



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4ZIV / pdb_00004ziv
Title : Crystal structure of AcrB triple mutant in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-28
Resolution : 3.16 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 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

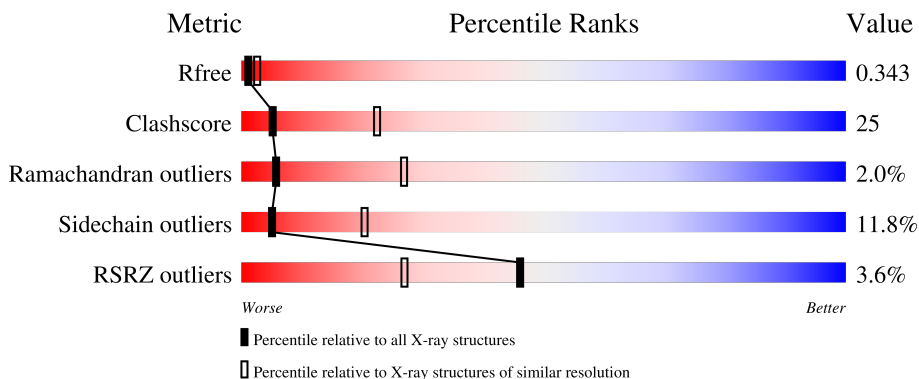
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	B	1101	X	-	-	-
2	LMT	C	1101	X	-	-	-

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.28Å 157.49Å 219.16Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	19.98 – 3.16 19.98 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-3.16) 97.3 (19.98-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.270 , 0.335 0.282 , 0.343	Depositor DCC
R_{free} test set	8816 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.075 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47736	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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 50.20 % 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 6.6875e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

3 Model quality

3.1 Standard geometry

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

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	0.83	4/8056 (0.0%)	1.26	49/10940 (0.4%)
1	B	0.84	1/8089 (0.0%)	1.28	65/10986 (0.6%)
1	C	0.86	1/8074 (0.0%)	1.29	56/10965 (0.5%)
1	D	0.78	3/8056 (0.0%)	1.23	61/10940 (0.6%)
1	E	0.77	2/8056 (0.0%)	1.22	50/10940 (0.5%)
1	F	0.81	2/8089 (0.0%)	1.27	63/10986 (0.6%)
All	All	0.82	13/48420 (0.0%)	1.26	344/65757 (0.5%)

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	C	0	1
1	D	0	2
1	F	0	2
All	All	0	5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1022	VAL	CA-CB	11.56	1.59	1.54
1	A	1022	VAL	CA-CB	9.21	1.58	1.54
1	E	905	VAL	CA-CB	8.10	1.58	1.54
1	D	905	VAL	CA-CB	7.43	1.57	1.54
1	C	897	ILE	CA-CB	7.23	1.58	1.54

The worst 5 of 344 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	TYR	CA-C-N	-12.51	108.13	120.52
1	A	35	TYR	C-N-CA	-12.51	108.13	120.52
1	C	1044	HIS	N-CA-C	12.51	119.04	108.78
1	E	515	TRP	N-CA-C	-10.77	99.32	111.82
1	A	39	ALA	CA-C-N	10.52	127.34	119.66

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	ILE	Peptide
1	D	1034	SER	Peptide
1	D	992	SER	Peptide
1	F	1036	LYS	Peptide
1	F	1039	ASP	Peptide

3.2 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	7907	0	8050	412	0
1	B	7939	0	8077	392	0
1	C	7924	0	8064	416	0
1	D	7907	0	8050	387	0
1	E	7907	0	8050	436	1
1	F	7939	0	8077	417	1
2	A	35	0	46	4	0
2	B	35	0	46	4	0
2	C	35	0	46	4	0
2	D	35	0	46	1	0
2	E	35	0	46	4	0
2	F	35	0	46	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47736	0	48644	2373	1

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 25.

The worst 5 of 2373 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:D:446:ALA:HB2	1:D:482:VAL:HG21	1.39	0.99
1:A:957:GLY:HA2	1:A:1042:HIS:HB2	1.41	0.99
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.46	0.98
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	1.97	0.97
1:F:578:LEU:HG	1:F:587:THR:HG22	1.46	0.95

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:ASP:OD1	1:F:529:ASP:OD2[2_555]	2.08	0.12

3.3 Torsion angles [i](#)

3.3.1 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	1040/1049 (99%)	939 (90%)	82 (8%)	19 (2%)	6	29
1	B	1044/1049 (100%)	925 (89%)	92 (9%)	27 (3%)	4	21
1	C	1042/1049 (99%)	931 (89%)	91 (9%)	20 (2%)	6	28
1	D	1040/1049 (99%)	941 (90%)	83 (8%)	16 (2%)	8	33
1	E	1040/1049 (99%)	919 (88%)	97 (9%)	24 (2%)	5	24
1	F	1044/1049 (100%)	936 (90%)	87 (8%)	21 (2%)	6	27
All	All	6250/6294 (99%)	5591 (90%)	532 (8%)	127 (2%)	6	27

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	675	GLY
1	A	1038	GLU
1	B	163	LYS
1	B	360	GLN

3.3.2 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	845/852 (99%)	769 (91%)	76 (9%)	9	30
1	B	849/852 (100%)	717 (84%)	132 (16%)	2	12
1	C	847/852 (99%)	753 (89%)	94 (11%)	6	22
1	D	845/852 (99%)	767 (91%)	78 (9%)	8	30
1	E	845/852 (99%)	715 (85%)	130 (15%)	2	12
1	F	849/852 (100%)	759 (89%)	90 (11%)	6	24
All	All	5080/5112 (99%)	4480 (88%)	600 (12%)	5	20

5 of 600 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	608	SER
1	F	703	LEU
1	E	714	THR
1	E	607	GLU
1	F	88	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	125	GLN
1	F	104	GLN
1	D	74	ASN
1	F	68	ASN

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Mol	Chain	Res	Type
1	E	623	ASN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 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	1042/1049 (99%)	0.14	33 (3%)	50	30	28, 63, 113, 139	0
1	B	1046/1049 (99%)	-0.14	21 (2%)	65	44	26, 57, 100, 161	0
1	C	1044/1049 (99%)	-0.00	38 (3%)	46	27	17, 56, 98, 173	0
1	D	1042/1049 (99%)	0.19	38 (3%)	46	27	21, 81, 133, 168	0
1	E	1042/1049 (99%)	0.24	37 (3%)	46	27	38, 77, 119, 154	0
1	F	1046/1049 (99%)	0.32	57 (5%)	31	18	29, 73, 120, 143	0
All	All	6262/6294 (99%)	0.12	224 (3%)	46	27	17, 68, 116, 173	0

The worst 5 of 224 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	ILE	7.5
1	F	856	GLY	7.3
1	C	69	MET	7.3
1	C	856	GLY	7.0
1	C	838	GLY	6.9

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

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

4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

4.4 Other polymers [i](#)

There are no such residues in this entry.