



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2025 – 01:04 pm BST

PDB ID : 9FHJ / pdb_00009fhj
Title : Crystallographic structure of AcrB V612N in TTT state
Authors : Lazarova, M.; Pos, K.M.
Deposited on : 2024-05-27
Resolution : 3.55 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

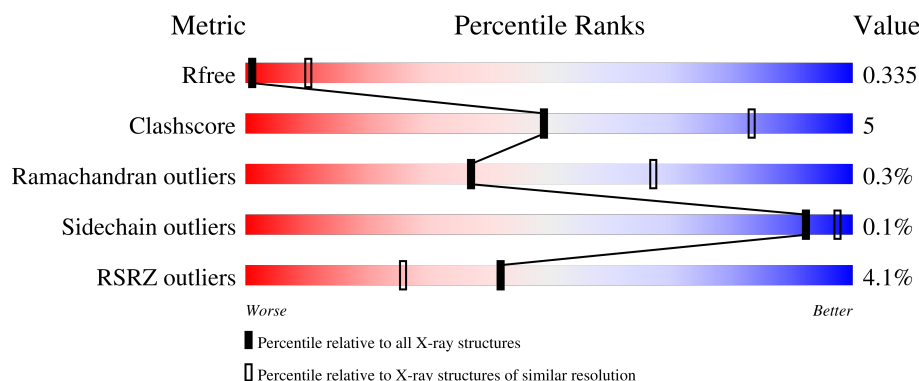
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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}	164625	1261 (3.62-3.50)
Clashscore	180529	1351 (3.62-3.50)
Ramachandran outliers	177936	1336 (3.62-3.50)
Sidechain outliers	177891	1337 (3.62-3.50)
RSRZ outliers	164620	1260 (3.62-3.50)

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 of 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	1057	
2	D	169	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9085 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1043	Total	C	N	O	S	0	0	0
			7934	5099	1313	1478	44			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	ASN	VAL	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	228.65Å 228.65Å 228.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.74 – 3.55 41.74 – 3.55	Depositor EDS
% Data completeness (in resolution range)	93.6 (41.74-3.55) 93.9 (41.74-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.20.1, REFMAC 5	Depositor
R, R_{free}	0.272 , 0.326 0.272 , 0.335	Depositor DCC
R_{free} test set	1233 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	205.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 139.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.068 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9085	wwPDB-VP
Average B, all atoms (Å ²)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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](#)

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	0.18	0/8085	0.38	0/10977
2	D	0.14	0/1170	0.29	0/1591
All	All	0.17	0/9255	0.37	0/12568

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	7934	0	8074	89	0
2	D	1151	0	1136	8	0
All	All	9085	0	9210	97	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 5.

All (97) 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:49:TYR:HD2	1:A:52:ALA:HB2	1.37	0.88
1:A:49:TYR:CD2	1:A:52:ALA:HB2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:THR:HG23	1:A:677:ALA:H	1.49	0.78
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.74	0.68
1:A:310:LEU:HD13	1:A:323:ILE:HG21	1.74	0.68
1:A:713:LEU:HD13	1:A:843:LEU:HD23	1.77	0.66
1:A:578:LEU:HD23	1:A:661:ALA:HB2	1.79	0.65
1:A:699:ARG:HD2	1:A:718:PRO:HB3	1.79	0.65
1:A:26:ALA:O	1:A:29:LYS:N	2.24	0.64
2:D:100:LEU:HD23	2:D:104:ALA:HB3	1.80	0.64
1:A:49:TYR:HB2	1:A:122:VAL:HG22	1.81	0.63
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.82	0.61
1:A:696:THR:OG1	1:A:825:MET:HE1	2.02	0.59
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.84	0.59
1:A:32:VAL:HG11	1:A:337:ILE:HD11	1.83	0.59
1:A:414:GLU:HG2	1:A:973:ARG:HH21	1.67	0.59
1:A:81:ASN:HD22	1:A:815:ARG:HE	1.51	0.58
2:D:100:LEU:HD22	2:D:135:TYR:CD2	2.39	0.57
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.88	0.55
1:A:81:ASN:HD22	1:A:815:ARG:NE	2.04	0.54
1:A:619:GLY:HA3	1:A:815:ARG:HD2	1.89	0.54
1:A:555:LEU:HD21	1:A:914:LEU:HD12	1.89	0.54
1:A:960:LEU:HD22	1:A:1027:VAL:HG22	1.91	0.53
1:A:396:PHE:HA	1:A:399:VAL:HG22	1.91	0.53
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.89	0.53
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.44	0.52
1:A:183:ALA:HB2	1:A:273:GLU:HG2	1.91	0.52
1:A:905:VAL:HG22	1:A:935:ILE:HG23	1.91	0.52
1:A:139:VAL:HB	1:A:327:TYR:HB3	1.91	0.52
1:A:342:LYS:O	1:A:346:GLU:HG3	2.10	0.51
1:A:108:GLN:HG2	1:A:129:VAL:HG11	1.93	0.51
1:A:184:MET:HB3	1:A:771:VAL:HG22	1.93	0.50
1:A:72:ILE:HD11	1:A:110:LYS:HG3	1.93	0.50
1:A:719:ASN:O	1:A:719:ASN:ND2	2.42	0.50
1:A:904:VAL:HG11	1:A:942:ALA:HB2	1.93	0.50
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.93	0.50
1:A:716:VAL:HA	1:A:828:LEU:O	2.12	0.50
1:A:548:ILE:HG23	1:A:910:ILE:CD1	2.42	0.49
1:A:676:THR:HG21	1:A:862:MET:HB2	1.95	0.49
2:D:100:LEU:HD11	2:D:132:LEU:HD23	1.95	0.48
1:A:314:GLU:HB2	1:A:315:PRO:HD3	1.95	0.48
1:A:888:LEU:HD21	1:A:901:VAL:HB	1.96	0.48
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ILE:O	1:A:910:ILE:HD11	2.14	0.47
2:D:42:ALA:O	2:D:50:PRO:HD3	2.15	0.47
1:A:921:LEU:HD22	1:A:1005:THR:HG21	1.95	0.47
1:A:187:TRP:NE1	1:A:269:GLU:OE2	2.48	0.47
1:A:55:LYS:NZ	1:A:59:ASP:OD2	2.43	0.47
1:A:973:ARG:HG2	1:A:977:MET:HE2	1.97	0.47
2:D:60:LEU:HD22	2:D:94:GLU:HG3	1.96	0.47
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.30	0.46
1:A:944:LEU:HB3	1:A:971:ARG:HD2	1.97	0.46
1:A:281:PHE:HE1	1:A:326:PRO:HB3	1.81	0.46
1:A:882:ILE:O	1:A:886:LEU:HD13	2.16	0.46
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.99	0.46
1:A:699:ARG:HD3	1:A:825:MET:SD	2.56	0.45
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.97	0.45
1:A:183:ALA:N	1:A:271:GLY:O	2.39	0.45
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.99	0.45
1:A:57:VAL:CG1	1:A:88:VAL:HB	2.47	0.44
1:A:706:ALA:HB1	1:A:713:LEU:HD23	1.98	0.44
2:D:60:LEU:HD13	2:D:94:GLU:HG2	2.00	0.44
1:A:676:THR:C	1:A:678:THR:H	2.25	0.44
1:A:293:LEU:HD11	1:A:299:ALA:HB2	1.99	0.44
1:A:888:LEU:HD23	1:A:898:PRO:HA	1.99	0.44
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.99	0.44
1:A:359:LEU:HD13	1:A:417:GLU:HG3	2.00	0.44
1:A:892:TYR:O	1:A:950:LYS:HE3	2.18	0.44
1:A:277:ILE:HD12	1:A:615:PHE:HD2	1.83	0.43
1:A:189:ASN:CG	1:A:192:GLU:HG2	2.42	0.43
1:A:169:THR:HG21	1:A:306:ILE:HA	2.00	0.43
1:A:318:PRO:HD2	1:A:321:LEU:HD12	2.00	0.43
1:A:520:PHE:CZ	1:A:972:LEU:HD22	2.53	0.43
2:D:138:ASP:HB3	2:D:141:ALA:HB2	2.00	0.43
1:A:448:VAL:HG13	1:A:884:VAL:HG13	2.01	0.42
1:A:338:HIS:O	1:A:342:LYS:HB2	2.19	0.42
1:A:158:VAL:O	1:A:163:LYS:N	2.49	0.42
1:A:416:VAL:HG22	1:A:431:THR:HA	2.00	0.42
1:A:719:ASN:HB3	1:A:826:GLU:HB3	2.00	0.42
1:A:951:ASP:O	1:A:955:LYS:HG2	2.20	0.42
1:A:360:GLN:HG2	1:A:513:PHE:CD1	2.55	0.41
1:A:512:PHE:CD1	1:A:512:PHE:N	2.87	0.41
1:A:415:ASN:HB3	1:A:434:SER:OG	2.20	0.41
1:A:445:ILE:HD11	1:A:944:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ILE:HG23	1:A:910:ILE:HD12	2.03	0.41
2:D:34:MET:HE2	2:D:69:ASN:HB3	2.02	0.41
1:A:75:LEU:HD23	1:A:76:MET:N	2.35	0.41
1:A:311:ALA:HA	1:A:314:GLU:HG2	2.03	0.41
1:A:317:PHE:HB3	1:A:321:LEU:HB2	2.03	0.41
1:A:574:THR:HA	1:A:665:ALA:HA	2.01	0.41
1:A:57:VAL:HG12	1:A:82:SER:HB3	2.03	0.40
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.56	0.40
1:A:173:GLY:O	1:A:174:ASP:HB2	2.21	0.40
1:A:572:PHE:CD2	1:A:648:THR:HG22	2.56	0.40
1:A:424:GLY:HA3	1:A:502:LYS:HB2	2.04	0.40
1:A:467:TYR:OH	1:A:928:GLN:OE1	2.30	0.40
1:A:739:LEU:HD13	1:A:799:VAL:HG11	2.03	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	1041/1057 (98%)	1002 (96%)	35 (3%)	4 (0%)	30	62
2	D	150/169 (89%)	145 (97%)	5 (3%)	0	100	100
All	All	1191/1226 (97%)	1147 (96%)	40 (3%)	4 (0%)	37	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	676	THR
1	A	26	ALA
1	A	174	ASP

5.3.2 Protein sidechains ⓘ

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	849/863 (98%)	848 (100%)	1 (0%)	92	97
2	D	117/132 (89%)	117 (100%)	0	100	100
All	All	966/995 (97%)	965 (100%)	1 (0%)	92	97

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

Mol	Chain	Res	Type
1	A	630	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	89	GLN
1	A	123	GLN
1	A	161	ASN
1	A	596	HIS
2	D	36	ASN
2	D	102	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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	1043/1057 (98%)	-0.32	49 (4%) 37 24	168, 191, 223, 252	0
2	D	152/169 (89%)	-0.70	0 100 100	174, 213, 238, 250	0
All	All	1195/1226 (97%)	-0.37	49 (4%) 42 26	168, 193, 227, 252	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	PHE	9.5
1	A	672	VAL	8.6
1	A	291	ILE	8.1
1	A	675	GLY	6.1
1	A	138	MET	6.0
1	A	290	GLY	6.0
1	A	573	MET	5.8
1	A	135	SER	5.6
1	A	175	VAL	5.2
1	A	668	LEU	5.0
1	A	139	VAL	4.8
1	A	669	PRO	4.8
1	A	137	LEU	4.5
1	A	674	LEU	4.5
1	A	300	LEU	4.2
1	A	19	ILE	4.0
1	A	542	LEU	4.0
1	A	327	TYR	3.9
1	A	666	PHE	3.9
1	A	864	TYR	3.8
1	A	693	GLU	3.6
1	A	628	PHE	3.6
1	A	677	ALA	3.4
1	A	299	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	214	VAL	3.4
1	A	333	VAL	3.3
1	A	980	LEU	3.1
1	A	174	ASP	2.9
1	A	329	THR	2.8
1	A	76	MET	2.8
1	A	563	PHE	2.7
1	A	176	GLN	2.7
1	A	292	LYS	2.7
1	A	561	SER	2.7
1	A	676	THR	2.6
1	A	170	SER	2.6
1	A	75	LEU	2.6
1	A	328	ASP	2.6
1	A	330	THR	2.5
1	A	562	SER	2.3
1	A	237	GLN	2.3
1	A	1025	PHE	2.3
1	A	236	ALA	2.2
1	A	817	GLU	2.2
1	A	673	GLU	2.1
1	A	140	VAL	2.1
1	A	301	ASP	2.1
1	A	33	ALA	2.1
1	A	1028	VAL	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 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.