



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:16 PM UTC

PDB ID : 1ZWW / pdb_00001zww
Title : Crystal structure of endophilin-A1 BAR domain
Authors : Weissenhorn, W.
Deposited on : 2005-06-06
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 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
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

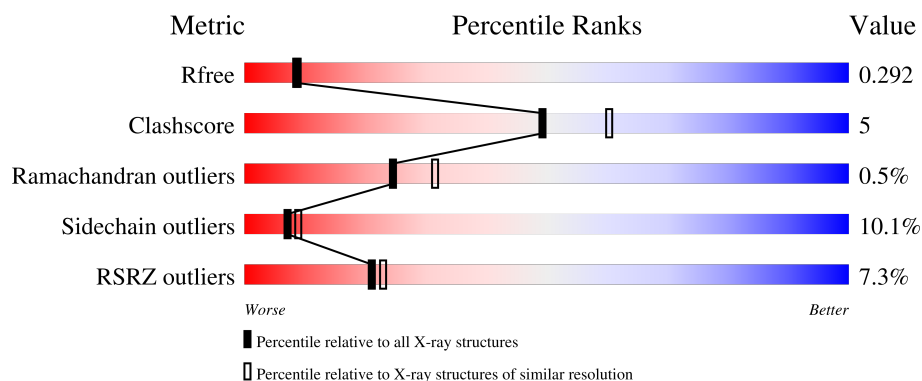
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	256	4% 62% 14% • 22%
1	B	256	7% 62% 13% • 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3060 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 SH3-containing GRB2-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1521	951	263	298	9			
1	B	196	Total	C	N	O	S	0	0	0
			1459	914	253	283	9			

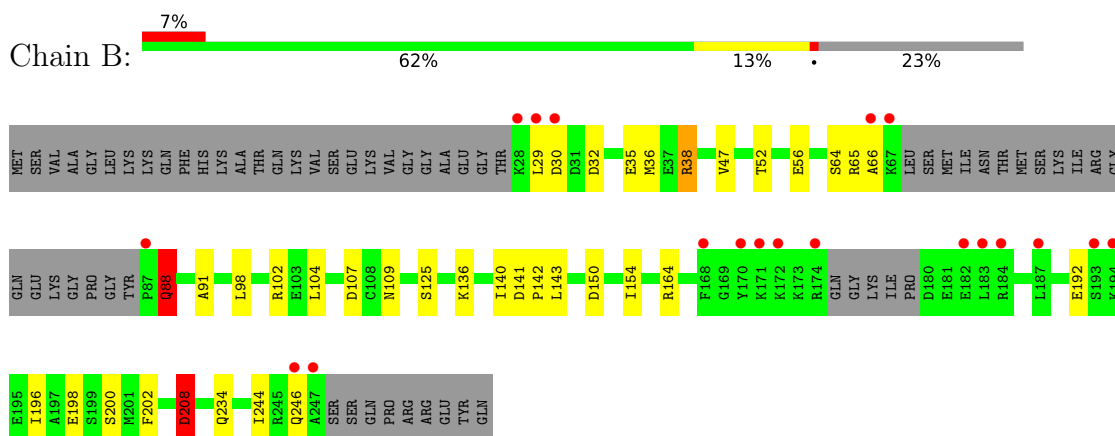
- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Cd	0	0
			6	6		
2	B	5	Total	Cd	0	0
			5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	38	Total	O	0	0
			38	38		

- Molecule 1: SH3-containing GRB2-like protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	40.70Å 121.65Å 244.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.30) 99.2 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.249 , 0.287 0.259 , 0.292	Depositor DCC
R_{free} test set	1382 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.854	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	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	3060	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% 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: CD

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	0.92	2/1539 (0.1%)	1.12	3/2073 (0.1%)
1	B	0.85	1/1475 (0.1%)	1.12	1/1993 (0.1%)
All	All	0.89	3/3014 (0.1%)	1.12	4/4066 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	GLU	CB-CG	7.17	1.74	1.52
1	A	120	ALA	CA-CB	-5.30	1.45	1.53
1	B	88	GLN	CG-CD	-5.12	1.39	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	GLN	CB-CG-CD	-8.50	98.15	112.60
1	A	126	GLU	N-CA-C	-7.51	103.03	111.14
1	A	61	ASN	CA-C-N	5.25	125.06	119.28
1	A	61	ASN	C-N-CA	5.25	125.06	119.28

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	1521	0	1448	17	2
1	B	1459	0	1354	18	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
3	A	31	0	0	1	0
3	B	38	0	0	1	0
All	All	3060	0	2802	31	2

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 (31) 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:B:36:MET:HE1	1:B:202:PHE:HB2	1.71	0.73
1:A:35:GLU:OE2	1:A:38:ARG:NH1	2.23	0.72
1:A:35:GLU:CD	1:A:38:ARG:NH1	2.50	0.69
1:A:35:GLU:CD	1:A:38:ARG:HH12	2.01	0.69
1:A:36:MET:HE1	1:A:198:GLU:HG3	1.84	0.59
1:B:192:GLU:O	1:B:196:ILE:HG12	2.04	0.58
1:A:172:LYS:O	1:A:175:GLN:HB2	2.09	0.53
1:B:136:LYS:HA	1:B:140:ILE:HB	1.91	0.52
1:A:97:MET:SD	1:A:117:VAL:HG12	2.51	0.51
1:B:91:ALA:HB2	1:B:125:SER:OG	2.11	0.50
1:B:36:MET:HE2	1:B:202:PHE:HA	1.93	0.50
1:A:209:ILE:HD11	1:B:244:ILE:HA	1.94	0.49
1:B:35:GLU:OE2	1:B:38:ARG:NH1	2.47	0.48
1:B:141:ASP:HB2	1:B:142:PRO:HD3	1.96	0.48
1:A:53:LYS:HE3	3:A:925:HOH:O	2.14	0.46
1:A:109:ASN:OD1	1:B:208:ASP:HB3	2.17	0.45
1:A:147:HIS:HA	1:A:151:LEU:HD12	1.98	0.44
1:B:98:LEU:O	1:B:102:ARG:HG2	2.18	0.44
1:B:52:THR:O	1:B:56:GLU:HG3	2.18	0.44
1:A:61:ASN:HA	1:A:62:PRO:HD3	1.88	0.43
1:B:36:MET:CE	1:B:202:PHE:HA	2.49	0.43
1:A:40:VAL:HG11	1:A:154:ILE:HG21	2.02	0.42
1:B:154:ILE:HG12	1:B:200:SER:HB3	2.02	0.42
1:A:38:ARG:O	1:A:42:VAL:HG23	2.19	0.42
1:B:36:MET:HE1	1:B:202:PHE:CB	2.45	0.42
1:A:197:ALA:O	1:A:201:MET:HG3	2.19	0.42
1:B:64:SER:C	1:B:66:ALA:H	2.28	0.41
1:A:162:GLU:OE2	1:A:165:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLN:HG2	3:B:923:HOH:O	2.21	0.41
1:A:212:VAL:HG21	1:B:109:ASN:HB3	2.02	0.41
1:A:103:GLU:O	1:B:38:ARG:NH2	2.52	0.41

All (2) 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:A:123:GLU:OE2	1:A:123:GLU:OE2[4_566]	2.01	0.19
1:A:119:GLU:OE2	1:A:126:GLU:OE1[4_566]	2.03	0.17

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	195/256 (76%)	190 (97%)	5 (3%)	0	100	100
1	B	190/256 (74%)	183 (96%)	5 (3%)	2 (1%)	11	13
All	All	385/512 (75%)	373 (97%)	10 (3%)	2 (0%)	24	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	65	ARG
1	B	208	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	155/223 (70%)	140 (90%)	15 (10%)	8	10
1	B	141/223 (63%)	126 (89%)	15 (11%)	6	8
All	All	296/446 (66%)	266 (90%)	30 (10%)	7	9

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	47	VAL
1	A	50	ILE
1	A	58	LEU
1	A	90	GLU
1	A	124	LEU
1	A	129	ASP
1	A	134	GLU
1	A	146	LEU
1	A	150	ASP
1	A	165	ARG
1	A	167	ASP
1	A	171	LYS
1	A	209	ILE
1	A	244	ILE
1	B	29	LEU
1	B	30	ASP
1	B	32	ASP
1	B	38	ARG
1	B	47	VAL
1	B	88	GLN
1	B	104	LEU
1	B	107	ASP
1	B	143	LEU
1	B	150	ASP
1	B	164	ARG
1	B	198	GLU
1	B	208	ASP
1	B	234	GLN
1	B	246	GLN

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	211	GLN
1	A	214	GLN
1	A	222	GLN
1	B	61	ASN
1	B	137	GLN
1	B	138	ASN
1	B	211	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are 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 [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

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	199/256 (77%)	0.43	10 (5%) 34 35	21, 45, 60, 83	0
1	B	196/256 (76%)	0.60	19 (9%) 13 15	21, 44, 87, 100	0
All	All	395/512 (77%)	0.51	29 (7%) 21 23	21, 45, 74, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	LYS	4.9
1	B	30	ASP	4.2
1	B	66	ALA	4.1
1	B	247	ALA	3.9
1	B	29	LEU	3.7
1	B	174	ARG	3.3
1	A	27	THR	3.3
1	B	187	LEU	3.3
1	A	107	ASP	3.3
1	B	67	LYS	3.2
1	A	195	GLU	3.1
1	B	28	LYS	3.0
1	B	184	ARG	2.7
1	A	109	ASN	2.7
1	B	183	LEU	2.6
1	B	168	PHE	2.6
1	B	182	GLU	2.5
1	B	87	PRO	2.5
1	B	170	TYR	2.4
1	B	172	LYS	2.4
1	A	29	LEU	2.4
1	A	203	ASN	2.3
1	A	63	ALA	2.3
1	A	169	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	171	LYS	2.2
1	A	188	GLU	2.1
1	B	246	GLN	2.1
1	A	244	ILE	2.1
1	B	193	SER	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 oligosaccharides 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(Å ²)	Q<0.9
2	CD	B	905	1/1	0.72	0.14	33,33,33,33	1
2	CD	A	902	1/1	0.84	0.09	24,24,24,24	1
2	CD	B	901	1/1	0.88	0.09	35,35,35,35	1
2	CD	B	904	1/1	0.92	0.11	30,30,30,30	1
2	CD	A	911	1/1	0.92	0.08	52,52,52,52	1
2	CD	B	910	1/1	0.94	0.06	80,80,80,80	1
2	CD	A	907	1/1	0.96	0.05	82,82,82,82	1
2	CD	A	906	1/1	0.96	0.11	78,78,78,78	1
2	CD	B	909	1/1	0.97	0.06	66,66,66,66	1
2	CD	A	900	1/1	0.98	0.07	57,57,57,57	1
2	CD	A	903	1/1	0.98	0.08	62,62,62,62	1

6.5 Other polymers [i](#)

There are no such residues in this entry.