



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:03 PM BST

PDB ID : 6X84
Title : Sn-glycerol-3-phosphate binding periplasmic protein UgpB from Escherichia coli - W169S, W172S
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Deposited on : 2020-06-01
Resolution : 1.25 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.14.4.dev1

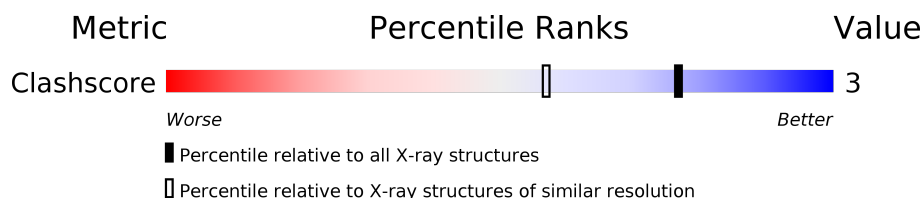
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	141614	1060 (1.28-1.24)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	416	94% 6%
1	B	416	95% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6954 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 sn-glycerol-3-phosphate-binding periplasmic protein UgpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	4	0
			3226	2048	536	626	16			
1	B	414	Total	C	N	O	S	0	1	0
			3066	1946	505	600	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0AG80
A	169	SER	TRP	engineered mutation	UNP P0AG80
A	172	SER	TRP	engineered mutation	UNP P0AG80
B	0	SER	-	expression tag	UNP P0AG80
B	169	SER	TRP	engineered mutation	UNP P0AG80
B	172	SER	TRP	engineered mutation	UNP P0AG80

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	414	Total	O	0	0
			414	414		
3	B	242	Total	O	0	0
			242	242		

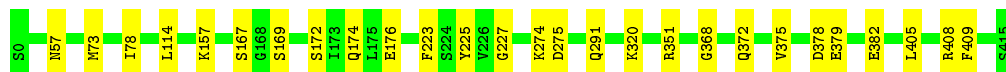
3 Residue-property plots [i](#)

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 failed to run properly.

- Molecule 1: sn-glycerol-3-phosphate-binding periplasmic protein UgpB

Chain A:  94% 6%



- Molecule 1: sn-glycerol-3-phosphate-binding periplasmic protein UgpB

Chain B:  95% 5%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.94Å 46.72Å 94.79Å 90.89° 98.53° 105.13°	Depositor
Resolution (Å)	46.80 – 1.25	Depositor
% Data completeness (in resolution range)	94.7 (46.80-1.25)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.25Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.158 , 0.186	Depositor
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.369	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6954	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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

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	0.57	0/3312	0.74	1/4486 (0.0%)
1	B	0.45	0/3146	0.64	0/4293
All	All	0.52	0/6458	0.69	1/8779 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ASP	CB-CG-OD1	6.03	123.73	118.30

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	A	3226	0	3115	22	0
1	B	3066	0	2803	19	0
2	B	6	0	8	0	0
3	A	414	0	0	5	1
3	B	242	0	0	3	1
All	All	6954	0	5926	37	1

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 3.

All (37) 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:408:ARG:HD2	1:B:147:GLN:HB3	1.67	0.77
1:A:73[B]:MET:SD	1:A:114:LEU:HD13	2.33	0.68
1:A:375:VAL:O	1:A:379:GLU:HG3	1.99	0.62
1:A:408:ARG:HH22	1:B:151:ASP:HB2	1.66	0.61
1:A:174:GLN:NE2	3:A:511:HOH:O	2.35	0.58
1:A:408:ARG:NH2	1:B:151:ASP:HB2	2.19	0.57
1:B:7:TRP:CE2	1:B:39:LYS:HE3	2.40	0.57
1:B:73[A]:MET:SD	1:B:366:ARG:HD3	2.44	0.57
1:A:320:LYS:NZ	3:A:510:HOH:O	2.35	0.56
1:B:401:ARG:NH1	3:B:601:HOH:O	2.21	0.56
1:A:169:SER:HB3	1:A:227:GLY:O	2.06	0.55
1:A:351:ARG:NH1	3:A:514:HOH:O	2.40	0.55
1:A:408:ARG:CD	1:B:147:GLN:HB3	2.39	0.51
1:A:73[B]:MET:CE	1:A:78:ILE:HD11	2.42	0.49
1:A:372:GLN:HB2	1:A:405[B]:LEU:HD23	1.95	0.49
1:A:73[B]:MET:CE	1:A:73[B]:MET:HA	2.44	0.48
1:B:7:TRP:CD2	1:B:39:LYS:HE3	2.50	0.47
1:A:167:SER:HG	1:A:223:PHE:HE1	1.64	0.46
1:B:79:LYS:HD2	1:B:84:VAL:HG22	1.98	0.46
1:B:201:GLU:O	1:B:204:LYS:HG2	2.17	0.45
1:B:186:PHE:CD2	1:B:365:LEU:HD11	2.52	0.45
1:A:368:GLY:HA3	1:A:409:PHE:CG	2.53	0.43
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.93	0.43
1:B:403:ASN:O	1:B:407:ARG:HG2	2.19	0.42
1:A:73[B]:MET:HE1	1:A:78:ILE:HD11	2.01	0.42
1:A:57:ASN:OD1	3:A:502:HOH:O	2.22	0.42
1:A:172:SER:O	1:A:176:GLU:HG3	2.20	0.41
1:B:238:ASN:HB3	3:B:797:HOH:O	2.21	0.41
1:A:225:TYR:CE2	1:A:382:GLU:HG2	2.55	0.41
1:A:157:LYS:HE2	1:A:157:LYS:HB3	1.77	0.41
1:B:199:VAL:HG22	3:B:683:HOH:O	2.20	0.41
1:B:186:PHE:HD2	1:B:365:LEU:HD11	1.86	0.41
1:B:79:LYS:HB2	1:B:79:LYS:HE2	1.87	0.41
1:A:274:LYS:HG2	1:A:275:ASP:OD1	2.21	0.41
1:B:102:SER:HB2	1:B:113:LEU:HD21	2.04	0.41
1:B:73[B]:MET:SD	1:B:114:LEU:HD13	2.62	0.40
1:A:291:GLN:OE1	3:A:503:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:881:HOH:O	3:B:823:HOH:O[1_556]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

1 ligand is 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		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	501	-	5,5,5	0.69	0	5,5,5	0.61	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
2	GOL	B	501	-	-	0/4/4/4	-

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.