



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2C08 / pdb_00002c08
Title : Rat endophilin A1 BAR domain
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Deposited on : 2005-08-26
Resolution : 2.90 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
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

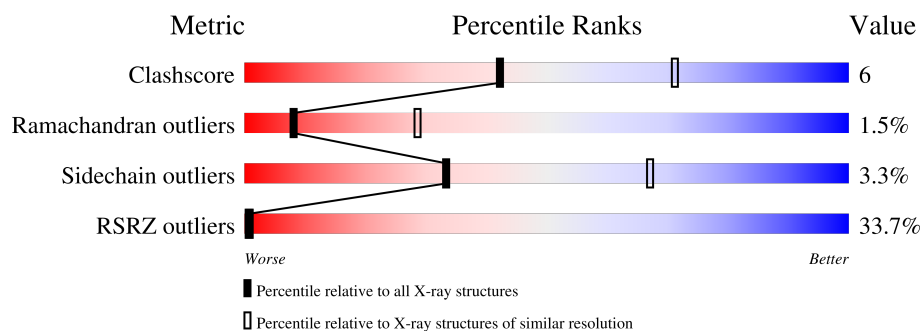
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	204	32% 84% 15% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1653 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.

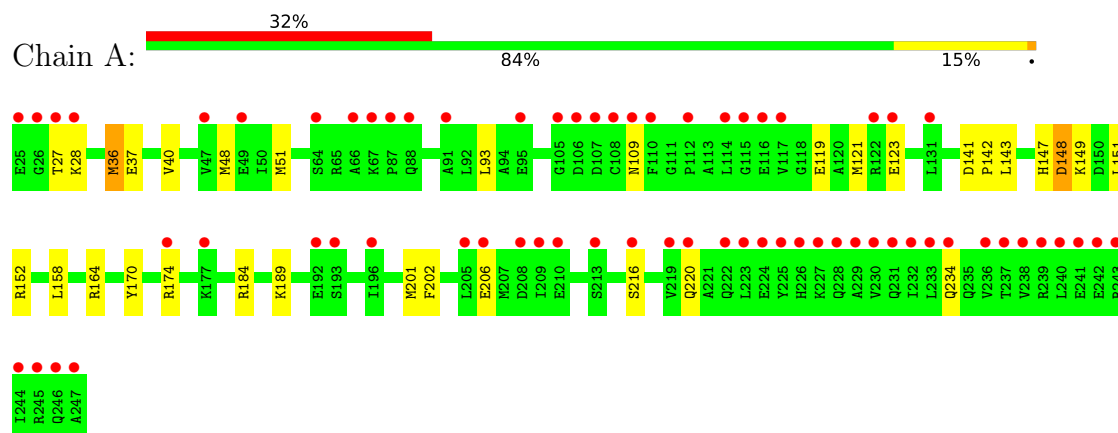
- Molecule 1 is a protein called SH3-CONTAINING GRB2-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	204	1653	1028	290	326	1	8	0	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SH3-CONTAINING GRB2-LIKE PROTEIN 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	126.58Å 126.58Å 101.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.44 – 2.90 89.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.44-2.90) 99.9 (89.44-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.279 , 0.295 0.273 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	1653	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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	0.55	0/1663	0.77	0/2210

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	1653	0	1658	21	0
All	All	1653	0	1658	21	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.

All (21) 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:164:ARG:HD3	1:A:189:LYS:HB3	1.66	0.76
1:A:48:MSE:HE3	1:A:147:HIS:CD2	2.24	0.73
1:A:158:LEU:HD11	1:A:201:MSE:HE3	1.79	0.65
1:A:147:HIS:HA	1:A:151:LEU:HD12	1.84	0.60
1:A:48:MSE:HA	1:A:48:MSE:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG21	1:A:201:MSE:HE2	1.88	0.55
1:A:148:ASP:O	1:A:152:ARG:CB	2.55	0.55
1:A:119:GLU:O	1:A:123:GLU:HG2	2.09	0.53
1:A:148:ASP:O	1:A:152:ARG:HB2	2.11	0.51
1:A:48:MSE:HE2	1:A:48:MSE:CA	2.43	0.49
1:A:37:GLU:HA	1:A:201:MSE:HE1	1.95	0.47
1:A:93:LEU:HD23	1:A:121:MSE:HE2	1.98	0.46
1:A:51:MSE:HE2	1:A:143:LEU:HB3	1.97	0.45
1:A:216:SER:O	1:A:220:GLN:HG2	2.16	0.45
1:A:170:TYR:CZ	1:A:174:ARG:HD2	2.52	0.45
1:A:37:GLU:HA	1:A:201:MSE:CE	2.47	0.44
1:A:40:VAL:CG2	1:A:201:MSE:HE2	2.48	0.43
1:A:158:LEU:HD11	1:A:201:MSE:CE	2.46	0.43
1:A:141:ASP:HB2	1:A:142:PRO:HD3	2.00	0.42
1:A:36:MSE:HE2	1:A:202:PHE:HA	2.03	0.41
1:A:48:MSE:CE	1:A:147:HIS:CD2	3.02	0.40

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	200/204 (98%)	185 (92%)	12 (6%)	3 (2%)	8 28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	28	LYS
1	A	148	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	181/173 (105%)	175 (97%)	6 (3%)	33 67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	36	MSE
1	A	109	ASN
1	A	184	ARG
1	A	206	GLU
1	A	234	GLN

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	144	GLN
1	A	147	HIS

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 [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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	67:LYS	C	87:PRO	N	12.45

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	196/204 (96%)	1.70	66 (33%) 1 1	41, 61, 78, 82	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	THR	5.0
1	A	209	ILE	4.9
1	A	247	ALA	4.8
1	A	245	ARG	4.7
1	A	246	GLN	4.5
1	A	238	VAL	4.4
1	A	67	LYS	4.2
1	A	240	LEU	4.1
1	A	231	GLN	4.0
1	A	109	ASN	3.9
1	A	66	ALA	3.8
1	A	87	PRO	3.7
1	A	28	LYS	3.6
1	A	232	ILE	3.6
1	A	223	LEU	3.3
1	A	234	GLN	3.3
1	A	25	GLU	3.2
1	A	243	ARG	3.2
1	A	95	GLU	3.1
1	A	230	VAL	3.1
1	A	27	THR	3.1
1	A	222	GLN	3.0
1	A	242	GLU	3.0
1	A	122	ARG	3.0
1	A	228	GLN	3.0
1	A	239	ARG	3.0
1	A	213	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	177	LYS	2.9
1	A	115	GLY	2.9
1	A	108	CYS	2.8
1	A	123	GLU	2.8
1	A	112	PRO	2.8
1	A	226	HIS	2.8
1	A	193	SER	2.8
1	A	244	ILE	2.7
1	A	219	VAL	2.7
1	A	233	LEU	2.7
1	A	205	LEU	2.6
1	A	229	ALA	2.6
1	A	64	SER	2.6
1	A	220	GLN	2.6
1	A	208	ASP	2.6
1	A	114	LEU	2.6
1	A	131	LEU	2.6
1	A	236	VAL	2.5
1	A	206	GLU	2.5
1	A	106	ASP	2.5
1	A	216	SER	2.4
1	A	105	GLY	2.4
1	A	88	GLN	2.4
1	A	241	GLU	2.3
1	A	107	ASP	2.3
1	A	116	GLU	2.2
1	A	192	GLU	2.2
1	A	91	ALA	2.2
1	A	227	LYS	2.1
1	A	110	PHE	2.1
1	A	210	GLU	2.1
1	A	224	GLU	2.1
1	A	174	ARG	2.1
1	A	49	GLU	2.1
1	A	225	TYR	2.1
1	A	47	VAL	2.0
1	A	196	ILE	2.0
1	A	26	GLY	2.0
1	A	117	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 oligosaccharides 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.