



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 05:50 AM EDT

PDB ID : 2H99
Title : Crystal structure of the effector binding domain of a BenM variant (R156H,T157S)
Authors : Ezezika, O.C.; Craven, S.H.; Neidle, E.L.; Momany, C.
Deposited on : 2006-06-09
Resolution : 1.85 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

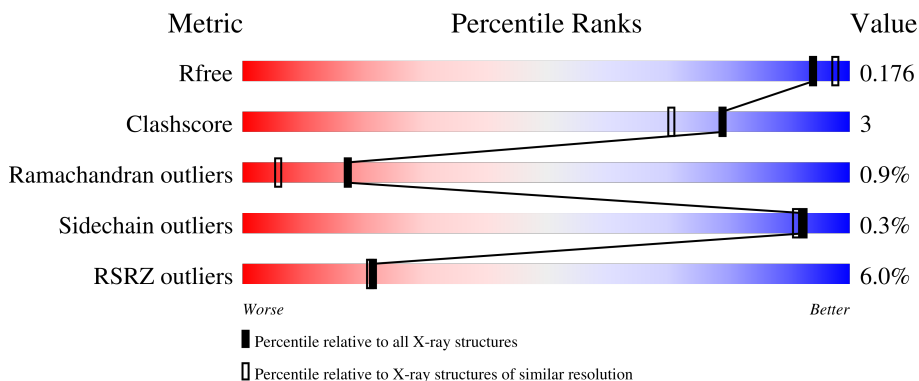
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	312	 5% 65% 5% 31%
1	B	312	 4% 63% 5% 30%

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
3	ACT	A	585	-	-	X	-
3	ACT	B	584	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4119 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 HTH-type transcriptional regulator benM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	Total 1736	C 1118	N 298	O 314	S 6	0	4	0
1	B	217	Total 1753	C 1127	N 302	O 319	S 5	0	5	0

There are 20 discrepancies between the modelled and reference sequences:

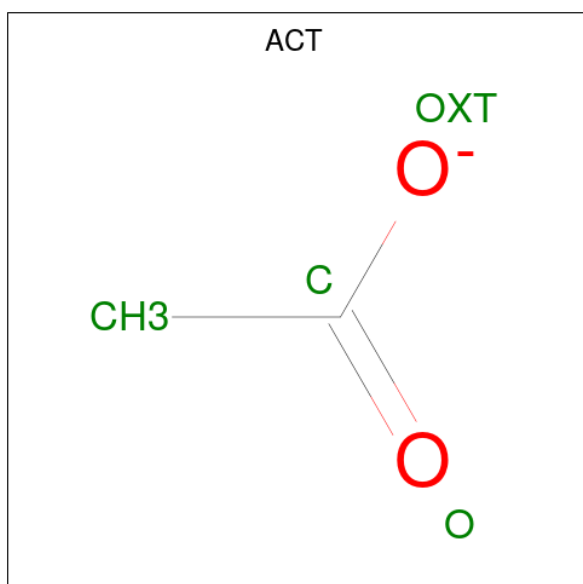
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	HIS	ARG	engineered mutation	UNP O68014
A	157	SER	THR	engineered mutation	UNP O68014
A	305	LEU	-	expression tag	UNP O68014
A	306	GLU	-	expression tag	UNP O68014
A	307	HIS	-	expression tag	UNP O68014
A	308	HIS	-	expression tag	UNP O68014
A	309	HIS	-	expression tag	UNP O68014
A	310	HIS	-	expression tag	UNP O68014
A	311	HIS	-	expression tag	UNP O68014
A	312	HIS	-	expression tag	UNP O68014
B	156	HIS	ARG	engineered mutation	UNP O68014
B	157	SER	THR	engineered mutation	UNP O68014
B	305	LEU	-	expression tag	UNP O68014
B	306	GLU	-	expression tag	UNP O68014
B	307	HIS	-	expression tag	UNP O68014
B	308	HIS	-	expression tag	UNP O68014
B	309	HIS	-	expression tag	UNP O68014
B	310	HIS	-	expression tag	UNP O68014
B	311	HIS	-	expression tag	UNP O68014
B	312	HIS	-	expression tag	UNP O68014

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

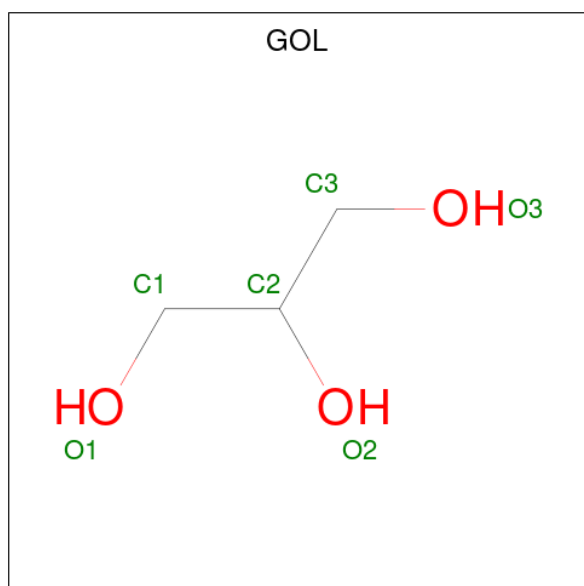


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	264	Total 264	O 264	0	0
6	B	314	Total 314	O 314	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.94Å 66.51Å 117.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 1.85 44.03 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.00-1.85) 99.6 (44.03-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.165 , 0.204 0.183 , 0.176	Depositor DCC
R_{free} test set	2222 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtrriage
Anisotropy	0.577	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4119	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: CL, ACT, GOL, SO4

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	0.32	0/1779	0.50	0/2413
1	B	0.34	0/1796	0.54	0/2437
All	All	0.33	0/3575	0.52	0/4850

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

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	1736	0	1769	7	0
1	B	1753	0	1781	12	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
3	A	12	0	9	3	0
3	B	8	0	6	3	0
4	B	1	0	0	0	0
5	B	6	0	8	0	0
6	A	264	0	0	2	0
6	B	314	0	0	1	0
All	All	4119	0	3573	20	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 3.

The worst 5 of 20 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:160:ARG:HH11	3:B:584:ACT:H1	1.35	0.90
1:B:104:LEU:H	3:B:584:ACT:H3	1.42	0.84
1:A:146[A]:ARG:HD2	6:A:616:HOH:O	2.02	0.58
3:A:585:ACT:H1	6:A:639:HOH:O	2.05	0.57
1:B:300:GLU:HB3	1:B:302:PRO:HA	1.86	0.57

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	216/312 (69%)	215 (100%)	0	1 (0%)	29	15
1	B	218/312 (70%)	215 (99%)	0	3 (1%)	11	3
All	All	434/624 (70%)	430 (99%)	0	4 (1%)	17	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	GLU
1	A	302	PRO
1	B	301	PRO
1	B	302	PRO

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	191/276 (69%)	191 (100%)	0	100	100
1	B	193/276 (70%)	192 (100%)	1 (0%)	88	86
All	All	384/552 (70%)	383 (100%)	1 (0%)	92	91

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

Mol	Chain	Res	Type
1	B	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	175	ASN
1	B	222	ASN
1	B	254	ASN
1	B	291	GLN
1	B	303	ASN

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

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	588	-	3,3,3	0.78	0	3,3,3	1.51	0
3	ACT	A	585	-	3,3,3	0.65	0	3,3,3	1.41	0
3	ACT	B	584	-	3,3,3	0.87	0	3,3,3	0.80	0
2	SO4	B	579	-	4,4,4	0.18	0	6,6,6	0.31	0
2	SO4	B	582	-	4,4,4	0.14	0	6,6,6	0.08	0
3	ACT	A	587	-	3,3,3	0.78	0	3,3,3	1.48	0
2	SO4	A	580	-	4,4,4	0.15	0	6,6,6	0.21	0
5	GOL	B	590	-	5,5,5	0.40	0	5,5,5	0.26	0
2	SO4	B	581	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	A	583	-	4,4,4	0.14	0	6,6,6	0.08	0
3	ACT	B	586	-	3,3,3	0.72	0	3,3,3	1.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	590	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	590	GOL	C1-C2-C3-O3
5	B	590	GOL	O1-C1-C2-C3
5	B	590	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	588	ACT	1	0
3	A	585	ACT	2	0
3	B	584	ACT	3	0

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	215/312 (68%)	0.33	15 (6%) 16 15	12, 20, 35, 50	0
1	B	217/312 (69%)	0.32	11 (5%) 28 26	11, 17, 31, 67	0
All	All	432/624 (69%)	0.32	26 (6%) 21 21	11, 19, 34, 67	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	304	TRP	14.2
1	B	304	TRP	13.2
1	A	303	ASN	13.0
1	B	301	PRO	10.2
1	B	303	ASN	8.4

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](#)

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(\AA^2)	Q<0.9
5	GOL	B	590	6/6	0.61	0.34	43,49,52,53	0
3	ACT	A	588	4/4	0.72	0.19	23,25,26,26	0
3	ACT	A	585	4/4	0.79	0.17	23,25,25,26	0
3	ACT	A	587	4/4	0.81	0.40	51,51,51,52	0
3	ACT	B	584	4/4	0.87	0.15	16,17,18,20	0
3	ACT	B	586	4/4	0.88	0.14	29,30,31,32	0
2	SO4	A	583	5/5	0.92	0.21	54,55,56,59	0
2	SO4	B	582	5/5	0.93	0.14	57,58,59,60	0
2	SO4	A	580	5/5	0.98	0.11	34,36,40,41	0
2	SO4	B	579	5/5	0.99	0.09	19,22,25,28	0
4	CL	B	589	1/1	1.00	0.08	16,16,16,16	0
2	SO4	B	581	5/5	1.00	0.07	12,13,14,15	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.