



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 11:12 AM BST

PDB ID : 6VJ9
Title : Crystal structure of GlpG in complex with peptide boronate inhibitor
Authors : Urban, S.; Cho, S.
Deposited on : 2020-01-15
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 ⓘ 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 : 2.14.4.dev1
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) : 2.14.4.dev1

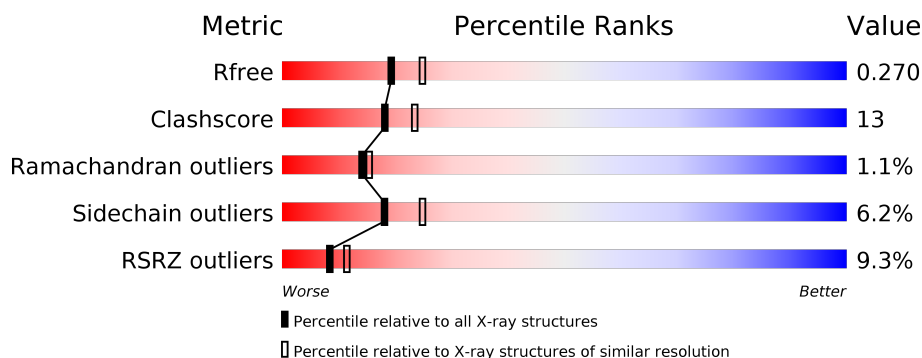
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 $\leq 5\%$. 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	194	
2	B	5	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1477 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 Rhomboid family intramembrane serine protease GlpG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1423	961	226	225	11			

There are 4 discrepancies between the modelled and reference sequences:

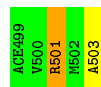
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLY	-	expression tag	UNP A0A4Q6HQP3
A	84	SER	-	expression tag	UNP A0A4Q6HQP3
A	85	HIS	-	expression tag	UNP A0A4Q6HQP3
A	86	MET	-	expression tag	UNP A0A4Q6HQP3

- Molecule 2 is a protein called ACE-VAL-ARG-MET-B2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	B	C	N	O	S	0	0
			35	1	20	7	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	1	Total	O	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	111.31Å 111.31Å 125.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.15 – 2.30 29.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.15-2.30) 99.9 (29.77-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.227 , 0.258 0.238 , 0.270	Depositor DCC
R_{free} test set	683 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1477	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: B2A, ACE

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	0.43	0/1472	0.78	1/2004 (0.0%)
2	B	0.69	0/26	1.46	0/33
All	All	0.44	0/1498	0.79	1/2037 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	168	ARG	CG-CD-NE	5.03	122.36	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	SER	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	1423	0	1421	35	0
2	B	35	0	40	7	0
3	A	18	0	0	2	0
3	B	1	0	0	0	0
All	All	1477	0	1461	39	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 13.

All (39) 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)
2:B:501:ARG:HH11	2:B:501:ARG:HG2	1.20	1.01
1:A:218:ASP:OD2	1:A:269:SER:HA	1.84	0.77
1:A:154:ASN:HD21	1:A:201:SER:HB3	1.55	0.69
1:A:98:TRP:CE2	1:A:102:ILE:HD11	2.27	0.69
2:B:501:ARG:NH1	2:B:501:ARG:HG2	1.95	0.69
1:A:154:ASN:ND2	1:A:201:SER:HB3	2.11	0.66
1:A:210:TYR:O	1:A:214:ARG:HB2	2.04	0.58
1:A:249:MET:CE	1:A:254:HIS:HE1	2.20	0.55
1:A:148:LEU:O	1:A:152:LEU:HB2	2.08	0.54
1:A:254:HIS:NE2	2:B:503:B2A:HA	2.23	0.54
1:A:215:GLY:HA2	1:A:223:ILE:O	2.08	0.53
3:A:301:HOH:O	2:B:501:ARG:HD2	2.10	0.51
1:A:149:MET:CE	1:A:149:MET:H	2.24	0.50
1:A:205:TYR:HE1	1:A:254:HIS:CG	2.30	0.50
1:A:188:VAL:HG21	1:A:256:ALA:HB2	1.94	0.49
1:A:173:LYS:HZ1	1:A:268:ASP:CG	2.16	0.49
1:A:184:LEU:HD13	1:A:260:VAL:CG2	2.43	0.48
1:A:244:LEU:O	1:A:246:GLY:N	2.46	0.48
1:A:270:LEU:O	1:A:271:ASN:C	2.51	0.47
1:A:107:VAL:O	1:A:111:MET:HG3	2.14	0.47
2:B:501:ARG:NH1	2:B:501:ARG:CG	2.72	0.47
1:A:149:MET:H	1:A:149:MET:HE3	1.78	0.47
1:A:249:MET:HE3	1:A:254:HIS:HE1	1.79	0.46
1:A:168:ARG:HD3	1:A:222:GLY:O	2.15	0.46
1:A:167:LYS:HD3	1:A:167:LYS:HA	1.59	0.45
1:A:125:TRP:NE1	1:A:190:GLN:HG2	2.31	0.45
1:A:254:HIS:HE2	2:B:503:B2A:HA	1.81	0.44
1:A:254:HIS:HE2	2:B:503:B2A:CA	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLY:CA	1:A:223:ILE:O	2.64	0.44
1:A:168:ARG:HD2	1:A:223:ILE:CD1	2.48	0.43
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.84	0.43
1:A:189:GLN:HB2	1:A:253:ALA:HB2	2.01	0.43
1:A:189:GLN:HE21	1:A:193:SER:HB2	1.85	0.42
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.53	0.42
1:A:168:ARG:NH1	3:A:302:HOH:O	2.52	0.41
1:A:214:ARG:O	1:A:218:ASP:HB3	2.21	0.41
1:A:249:MET:CE	1:A:254:HIS:CE1	3.02	0.41
1:A:128:ASP:OD1	1:A:130:THR:HG23	2.21	0.41
1:A:146:PHE:H	1:A:150:HIS:HD1	1.69	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	177/194 (91%)	168 (95%)	7 (4%)	2 (1%)	14	15
2	B	3/5 (60%)	3 (100%)	0	0	100	100
All	All	180/199 (90%)	171 (95%)	7 (4%)	2 (1%)	14	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	PHE
1	A	218	ASP

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	142/154 (92%)	134 (94%)	8 (6%)	21	29
2	B	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	145/157 (92%)	136 (94%)	9 (6%)	18	25

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	149	MET
1	A	167	LYS
1	A	184	LEU
1	A	191	LYS
1	A	214	ARG
1	A	220	GLN
1	A	234	LEU
2	B	501	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue 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	B2A	B	503	1,2	1,5,5	1.75	0	0,6,6	0.00	-

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	B2A	B	503	1,2	-	0/0/4/4	-

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	B2A	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	179/194 (92%)	0.41	17 (9%) 8 11	37, 58, 94, 154	0
2	B	3/5 (60%)	0.12	0 100 100	66, 66, 68, 73	0
All	All	182/199 (91%)	0.41	17 (9%) 8 11	37, 59, 93, 154	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	GLN	9.7
1	A	241	TRP	5.1
1	A	122	TRP	4.7
1	A	221	SER	4.6
1	A	168	ARG	4.3
1	A	222	GLY	4.2
1	A	135	PHE	4.0
1	A	244	LEU	3.7
1	A	118	GLU	2.5
1	A	271	ASN	2.5
1	A	270	LEU	2.4
1	A	242	PHE	2.4
1	A	113	ILE	2.3
1	A	200	LEU	2.3
1	A	114	LEU	2.3
1	A	240	GLY	2.2
1	A	153	PHE	2.2

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

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	B2A	B	503	6/6	0.93	0.19	49,61,74,74	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.