/1/6/6
17	CLA	J	367	1	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	J	368	-	3/3/13/25	0/0/92/135	0/0/9/9
21	BCR	K	47	-	-	0/21/23/63	0/0/0/2
17	CLA	L	1107	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1108	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1109	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1110	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1111	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1112	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1113	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1114	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1115	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1116	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1117	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1118	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1119	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1120	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1121	2	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	L	1122	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1078	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1079	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1080	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1081	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1082	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1083	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1084	-	3/3/13/25	0/0/92/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	M	1085	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1086	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1087	3	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	M	1088	-	3/3/13/25	0/0/92/135	0/0/9/9
17	CLA	N	354	4	1/1/13/25	0/0/92/135	0/0/9/9
17	CLA	N	355	-	2/2/13/25	0/0/92/135	0/0/9/9
17	CLA	N	356	-	2/2/13/25	0/0/92/135	0/0/9/9
18	PHO	N	357	-	-	0/15/60/103	0/1/6/6
17	CLA	N	358	4	3/3/13/25	0/0/92/135	0/0/9/9
20	PLA	N	359	-	-	0/0/0/23	0/1/1/1
19	HEM	P	92	-	-	0/0/40/54	0/0/8/8
17	CLA	R	221	-	2/2/13/25	0/0/92/135	0/0/9/9
19	HEM	V	138	13	-	0/0/40/54	0/0/8/8
17	CLA	W	64	-	3/3/13/25	0/0/92/135	0/0/9/9

The worst 5 of 316 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	92	HEM	C2D-C1D	-8.41	1.38	1.50
19	0	138	HEM	C2D-C1D	-8.38	1.38	1.50
19	V	138	HEM	C2D-C1D	-8.34	1.38	1.50
19	E	84	HEM	C2D-C1D	-8.28	1.38	1.50
19	V	138	HEM	C2B-C1B	-7.32	1.39	1.50

The worst 5 of 729 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	365	CLA	OBD-CAD-CBD	-7.98	109.14	125.98
19	0	138	HEM	C3D-C4D-CHA	-7.10	116.89	124.06
19	P	92	HEM	C3D-C4D-CHA	-7.06	116.93	124.06
19	V	138	HEM	C3D-C4D-CHA	-7.01	116.98	124.06
19	E	84	HEM	C3D-C4D-CHA	-6.98	117.01	124.06

5 of 207 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	L	1111	CLA	NC
17	L	1111	CLA	ND
17	L	1111	CLA	NA
17	J	367	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	J	367	CLA	ND

There are no torsion outliers.

There are no ring outliers.

70 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	0	138	HEM	8	0
17	A	365	CLA	5	0
17	A	366	CLA	5	0
18	A	367	PHO	20	0
17	A	368	CLA	24	0
17	A	369	CLA	2	0
17	B	1107	CLA	11	0
17	B	1108	CLA	8	0
17	B	1109	CLA	13	0
17	B	1110	CLA	10	0
17	B	1111	CLA	19	0
17	B	1112	CLA	3	0
17	B	1113	CLA	3	0
17	B	1114	CLA	14	0
17	B	1116	CLA	7	0
17	B	1117	CLA	12	0
17	B	1118	CLA	6	0
17	B	1119	CLA	14	0
17	B	1120	CLA	5	0
17	B	1121	CLA	3	0
17	C	1078	CLA	11	0
17	C	1079	CLA	15	0
17	C	1080	CLA	11	0
17	C	1081	CLA	5	0
17	C	1082	CLA	11	0
17	C	1083	CLA	6	0
17	C	1085	CLA	3	0
17	C	1086	CLA	9	0
17	C	1087	CLA	3	0
17	C	1088	CLA	14	0
17	C	1089	CLA	24	0
17	D	354	CLA	7	0
18	D	356	PHO	8	0
17	D	357	CLA	5	0
21	D	359	BCR	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	J	365	CLA	2	0
18	J	366	PHO	19	0
17	J	367	CLA	21	0
21	K	47	BCR	1	0
17	L	1107	CLA	9	0
17	L	1108	CLA	13	0
17	L	1109	CLA	13	0
17	L	1110	CLA	6	0
17	L	1111	CLA	16	0
17	L	1112	CLA	3	0
17	L	1113	CLA	4	0
17	L	1114	CLA	12	0
17	L	1115	CLA	2	0
17	L	1117	CLA	12	0
17	L	1118	CLA	6	0
17	L	1119	CLA	23	0
17	L	1120	CLA	22	0
17	L	1121	CLA	3	0
17	M	1078	CLA	3	0
17	M	1079	CLA	16	0
17	M	1080	CLA	1	0
17	M	1081	CLA	14	0
17	M	1082	CLA	6	0
17	M	1084	CLA	3	0
17	M	1085	CLA	4	0
17	M	1086	CLA	3	0
17	M	1087	CLA	11	0
17	M	1088	CLA	15	0
17	N	354	CLA	4	0
17	N	355	CLA	4	0
17	N	356	CLA	1	0
18	N	357	PHO	28	0
17	N	358	CLA	1	0
19	V	138	HEM	8	0
17	W	64	CLA	15	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 ⓘ

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.