



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5FEI
Title : Crystal structure of the bacteriophage phi29 tail knob protein gp9 truncation variant
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Deposited on : 2015-12-17
Resolution : 2.60 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

<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 : 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

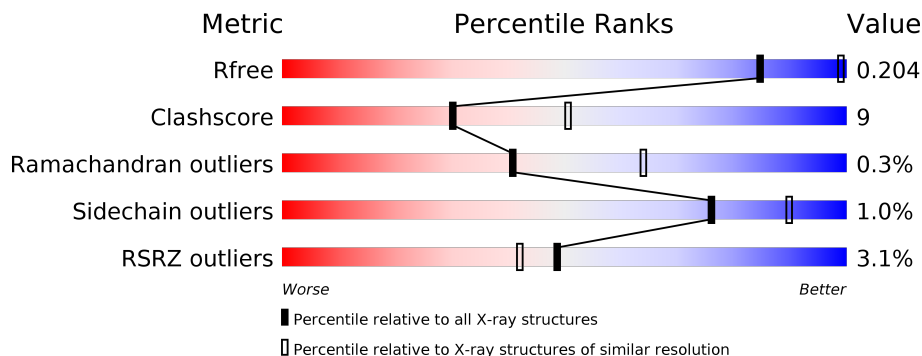
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	605	 2% 71% 13% 16%
1	B	605	 3% 69% 15% 15%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8628 atoms, of which 20 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 Distal tube protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	509	4122	2627	683	795	17	0	0	0
1	B	512	4145	2640	688	799	18	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	ARG	see sequence details	UNP P04331
A	121	ILE	MET	see sequence details	UNP P04331
A	600	HIS	-	expression tag	UNP P04331
A	601	HIS	-	expression tag	UNP P04331
A	602	HIS	-	expression tag	UNP P04331
A	603	HIS	-	expression tag	UNP P04331
A	604	HIS	-	expression tag	UNP P04331
A	605	HIS	-	expression tag	UNP P04331
B	41	SER	ARG	see sequence details	UNP P04331
B	121	ILE	MET	see sequence details	UNP P04331
B	600	HIS	-	expression tag	UNP P04331
B	601	HIS	-	expression tag	UNP P04331
B	602	HIS	-	expression tag	UNP P04331
B	603	HIS	-	expression tag	UNP P04331
B	604	HIS	-	expression tag	UNP P04331
B	605	HIS	-	expression tag	UNP P04331

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	17	4	10	3	0	0
2	A	1	17	4	10	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	172	172	172	0	0
3	B	155	155	155	0	0

16588	L598	HIS	HIS	HIS	HIS	HIS	HIS
	R699	HIS	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	184.67Å 184.67Å 184.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 2.60 49.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.35-2.60) 97.3 (49.36-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.85 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.201 0.170 , 0.204	Depositor DCC
R_{free} test set	3256 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8628	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: PEG

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	0.46	0/4218	0.59	0/5707
1	B	0.44	0/4241	0.59	0/5735
All	All	0.45	0/8459	0.59	0/11442

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	GLY	Peptide

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	4122	0	3988	63	0
1	B	4145	0	4010	91	0
2	A	14	20	20	0	0
3	A	172	0	0	3	0
3	B	155	0	0	2	0
All	All	8608	20	8018	151	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 9.

The worst 5 of 151 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:57:ARG:HD2	1:A:60:LYS:HE2	1.28	1.12
1:B:101:ASN:HB3	1:B:104:VAL:HG22	1.33	1.05
1:B:176:ILE:HD12	1:B:238:MET:HE1	1.49	0.91
1:B:176:ILE:HG12	1:B:255:MET:HE2	1.51	0.90
1:A:55:GLY:HA2	1:A:56:PHE:HB2	1.53	0.89

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	505/605 (84%)	484 (96%)	20 (4%)	1 (0%)	47	71
1	B	508/605 (84%)	491 (97%)	15 (3%)	2 (0%)	34	57
All	All	1013/1210 (84%)	975 (96%)	35 (4%)	3 (0%)	41	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	PHE
1	B	189	GLU
1	A	56	PHE

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	458/528 (87%)	454 (99%)	4 (1%)	78 91
1	B	460/528 (87%)	455 (99%)	5 (1%)	73 88
All	All	918/1056 (87%)	909 (99%)	9 (1%)	76 90

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	LEU
1	B	588	ASN
1	B	328	MET
1	A	138	ASP
1	B	123	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	B	212	HIS

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](#)

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		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	A	701	-	6,6,6	0.67	0	5,5,5	0.60	0
2	PEG	A	702	-	6,6,6	0.86	0	5,5,5	0.73	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	PEG	A	701	-	-	2/4/4/4	-
2	PEG	A	702	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	PEG	O1-C1-C2-O2
2	A	701	PEG	O1-C1-C2-O2
2	A	701	PEG	O2-C3-C4-O4
2	A	702	PEG	C1-C2-O2-C3

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, 95th 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>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	509/605 (84%)	-0.53	13 (2%) 56 50	19, 36, 92, 151	0
1	B	512/605 (84%)	-0.37	19 (3%) 41 34	20, 41, 108, 159	0
All	All	1021/1210 (84%)	-0.45	32 (3%) 49 42	19, 38, 103, 159	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ASN	4.6
1	B	57	ARG	4.5
1	B	100	LYS	4.4
1	B	106	TYR	4.0
1	B	99	PHE	3.7

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, 95th 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	B-factors(\AA^2)	Q<0.9
2	PEG	A	702	7/7	0.84	0.21	43,54,67,67	0
2	PEG	A	701	7/7	0.90	0.16	40,59,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.