

Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2021 – 03:23 PM EST

PDB ID : 1XFJ

Title : Crystal structure of protein CC 0490 from Caulobacter crescentus, Pfam

DUF152

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Deposited on : 2004-09-14

Resolution : 1.75 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED EDS : NOT EXECUTED

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

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

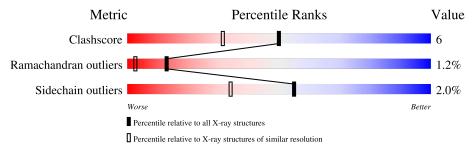
Validation Pipeline (wwPDB-VP) : 2.16

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 1.75 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 of 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	261	86%	11%	

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
4	GOL	A	271	_	X	-	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2202 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.

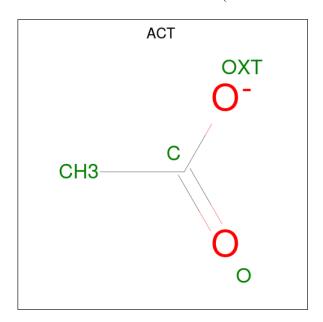
• Molecule 1 is a protein called conserved hypothetical protein.

Mo	l Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	256	Total 1935	C 1215	N 347	O 366	S 5	Se 2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	•
A	110	MSE		modified residue	
A	149	MSE	MET	modified residue	UNP Q9AAV3

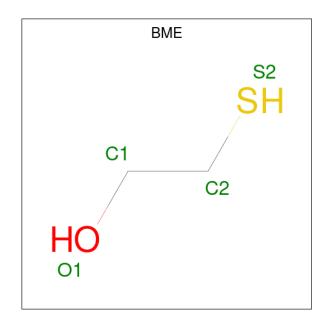
• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



N	/Iol	Chain	Residues	Atoms			ZeroOcc	AltConf
	2	A	1	Total 4	C 2	O 2	0	0



• Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 1	S 1	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	253	Total O 253 253	0	0

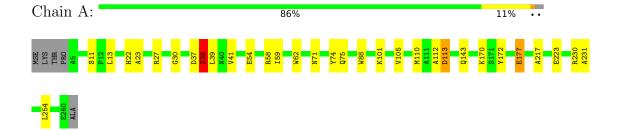


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: conserved hypothetical protein





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	39.81Å 66.83Å 43.17Å	Depositor	
a, b, c, α , β , γ	90.00° 110.60° 90.00°	Depositor	
Resolution (Å)	50.00 - 1.75	Depositor	
% Data completeness	(Not available) (50.00-1.75)	Depositor	
(in resolution range)	(1100 available) (90.00 1.19)		
R_{merge}	0.05	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	CNS	Depositor	
R, R_{free}	0.180 , 0.220	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2202	wwPDB-VP	
Average B, all atoms (Å ²)	9.0	wwPDB-VP	



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: GOL, ACT, BME

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).

Mal	Chain	Bond	lengths	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.29	0/1978	0.61	1/2683 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	A	74	TYR	N-CA-C	-6.38	93.78	111.00

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	A	1935	0	1870	22	0
2	A	4	0	3	0	0
3	A	4	0	4	0	0
4	A	6	0	3	1	0
5	A	253	0	0	1	0
All	All	2202	0	1880	22	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 6.



All (22) 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)
1:A:11:SER:H	1:A:22:HIS:HE1	1.36	0.73
1:A:75:GLN:HE22	1:A:110:MSE:H	1.38	0.71
1:A:59:ILE:HG21	1:A:254:LEU:HD23	1.79	0.63
1:A:27:ARG:O	1:A:38:SER:HB3	2.00	0.62
1:A:13:LEU:HD22	1:A:223:GLU:HG2	1.82	0.61
1:A:11:SER:H	1:A:22:HIS:CE1	2.17	0.59
1:A:170:LYS:HZ2	1:A:231:ALA:HB2	1.69	0.57
1:A:71:ASN:ND2	1:A:105:VAL:HG13	2.23	0.54
1:A:41:VAL:HG21	1:A:254:LEU:HB2	1.93	0.51
1:A:112:ALA:O	1:A:113:ASP:HB2	2.11	0.50
1:A:112:ALA:O	1:A:113:ASP:CB	2.59	0.50
1:A:75:GLN:NE2	1:A:110:MSE:H	2.06	0.49
1:A:170:LYS:NZ	1:A:231:ALA:HB2	2.30	0.47
1:A:177:GLU:H	1:A:177:GLU:CD	2.18	0.47
1:A:30:GLY:N	1:A:38:SER:OG	2.47	0.47
1:A:54:GLU:O	1:A:58:ARG:HG3	2.15	0.46
1:A:71:ASN:HB3	1:A:88:TRP:CZ3	2.51	0.45
1:A:143:GLN:HE22	1:A:217:ALA:HA	1.82	0.44
1:A:38:SER:HB2	4:A:271:GOL:O1	2.19	0.42
1:A:23:ALA:HB2	1:A:62:TRP:CH2	2.55	0.42
1:A:101:LYS:HE2	5:A:421:HOH:O	2.20	0.41
1:A:38:SER:HB3	1:A:39:LEU:H	1.62	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	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	254/261 (97%)	243 (96%)	8 (3%)	3 (1%)	13 3



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	38	SER
1	A	113	ASP

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	Analysed Rotameric C		Percentiles	
1	A	197/198 (100%)	193 (98%)	4 (2%)	55 34	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	172	TYR
1	A	177	GLU
1	A	230	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	22	HIS
1	A	71	ASN
1	A	75	GLN
1	A	77	HIS
1	A	143	GLN
1	A	239	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	272	-	1,3,3	2.52	1 (100%)	0,3,3	0.00	-
4	GOL	A	271	-	5,5,5	4.42	5 (100%)	5,5,5	5.70	3 (60%)
3	BME	A	273	-	3,3,3	1.63	1 (33%)	1,2,2	0.06	0

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
4	GOL	A	271	-	-	2/4/4/4	-
3	BME	A	273	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\mathring{A}})$	Ideal(A)
4	A	271	GOL	C3-C2	-7.39	1.21	1.51
4	A	271	GOL	O1-C1	-4.05	1.25	1.42
4	A	271	GOL	O3-C3	3.28	1.56	1.42
4	A	271	GOL	C1-C2	-2.96	1.39	1.51
3	A	273	BME	O1-C1	-2.75	1.27	1.42

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M	lol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(A)
4	4	A	271	GOL	O2-C2	-2.66	1.35	1.43
4	2	A	272	ACT	СН3-С	2.52	1.52	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
4	A	271	GOL	O3-C3-C2	10.17	158.96	110.20
4	A	271	GOL	O2-C2-C3	6.95	139.72	109.12
4	A	271	GOL	O1-C1-C2	3.14	125.28	110.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	271	GOL	C1-C2-C3-O3
4	A	271	GOL	O1-C1-C2-O2
3	A	273	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	271	GOL	1	0

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

