



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6IR5
Title : P domain of GII.3-TV24
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Deposited on : 2018-11-10
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
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

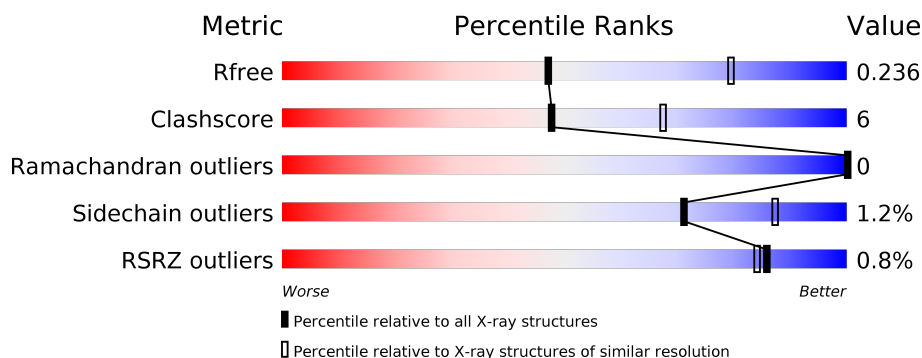
1 Overall quality at a glance

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	327	<div> <div>77%</div> <div>14%</div> <div>8%</div> </div>
1	B	327	<div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
1	C	327	<div> <div>78%</div> <div>14%</div> <div>7%</div> </div>
1	D	327	<div> <div>78%</div> <div>14%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9865 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 VP1 Capsid protein.

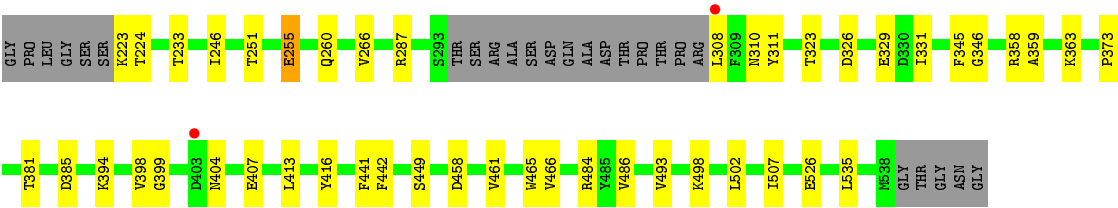
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2352	1498	396	450	8			
1	B	302	Total	C	N	O	S	0	0	0
			2359	1502	397	452	8			
1	C	304	Total	C	N	O	S	0	0	0
			2380	1514	403	455	8			
1	D	302	Total	C	N	O	S	0	0	0
			2367	1507	401	451	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	GLY	-	expression tag	UNP Q66296
A	218	PRO	-	expression tag	UNP Q66296
A	219	LEU	-	expression tag	UNP Q66296
A	220	GLY	-	expression tag	UNP Q66296
A	221	SER	-	expression tag	UNP Q66296
B	217	GLY	-	expression tag	UNP Q66296
B	218	PRO	-	expression tag	UNP Q66296
B	219	LEU	-	expression tag	UNP Q66296
B	220	GLY	-	expression tag	UNP Q66296
B	221	SER	-	expression tag	UNP Q66296
C	217	GLY	-	expression tag	UNP Q66296
C	218	PRO	-	expression tag	UNP Q66296
C	219	LEU	-	expression tag	UNP Q66296
C	220	GLY	-	expression tag	UNP Q66296
C	221	SER	-	expression tag	UNP Q66296
D	217	GLY	-	expression tag	UNP Q66296
D	218	PRO	-	expression tag	UNP Q66296
D	219	LEU	-	expression tag	UNP Q66296
D	220	GLY	-	expression tag	UNP Q66296
D	221	SER	-	expression tag	UNP Q66296

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	129	Total 129	O 129	0	0
2	B	96	Total 96	O 96	0	0
2	C	94	Total 94	O 94	0	0
2	D	88	Total 88	O 88	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	121.97Å 121.97Å 216.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.49 – 2.60 49.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.49-2.60) 99.7 (49.49-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.199 , 0.235 0.202 , 0.236	Depositor DCC
R_{free} test set	2586 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9865	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7841e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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	0/2421	0.49	0/3311
1	B	0.30	0/2428	0.47	0/3321
1	C	0.56	0/2449	0.52	0/3347
1	D	0.50	0/2436	0.49	0/3329
All	All	0.47	0/9734	0.49	0/13308

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	2352	0	2258	41	0
1	B	2359	0	2265	19	0
1	C	2380	0	2294	32	0
1	D	2367	0	2282	30	0
2	A	129	0	0	1	0
2	B	96	0	0	1	0
2	C	94	0	0	2	0
2	D	88	0	0	0	0
All	All	9865	0	9099	114	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.

The worst 5 of 114 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:422:HIS:ND1	1:A:424:MET:HE3	1.76	1.00
1:A:422:HIS:CE1	1:A:424:MET:CE	2.59	0.86
1:B:233:THR:HG22	1:B:235:SER:H	1.45	0.81
1:D:308:LEU:CD2	1:D:310:ASN:HB3	2.12	0.79
1:C:390:ASN:HB2	1:D:323:THR:HG22	1.66	0.77

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	297/327 (91%)	294 (99%)	3 (1%)	0	100	100
1	B	298/327 (91%)	295 (99%)	3 (1%)	0	100	100
1	C	300/327 (92%)	298 (99%)	2 (1%)	0	100	100
1	D	298/327 (91%)	295 (99%)	3 (1%)	0	100	100
All	All	1193/1308 (91%)	1182 (99%)	11 (1%)	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	263/283 (93%)	259 (98%)	4 (2%)	65	83
1	B	264/283 (93%)	262 (99%)	2 (1%)	81	92
1	C	267/283 (94%)	263 (98%)	4 (2%)	65	83
1	D	265/283 (94%)	262 (99%)	3 (1%)	73	88
All	All	1059/1132 (94%)	1046 (99%)	13 (1%)	71	87

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	368	SER
1	C	255	GLU
1	D	233	THR
1	B	225	LYS
1	C	341	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	C	310	ASN
1	D	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	301/327 (92%)	-0.41	1 (0%) 94 93	20, 31, 52, 71	0
1	B	302/327 (92%)	-0.39	3 (0%) 82 80	22, 31, 53, 72	0
1	C	304/327 (92%)	-0.38	4 (1%) 77 73	22, 33, 57, 85	0
1	D	302/327 (92%)	-0.35	2 (0%) 87 86	22, 34, 60, 85	0
All	All	1209/1308 (92%)	-0.38	10 (0%) 86 84	20, 33, 57, 85	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	PHE	5.3
1	B	420	PHE	5.1
1	B	294	THR	4.2
1	C	295	SER	3.4
1	B	370	ARG	2.6

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.