

wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2020 – 11:55 pm BST

PDB ID : 5NG7

> Title Novel epoxide hydrolases belonging to the alpha/beta hydrolases superfamily

> > in metagenomes from hot environments

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1.39 Å(reported) Resolution

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

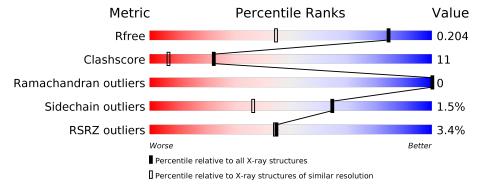
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.39 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 on 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 <=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	299	81%	14%	
1	В	299	85%	12%	•



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6046 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.

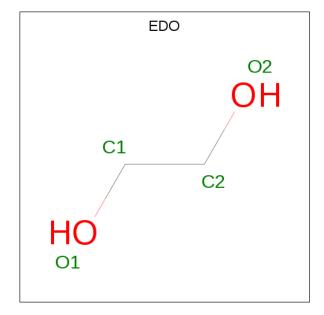
• Molecule 1 is a protein called epoxide hydrolase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	292	Total 2783	C 1875	1 1	O 462	S 11	0	63	0
1	В	290	Total 2618	C 1739	N 424	O 446	S 9	0	41	0

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	2	Total Cl 2 2	0	0
2	A	1	Total Cl 1 1	0	0

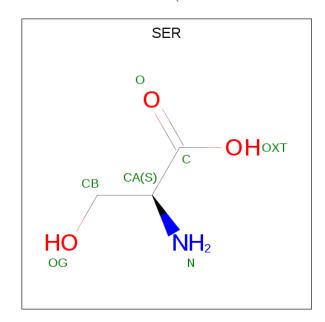
• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).





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	В	1	Total C O 4 2 2	0	0

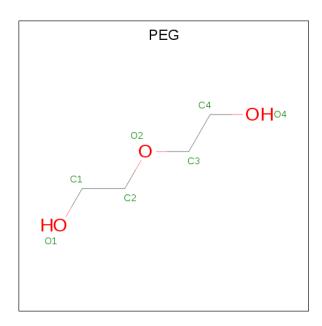
• Molecule 4 is SERINE (three-letter code: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
1	R	1	Total	С	N	О	0	0
4	ט	1	7	3	1	3		

 $\bullet \ \ Molecule \ 5 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 7 4 3	0	0

• Molecule 6 is water.

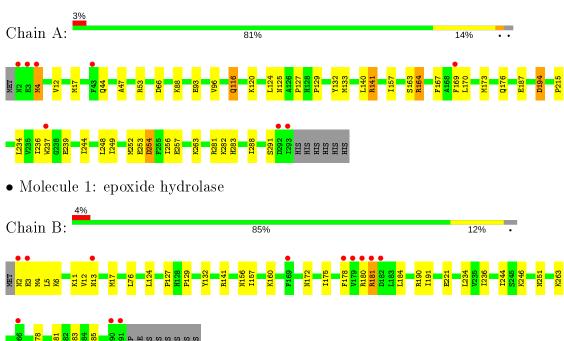
\mathbf{Mol}	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
6	A	347	Total O 347 347	0	0
6	В	269	Total O 269 269	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: epoxide hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	163.94Å 46.22Å 73.87Å	Depositor
a, b, c, α , β , γ	90.00° 106.94° 90.00°	Depositor
Resolution (Å)	39.51 - 1.39	Depositor
resolution (A)	39.51 - 1.39	EDS
% Data completeness	98.2 (39.51-1.39)	Depositor
(in resolution range)	98.2 (39.51-1.39)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	1.48 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
P. P.	0.173 , 0.204	Depositor
R, R_{free}	0.173 , 0.204	DCC
R_{free} test set	5200 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 42.8	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6046	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, CL

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		
MIOI		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.72	0/3035	0.85	1/4100 (0.0%)	
1	В	0.69	0/2799	0.82	0/3784	
All	All	0.70	0/5834	0.83	1/7884 (0.0%)	

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	66	ASP	CB-CG-OD2	-5.55	113.30	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254[B]	ASP	Peptide

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



All

All

6046

0

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2783	0	3002	96	0
1	В	2618	0	2773	35	0
2	A	1	0	0	0	0
2	В	2	0	0	0	0
3	A	8	0	12	3	0
3	В	4	0	6	0	0
4	В	7	0	4	0	0
5	В	7	0	10	2	0
6	A	347	0	0	16	3
6	В	269	0	0	5	3

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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 11.

129

3

5807

The worst 5 of 129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:169[B]:PHE:CZ	1:A:173[B]:MET:HE3	1.30	1.66
1:A:169[B]:PHE:CZ	1:A:173[B]:MET:CE	1.90	1.50
1:A:132[B]:TYR:CD1	1:A:133[B]:MET:HE2	1.43	1.50
1:A:169[B]:PHE:CE1	1:A:173[B]:MET:CE	2.00	1.43
1:A:132[B]:TYR:CD1	1:A:133[B]:MET:CE	2.05	1.39

All (3) 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	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (ext{\AA}) \end{aligned}$
6:A:559:HOH:O	6:B:633:HOH:O[4_555]	1.98	0.22
6:A:405:HOH:O	6:B:426:HOH:O[4_555]	1.99	0.21
6:A:496:HOH:O	6:B:446:HOH:O[3_455]	2.16	0.04

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	Perce	\mathbf{ntiles}
1	A	353/299 (118%)	339 (96%)	14 (4%)	0	100	100
1	В	$329/299 \; (110\%)$	315 (96%)	14 (4%)	0	100	100
All	All	682/598 (114%)	654 (96%)	28 (4%)	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	Analysed Rotameric Outliers		Percentiles		
1	A	322/267 (121%)	311 (97%)	11 (3%)	37 8		
1	В	$298/267 \ (112\%)$	296 (99%)	2 (1%)	84 66		
All	All	620/534 (116%)	607 (98%)	13 (2%)	65 21		

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164[A]	ARG
1	A	164[B]	ARG
1	A	282[B]	LYS
1	A	141[B]	ARG
1	A	282[A]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	165	ASN
1	В	144	GLN
1	В	176	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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		B	ond leng	${ m gths}$	В	ond ang	gles			
10101	Type	Chain	ites	Ites	ites	Ites Lilik	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	В	304	_	3,3,3	0.49	0	2,2,2	0.27	0			
3	EDO	A	302	_	3,3,3	0.33	0	2,2,2	0.65	0			
5	PEG	В	305	_	6,6,6	0.56	0	5,5,5	0.35	0			
3	EDO	A	303	_	3,3,3	0.43	0	2,2,2	0.33	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.

\mathbf{N}	Iol	\mathbf{Type}	Chain	${ m Res}$	Link	Chirals	Torsions	Rings
	3	EDO	В	304	_	-	1/1/1/1	-
	3	EDO	A	302	-	-	1/1/1/1	-
	5	PEG	В	305	-	-	2/4/4/4	-
	3	EDO	A	303	_	-	1/1/1/1	-

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	305	PEG	O1-C1-C2-O2
3	A	303	EDO	O1-C1-C2-O2
3	В	304	EDO	O1-C1-C2-O2
3	A	302	EDO	O1-C1-C2-O2
5	В	305	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	305	PEG	2	0
3	A	303	EDO	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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	292/299 (97%)	-0.15	8 (2%) 54 54	11, 19, 33, 131	0
1	В	290/299~(96%)	-0.01	12 (4%) 37 37	11, 21, 43, 107	0
All	All	582/598 (97%)	-0.08	20 (3%) 45 44	11, 20, 41, 131	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	В	2	ASN	6.3
1	A	3	GLU	5.5
1	В	291	SER	5.5
1	В	3[A]	GLU	5.2
1	A	293	ILE	5.2

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 carbohydrates 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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
5	PEG	В	305	7/7	0.78	0.15	34,45,54,57	7
4	SER	В	303	7/7	0.79	0.16	41,54,63,72	0
3	EDO	В	304	4/4	0.82	0.19	44,52,55,57	0
3	EDO	A	303	4/4	0.86	0.18	27,27,28,37	4
2	CL	В	302	1/1	0.93	0.10	28,28,28,28	1
3	EDO	A	302	4/4	0.95	0.18	34,41,47,49	0
2	CL	В	301	1/1	0.98	0.04	31,31,31,31	0
2	CL	A	301	1/1	0.99	0.03	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.

