

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 07:50 am BST

PDB ID : 5NMU

Title : Structure of hexameric CBS-CP12 protein from bloom-forming cyanobacteria Authors : Hackenberg, C.; Hakanpaa, J.; Antonyuk, S.V.; Dittmann, E.; Lamzin, V.S.

Deposited on : 2017-04-07

Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/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 Xtriage (Phenix) : 1.13

EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

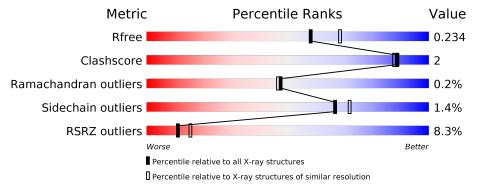
Validation Pipeline (wwPDB-VP) : 2.11

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 2.15 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	208	80%	5%	15%
1	В	208	77%	5% •	17%
1	С	208	76%	6%	18%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4196 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 CBS-CP12.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	Λ	177	Total	С	N	О	S	0	0	0	0
1	A	111	1375	872	237	258	8	0	U		
1	D	173	Total	С	N	О	S	0	0	0	
1	Б	173	1331	846	228	250	7	0			
1	1 C	C 171	Total	С	N	О	S	0	0	0	
	171	1295	827	221	240	7	0	U			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A8YJ50
A	2	PRO	-	expression tag	UNP A8YJ50
A	3	MET	_	expression tag	UNP A8YJ50
A	4	VAL	_	expression tag	UNP A8YJ50
В	1	GLY	-	expression tag	UNP A8YJ50
В	2	PRO	_	expression tag	UNP A8YJ50
В	3	MET	-	expression tag	UNP A8YJ50
В	4	VAL	_	expression tag	UNP A8YJ50
С	1	GLY	-	expression tag	UNP A8YJ50
С	2	PRO	-	expression tag	UNP A8YJ50
С	3	MET	-	expression tag	UNP A8YJ50
С	4	VAL	-	expression tag	UNP A8YJ50

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Cl 1 1	0	0
2	A	2	Total Cl 2 2	0	0
2	С	1	Total Cl 1 1	0	0



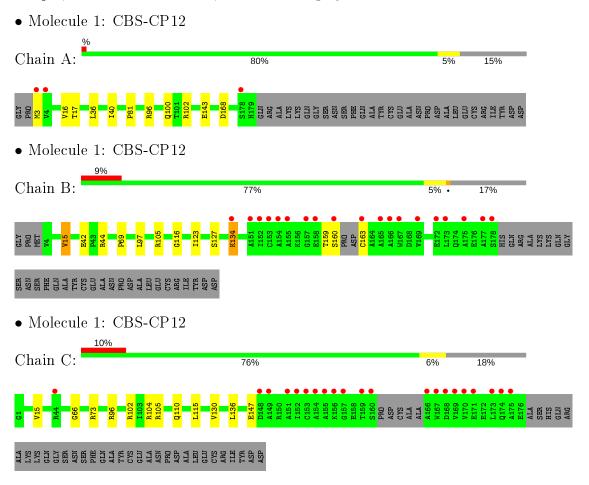
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	80	Total O 80 80	0	0
3	В	68	Total O 68 68	0	0
3	С	43	Total O 43 43	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 the various outlier classes 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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	81.61Å 124.02Å 118.45Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.58 - 2.15	Depositor
Resolution (A)	38.58 - 2.15	EDS
% Data completeness	97.1 (38.58-2.15)	Depositor
(in resolution range)	97.2 (38.58-2.15)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.34 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
D D.	0.178 , 0.234	Depositor
R, R_{free}	0.187 , 0.234	DCC
R_{free} test set	1643 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 40.5	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4196	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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	Chain	Bond	lengths	Bo	nd angles
	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.84	0/1396	0.95	2/1889 (0.1%)
1	В	0.70	0/1349	0.88	$2/1824 \ (0.1\%)$
1	С	0.68	0/1314	0.86	4/1777 (0.2%)
All	All	0.75	0/4059	0.90	8/5490 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	168	ASP	CB-CG-OD1	7.20	124.78	118.30
1	В	105	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	В	105	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	С	105	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	С	104	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	С	105	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	С	73	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	96	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	Α	1375	0	1407	5	0
1	В	1331	0	1363	10	0
1	С	1295	0	1308	4	0
2	A	2	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
3	A	80	0	0	1	0
3	В	68	0	0	2	0
3	С	43	0	0	0	0
All	All	4196	0	4078	15	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 2.

All (15) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:C:96:ARG:HD2	1:C:136:LEU:HD22	1.83	0.60
1:A:143:GLU:OE2	1:B:44:ARG:NH2	2.36	0.59
1:B:42:GLU:HB3	3:B:402:HOH:O	2.05	0.57
1:A:100:GLN:NE2	3:A:402:HOH:O	2.42	0.52
1:B:42:GLU:CB	3:B:402:HOH:O	2.58	0.52
1:B:123:ILE:O	1:B:127:SER:HB3	2.10	0.51
1:B:69:PRO:HG2	1:C:130:VAL:HA	1.99	0.45
1:A:81:PRO:HG2	1:B:97:LEU:HB2	1.98	0.45
1:A:16:VAL:HG21	1:A:36:LEU:HD11	1.98	0.44
1:B:159:THR:O	1:B:160:SER:OG	2.27	0.44
1:B:160:SER:HB2	1:B:163:CYS:N	2.34	0.43
1:B:134:LYS:O	1:C:66:GLY:HA3	2.19	0.43
1:B:15:VAL:HG11	1:B:116:GLY:C	2.41	0.40
1:C:110:GLN:HB2	1:C:115:LEU:HD11	2.02	0.40
1:A:17:THR:HA	1:A:40:ILE:O	2.21	0.40

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	${f Analysed}$	Favoured	Allowed	$\mathbf{Outliers}$	Perce	\mathbf{ntiles}
1	A	175/208~(84%)	174 (99%)	1 (1%)	0	100	100
1	В	169/208~(81%)	166 (98%)	3 (2%)	0	100	100
1	С	167/208 (80%)	158 (95%)	8 (5%)	1 (1%)	25	18
All	All	511/624 (82%)	498 (98%)	12 (2%)	1 (0%)	47	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	147	GLU

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	147/173~(85%)	145 (99%)	2 (1%)	67 72
1	В	141/173 (82%)	139 (99%)	2 (1%)	67 72
1	С	132/173 (76%)	130 (98%)	2 (2%)	65 69
All	All	420/519 (81%)	414 (99%)	6 (1%)	67 72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	102	ARG
1	В	15	VAL
1	В	134	LYS
1	С	15	VAL
1	C	102	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	100	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	177/208~(85%)	-0.27	3 (1%) 70 76	31, 43, 63, 104	0
1	В	173/208 (83%)	0.37	19 (10%) 5 8	30, 47, 107, 128	1 (0%)
1	С	171/208 (82%)	0.25	21 (12%) 4 5	34, 54, 126, 134	0
All	All	521/624 (83%)	0.11	43 (8%) 11 15	30, 46, 107, 134	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	152	ILE	7.9
1	В	166	ALA	6.6
1	В	155	ALA	6.2
1	С	167	TRP	6.1
1	С	169	VAL	5.6
1	В	151	ALA	5.3
1	С	149	ALA	5.2
1	С	166	ALA	4.3
1	В	167	TRP	4.3
1	С	171	GLU	4.2
1	A	3	MET	4.2
1	В	152	ILE	4.2
1	С	153	CYS	4.1
1	С	159	THR	4.0
1	С	151	ALA	4.0
1	С	173	LEU	3.9
1	В	169	VAL	3.8
1	В	172	GLU	3.8
1	В	134	LYS	3.8
1	С	170	VAL	3.6
1	С	154	ALA	3.5
1	В	154	ALA	3.5
1	С	160	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	В	160	SER	3.5
1	В	165	ALA	3.0
1	С	157	GLY	3.0
1	В	173	LEU	3.0
1	С	175	ALA	3.0
1	С	168	ASP	3.0
1	A	4	VAL	2.7
1	В	177	ALA	2.7
1	С	155	ALA	2.6
1	С	174	GLN	2.5
1	С	156	LYS	2.4
1	В	163	CYS	2.3
1	В	158	GLU	2.3
1	В	157	GLY	2.2
1	В	175	ALA	2.2
1	С	148	ASP	2.2
1	С	44	ARG	2.2
1	В	178	SER	2.0
1	A	178	SER	2.0
1	В	153	CYS	2.0

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. 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	${f B-factors}({f \AA}^2)$	Q<0.9
2	CL	A	302	1/1	0.97	0.11	53,53,53,53	0
2	CL	С	301	1/1	0.99	0.13	44,44,44,44	0
2	CL	A	301	1/1	1.00	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	CL	В	301	1/1	1.00	0.10	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.

