



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2024 – 01:53 pm BST

PDB ID : 8RIT
Title : Dimeric mutant S103D of the BTB domain of ZBTB8A from *Xenopus laevis*
Authors : Coste, F.; Suskiewicz, M.J.
Deposited on : 2023-12-19
Resolution : 3.75 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

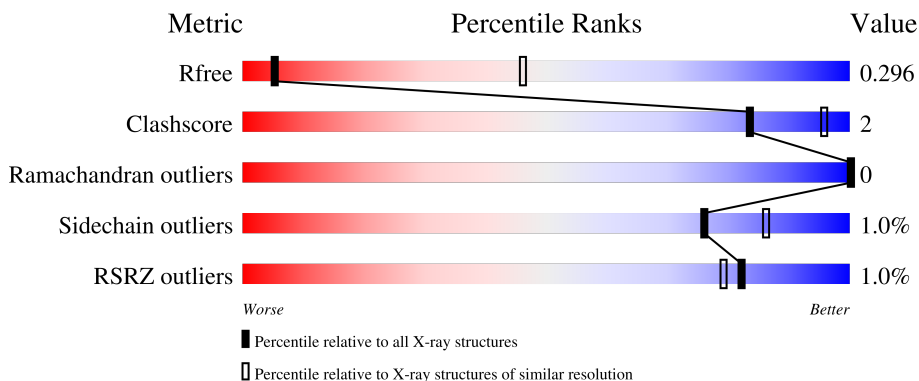
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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.



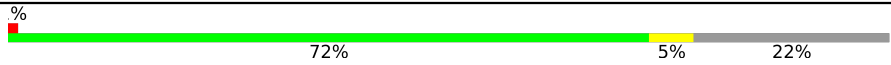
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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	156	 72% 5% 22%
1	B	156	 72% 24%
1	D	156	 72% 23%
1	E	156	 73% 22%
1	G	156	 71% 6% 22%

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Mol	Chain	Length	Quality of chain
1	H	156	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '72%', a yellow segment in the middle labeled '5%', and a grey segment on the right labeled '22%'. A small red square is positioned at the beginning of the bar, and a '%' symbol is located above the bar.</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5226 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 Zinc finger and BTB domain-containing protein 8A.1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	121	894	571	145	170	8	0	0	0
1	B	119	882	564	141	168	9	0	0	0
1	D	120	853	545	138	164	6	0	0	0
1	E	121	865	552	142	163	8	0	0	0
1	G	121	855	545	136	167	7	0	0	0
1	H	121	877	562	140	168	7	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q0IH98
A	0	GLY	-	expression tag	UNP Q0IH98
A	103	ASP	SER	engineered mutation	UNP Q0IH98
A	148	GLU	-	expression tag	UNP Q0IH98
A	149	HIS	-	expression tag	UNP Q0IH98
A	150	HIS	-	expression tag	UNP Q0IH98
A	151	HIS	-	expression tag	UNP Q0IH98
A	152	HIS	-	expression tag	UNP Q0IH98
A	153	HIS	-	expression tag	UNP Q0IH98
A	154	HIS	-	expression tag	UNP Q0IH98
B	-1	MET	-	initiating methionine	UNP Q0IH98
B	0	GLY	-	expression tag	UNP Q0IH98
B	103	ASP	SER	engineered mutation	UNP Q0IH98
B	148	GLU	-	expression tag	UNP Q0IH98
B	149	HIS	-	expression tag	UNP Q0IH98
B	150	HIS	-	expression tag	UNP Q0IH98
B	151	HIS	-	expression tag	UNP Q0IH98

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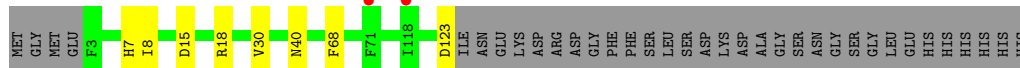
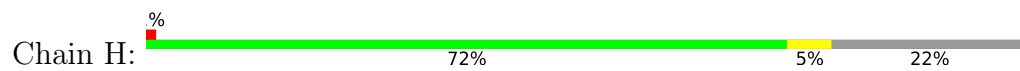
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Chain	Residue	Modelled	Actual	Comment	Reference
B	152	HIS	-	expression tag	UNP Q0IH98
B	153	HIS	-	expression tag	UNP Q0IH98
B	154	HIS	-	expression tag	UNP Q0IH98
D	-1	MET	-	initiating methionine	UNP Q0IH98
D	0	GLY	-	expression tag	UNP Q0IH98
D	103	ASP	SER	engineered mutation	UNP Q0IH98
D	148	GLU	-	expression tag	UNP Q0IH98
D	149	HIS	-	expression tag	UNP Q0IH98
D	150	HIS	-	expression tag	UNP Q0IH98
D	151	HIS	-	expression tag	UNP Q0IH98
D	152	HIS	-	expression tag	UNP Q0IH98
D	153	HIS	-	expression tag	UNP Q0IH98
D	154	HIS	-	expression tag	UNP Q0IH98
E	-1	MET	-	initiating methionine	UNP Q0IH98
E	0	GLY	-	expression tag	UNP Q0IH98
E	103	ASP	SER	engineered mutation	UNP Q0IH98
E	148	GLU	-	expression tag	UNP Q0IH98
E	149	HIS	-	expression tag	UNP Q0IH98
E	150	HIS	-	expression tag	UNP Q0IH98
E	151	HIS	-	expression tag	UNP Q0IH98
E	152	HIS	-	expression tag	UNP Q0IH98
E	153	HIS	-	expression tag	UNP Q0IH98
E	154	HIS	-	expression tag	UNP Q0IH98
G	-1	MET	-	initiating methionine	UNP Q0IH98
G	0	GLY	-	expression tag	UNP Q0IH98
G	103	ASP	SER	engineered mutation	UNP Q0IH98
G	148	GLU	-	expression tag	UNP Q0IH98
G	149	HIS	-	expression tag	UNP Q0IH98
G	150	HIS	-	expression tag	UNP Q0IH98
G	151	HIS	-	expression tag	UNP Q0IH98
G	152	HIS	-	expression tag	UNP Q0IH98
G	153	HIS	-	expression tag	UNP Q0IH98
G	154	HIS	-	expression tag	UNP Q0IH98
H	-1	MET	-	initiating methionine	UNP Q0IH98
H	0	GLY	-	expression tag	UNP Q0IH98
H	103	ASP	SER	engineered mutation	UNP Q0IH98
H	148	GLU	-	expression tag	UNP Q0IH98
H	149	HIS	-	expression tag	UNP Q0IH98
H	150	HIS	-	expression tag	UNP Q0IH98
H	151	HIS	-	expression tag	UNP Q0IH98
H	152	HIS	-	expression tag	UNP Q0IH98
H	153	HIS	-	expression tag	UNP Q0IH98

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Chain	Residue	Modelled	Actual	Comment	Reference
H	154	HIS	-	expression tag	UNP Q0IH98



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.99Å 61.99Å 71.49Å 90.00° 91.52° 90.00°	Depositor
Resolution (Å)	71.46 – 3.75 129.95 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (71.46-3.75) 91.6 (129.95-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.78Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.244 , 0.295 0.244 , 0.296	Depositor DCC
R_{free} test set	568 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtrriage
Anisotropy	0.755	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 107.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtrriage'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](#)

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	0.25	0/912	0.39	0/1240
1	B	0.24	0/899	0.39	0/1222
1	D	0.24	0/870	0.38	0/1188
1	E	0.24	0/881	0.38	0/1200
1	G	0.24	0/871	0.37	0/1190
1	H	0.24	0/895	0.38	0/1220
All	All	0.24	0/5328	0.38	0/7260

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	894	0	814	4	0
1	B	882	0	813	4	0
1	D	853	0	751	4	0
1	E	865	0	781	4	0
1	G	855	0	753	7	0
1	H	877	0	784	5	0
All	All	5226	0	4696	24	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 2.

All (24) 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:30:VAL:HG12	1:B:68:PHE:HB2	1.60	0.81
1:A:30:VAL:HG12	1:A:68:PHE:HB2	1.66	0.77
1:E:30:VAL:HG12	1:E:68:PHE:HB2	1.65	0.77
1:H:30:VAL:HG12	1:H:68:PHE:HB2	1.66	0.76
1:G:30:VAL:HG12	1:G:68:PHE:HB2	1.68	0.74
1:D:30:VAL:HG12	1:D:68:PHE:HB2	1.73	0.70
1:E:52:LEU:O	1:E:55:GLN:NE2	2.36	0.58
1:E:18:ARG:NH2	1:E:81:ASP:OD1	2.35	0.55
1:G:7:HIS:HB3	1:H:7:HIS:HB3	1.94	0.49
1:G:38:HIS:H	1:G:84:TYR:HH	1.63	0.46
1:G:17:GLN:HE22	1:H:40:ASN:HA	1.83	0.44
1:A:18:ARG:HG3	1:A:36:LYS:O	2.18	0.44
1:G:7:HIS:CD2	1:H:8:ILE:HD13	2.53	0.44
1:D:69:ASP:N	1:D:69:ASP:OD1	2.52	0.43
1:G:31:GLU:HB3	1:G:73:ALA:HB2	2.00	0.43
1:B:43:PHE:CD1	1:B:50:LYS:HA	2.54	0.42
1:B:122:LEU:HD13	1:E:48:TYR:CZ	2.55	0.42
1:A:4:SER:HB3	1:A:7:HIS:ND1	2.35	0.41
1:A:43:PHE:CD2	1:A:50:LYS:HA	2.55	0.41
1:D:11:LEU:HD11	1:D:84:TYR:HA	2.02	0.41
1:H:15:ASP:O	1:H:18:ARG:HG3	2.21	0.41
1:D:41:VAL:HG11	1:D:84:TYR:CE1	2.56	0.41
1:G:103:ASP:OD1	1:G:104:TYR:N	2.54	0.40
1:B:109:ASP:N	1:B:109:ASP:OD1	2.54	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	119/156 (76%)	115 (97%)	4 (3%)	0	100	100
1	B	117/156 (75%)	113 (97%)	4 (3%)	0	100	100
1	D	118/156 (76%)	115 (98%)	3 (2%)	0	100	100
1	E	119/156 (76%)	115 (97%)	4 (3%)	0	100	100
1	G	119/156 (76%)	115 (97%)	4 (3%)	0	100	100
1	H	119/156 (76%)	114 (96%)	5 (4%)	0	100	100
All	All	711/936 (76%)	687 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	92/137 (67%)	90 (98%)	2 (2%)	52	73
1	B	92/137 (67%)	92 (100%)	0	100	100
1	D	83/137 (61%)	82 (99%)	1 (1%)	71	84
1	E	86/137 (63%)	85 (99%)	1 (1%)	71	84
1	G	84/137 (61%)	84 (100%)	0	100	100
1	H	88/137 (64%)	87 (99%)	1 (1%)	73	85
All	All	525/822 (64%)	520 (99%)	5 (1%)	76	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	55	GLN
1	D	31	GLU
1	E	55	GLN
1	H	123	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 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 [i](#)

There are no chain breaks in this entry.

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

6.1 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	121/156 (77%)	0.11	0 100 100	87, 116, 180, 241	0
1	B	119/156 (76%)	0.04	0 100 100	89, 119, 166, 212	0
1	D	120/156 (76%)	0.18	2 (1%) 70 65	118, 157, 212, 223	0
1	E	121/156 (77%)	0.02	1 (0%) 86 84	99, 151, 197, 213	0
1	G	121/156 (77%)	-0.08	2 (1%) 70 65	130, 161, 210, 230	0
1	H	121/156 (77%)	0.06	2 (1%) 70 65	134, 160, 203, 231	0
All	All	723/936 (77%)	0.05	7 (0%) 82 79	87, 146, 203, 241	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	118	ILE	3.5
1	G	118	ILE	3.0
1	D	68	PHE	2.7
1	G	45	SER	2.7
1	D	26	CYS	2.1
1	H	118	ILE	2.1
1	H	71	PHE	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.