

Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2020 - 03:00 PM BST

PDB ID : 6XZ5

Title : RovC - regulator of virulence interconnected with the Csr system

Authors : Sadana, P.; Scrima, A.

Deposited on : 2020-02-02

Resolution : 2.30 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

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)

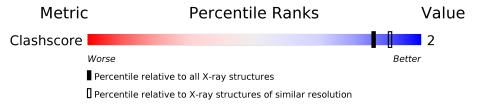
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.30 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	$(\# ext{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$	
Clashscore	141614	5643 (2.30-2.30)	

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	A	252	80%	5%	15%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1732 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.

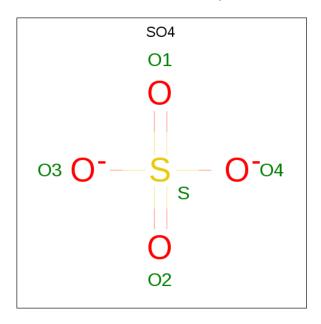
• Molecule 1 is a protein called Uncharacterized protein, RovC, Uncharacterized protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	214	Total	С	N	О	S	0	0	0
1	11	214	1682	1079	293	304	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLN	_	expression tag	UNP A0A0H3B5N9
A	-3	GLY	-	expression tag	UNP A0A0H3B5N9
A	-2	GLY	-	expression tag	UNP A0A0H3B5N9
A	-1	GLY	-	expression tag	UNP A0A0H3B5N9
A	0	ARG	_	expression tag	UNP A0A0H3B5N9

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	40	Total O 40 40	0	0

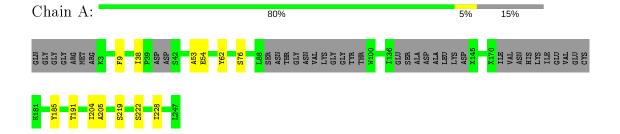


3 Residue-property plots (i)

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 failed to run properly.

• Molecule 1: Uncharacterized protein, RovC, Uncharacterized protein





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants	97.28	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.44 - 2.30	Depositor
% Data completeness	96.2 (33.44-2.30)	Depositor
(in resolution range)	, ,	-
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.229 , 0.274	Depositor
Wilson B-factor (A^2)	39.1	Xtriage
Anisotropy	0.170	Xtriage
L-test for twinning ²	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,l	Xtriage
Total number of atoms	1732	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.58% 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: SO4

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	0.24	0/1588	0.39	0/2138	

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 (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	1682	0	1552	7	0
2	A	10	0	0	0	0
3	A	40	0	0	0	0
All	All	1732	0	1552	7	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 (7) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-1 Atom-2		$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:53:ALA:HB2	1:A:62:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${f distance}({f \AA})$	$ \text{overlap } (\text{\AA})$	
1:A:205:ALA:HB2	1:A:228:ILE:HG13	1.96	0.48	
1:A:191:THR:HG23	1:A:204:ILE:HG21	1.96	0.47	
1:A:219:SER:HB2	1:A:222:SER:HB3	1.96	0.47	
1:A:54:GLU:HG3	1:A:76:SER:HB2	1.97	0.46	
1:A:38:ILE:H	1:A:38:ILE:HD12	1.84	0.42	
1:A:9:PHE:CE1	1:A:185:TYR:HB3	2.55	0.41	

There are no symmetry-related clashes.

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)

2 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			
	туре				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	302	_	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.05	0

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)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

