



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6RNQ
Title : Crystal structure of the dimerization domain of Gemin5 at 1.95 Å
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Deposited on : 2019-05-09
Resolution : 1.95 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
Xtriage (Phenix)	:	1.13
EDS	:	2.4
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

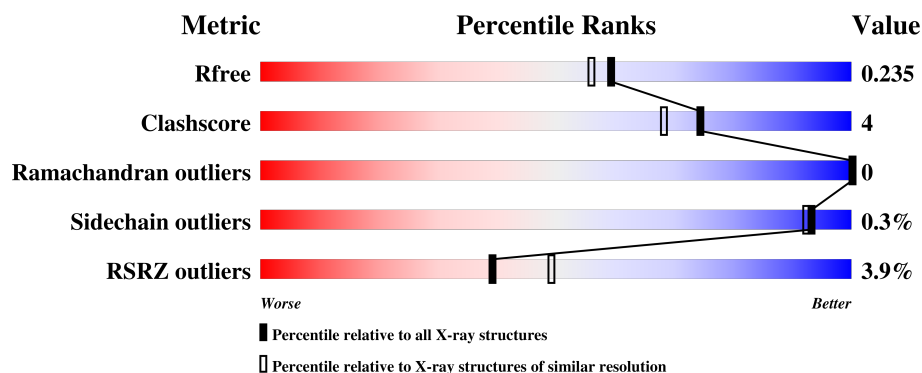
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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. 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	252	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	B	252	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7707 atoms, of which 3813 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 Gem-associated protein 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	H	N	O	S	0	0	0
			3816	1215	1906	334	353	8			
1	B	245	Total	C	H	N	O	S	0	0	0
			3816	1215	1907	334	352	8			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	42	Total	O	0	0
			42	42		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.22Å 54.97Å 103.64Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	100.40 – 1.95 100.43 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (100.40-1.95) 86.2 (100.43-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.211 , 0.235 0.210 , 0.235	Depositor DCC
R_{free} test set	2539 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7707	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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

5.1 Standard geometry

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

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	0.37	0/1948	0.45	0/2635
1	B	0.74	0/1947	0.56	0/2635
All	All	0.59	0/3895	0.51	0/5270

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

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	1910	1906	1906	19	0
1	B	1909	1907	1906	12	0
2	B	1	0	0	0	0
3	A	32	0	0	0	0
3	B	42	0	0	0	0
All	All	3894	3813	3812	27	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 4.

All (27) 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:1046:TYR:HE2	1:A:1058:VAL:HG21	1.47	0.79
1:B:846:ARG:HD2	1:B:921:LEU:HD11	1.68	0.76
1:A:1046:TYR:CE2	1:A:1058:VAL:HG21	2.24	0.72
1:A:958:TYR:OH	1:B:954:PRO:O	2.08	0.67
1:A:926:MET:HG3	1:A:935:VAL:HG21	1.82	0.62
1:A:1070:THR:HG21	1:B:864:HIS:HB3	1.86	0.56
1:B:906:ILE:HG23	1:B:925:LEU:HG	1.88	0.54
1:A:897:THR:HG22	1:A:898:ASP:N	2.23	0.53
1:A:848:LEU:HD12	1:B:979:VAL:HG11	1.91	0.52
1:A:927:LEU:HD22	1:A:952:MET:SD	2.50	0.52
1:B:1052:ALA:HB1	1:B:1078:VAL:HG21	1.90	0.52
1:B:1049:ALA:O	1:B:1050:THR:OG1	2.25	0.51
1:A:1033:LEU:HD13	1:A:1041:VAL:HG12	1.91	0.51
1:A:1078:VAL:HG12	1:A:1078:VAL:O	2.12	0.50
1:A:1052:ALA:HB1	1:A:1078:VAL:HG21	1.94	0.49
1:A:933:LYS:HG3	1:A:956:ALA:HB1	1.96	0.47
1:A:927:LEU:HD13	1:A:932:LEU:HD22	1.96	0.47
1:B:846:ARG:CD	1:B:921:LEU:HD11	2.44	0.45
1:A:926:MET:CG	1:A:935:VAL:HG21	2.46	0.44
1:B:1093:GLN:HA	1:B:1093:GLN:OE1	2.17	0.44
1:B:920:GLU:OE2	1:B:920:GLU:N	2.40	0.44
1:A:1074:LEU:O	1:A:1074:LEU:HD23	2.18	0.42
1:A:987:SER:O	1:B:955:ALA:HB2	2.19	0.42
1:A:1052:ALA:CB	1:A:1078:VAL:HG21	2.49	0.42
1:A:931:ASP:CG	1:A:931:ASP:O	2.58	0.42
1:B:993:GLU:N	1:B:993:GLU:OE1	2.43	0.42
1:A:1078:VAL:CG1	1:A:1078:VAL:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	241/252 (96%)	237 (98%)	4 (2%)	0	100	100
1	B	241/252 (96%)	235 (98%)	6 (2%)	0	100	100
All	All	482/504 (96%)	472 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	194/201 (96%)	194 (100%)	0	100	100
1	B	194/201 (96%)	193 (100%)	1 (0%)	90	89
All	All	388/402 (96%)	387 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	976	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	245/252 (97%)	0.56	11 (4%) 33 43	40, 57, 81, 113	0
1	B	245/252 (97%)	0.45	8 (3%) 46 56	40, 57, 79, 127	0
All	All	490/504 (97%)	0.51	19 (3%) 39 49	40, 57, 81, 127	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1096	LEU	4.2
1	A	885	ALA	3.8
1	A	1096	LEU	3.6
1	B	1089	LEU	3.6
1	A	974	PHE	3.6
1	B	886	ASP	3.5
1	A	887	VAL	3.4
1	A	932	LEU	3.3
1	A	846	ARG	3.3
1	A	886	ASP	3.1
1	B	888	GLU	2.5
1	A	884	SER	2.5
1	B	911	LYS	2.4
1	A	942	ARG	2.3
1	B	885	ALA	2.1
1	B	927	LEU	2.1
1	A	937	GLN	2.1
1	A	931	ASP	2.0
1	B	974	PHE	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, 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	K	B	1101	1/1	0.83	0.55	166,166,166,166	0

6.5 Other polymers [i](#)

There are no such residues in this entry.