



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:56 PM GMT

PDB ID : 3G02
Title : Structure of enantioselective mutant of epoxide hydrolase from *Aspergillus niger* generated by directed evolution
Authors : Naworyta, A.; Mowbray, S.L.
Deposited on : 2009-01-27
Resolution : 1.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

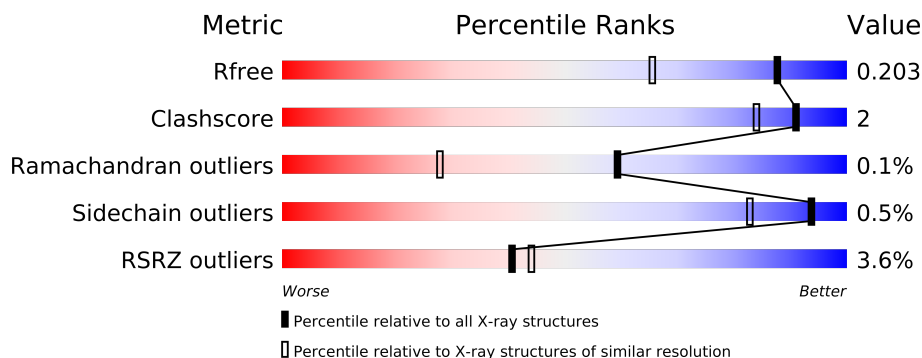
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.50 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}	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	408	
1	B	408	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7069 atoms, of which 0 are hydrogen and 0 are deuterium.

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	387	Total	C	N	O	S	0	14	0
			3198	2082	515	590	11			
1	B	380	Total	C	N	O	S	0	14	0
			3156	2054	511	579	12			

There are 46 discrepancies between the modelled and reference sequences:

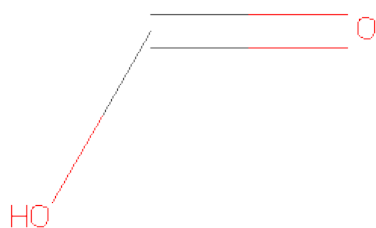
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP Q9UR30
A	1	ASN	-	EXPRESSION TAG	UNP Q9UR30
A	2	HIS	-	EXPRESSION TAG	UNP Q9UR30
A	3	LYS	-	EXPRESSION TAG	UNP Q9UR30
A	4	ALA	-	EXPRESSION TAG	UNP Q9UR30
A	215	PHE	LEU	ENGINEERED	UNP Q9UR30
A	217	ASN	ALA	ENGINEERED	UNP Q9UR30
A	219	SER	ARG	ENGINEERED	UNP Q9UR30
A	249	TYR	LEU	ENGINEERED	UNP Q9UR30
A	317	TRP	THR	ENGINEERED	UNP Q9UR30
A	318	VAL	THR	ENGINEERED	UNP Q9UR30
A	329	PRO	MET	ENGINEERED	UNP Q9UR30
A	330	TYR	LEU	ENGINEERED	UNP Q9UR30
A	350	VAL	CYS	ENGINEERED	UNP Q9UR30
A	399	GLY	-	EXPRESSION TAG	UNP Q9UR30
A	400	ARG	-	EXPRESSION TAG	UNP Q9UR30
A	401	SER	-	EXPRESSION TAG	UNP Q9UR30
A	402	HIS	-	EXPRESSION TAG	UNP Q9UR30
A	403	HIS	-	EXPRESSION TAG	UNP Q9UR30
A	404	HIS	-	EXPRESSION TAG	UNP Q9UR30
A	405	HIS	-	EXPRESSION TAG	UNP Q9UR30
A	406	HIS	-	EXPRESSION TAG	UNP Q9UR30
A	407	HIS	-	EXPRESSION TAG	UNP Q9UR30
B	0	MET	-	INITIATING METHIONINE	UNP Q9UR30
B	1	ASN	-	EXPRESSION TAG	UNP Q9UR30

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	HIS	-	EXPRESSION TAG	UNP Q9UR30
B	3	LYS	-	EXPRESSION TAG	UNP Q9UR30
B	4	ALA	-	EXPRESSION TAG	UNP Q9UR30
B	215	PHE	LEU	ENGINEERED	UNP Q9UR30
B	217	ASN	ALA	ENGINEERED	UNP Q9UR30
B	219	SER	ARG	ENGINEERED	UNP Q9UR30
B	249	TYR	LEU	ENGINEERED	UNP Q9UR30
B	317	TRP	THR	ENGINEERED	UNP Q9UR30
B	318	VAL	THR	ENGINEERED	UNP Q9UR30
B	329	PRO	MET	ENGINEERED	UNP Q9UR30
B	330	TYR	LEU	ENGINEERED	UNP Q9UR30
B	350	VAL	CYS	ENGINEERED	UNP Q9UR30
B	399	GLY	-	EXPRESSION TAG	UNP Q9UR30
B	400	ARG	-	EXPRESSION TAG	UNP Q9UR30
B	401	SER	-	EXPRESSION TAG	UNP Q9UR30
B	402	HIS	-	EXPRESSION TAG	UNP Q9UR30
B	403	HIS	-	EXPRESSION TAG	UNP Q9UR30
B	404	HIS	-	EXPRESSION TAG	UNP Q9UR30
B	405	HIS	-	EXPRESSION TAG	UNP Q9UR30
B	406	HIS	-	EXPRESSION TAG	UNP Q9UR30
B	407	HIS	-	EXPRESSION TAG	UNP Q9UR30

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	377	Total	O	0	0
			377	377		
3	B	329	Total	O	0	0
			329	329		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.87Å 89.67Å 75.34Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	28.91 – 1.50 28.91 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (28.91-1.50) 95.0 (28.91-1.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.53 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.183 , 0.204 0.184 , 0.203	Depositor DCC
R_{free} test set	6102 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 120660 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7069	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT

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	0.35	0/3300	0.48	0/4494
1	B	0.34	0/3254	0.48	0/4425
All	All	0.35	0/6554	0.48	0/8919

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3198	0	3104	15	0
1	B	3156	0	3057	11	0
2	A	6	0	2	0	0
2	B	3	0	1	0	0
3	A	377	0	0	2	0
3	B	329	0	0	0	0
All	All	7069	0	6164	25	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (25) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:MET:HG3	3:A:571:HOH:O	1.40	1.18
3:A:571:HOH:O	1:B:253[B]:MET:SD	2.37	0.83
1:A:39[A]:LYS:HE2	1:B:34:LEU:HD11	1.76	0.67
1:B:119:GLY:HA3	1:B:123[A]:GLU:OE1	1.95	0.65
1:A:119:GLY:HA3	1:A:123[B]:GLU:OE2	1.98	0.63
1:A:318[B]:VAL:CG2	1:A:319:PRO:HD3	2.35	0.57
1:A:40:ILE:HD13	1:A:62[B]:THR:CG2	2.34	0.56
1:A:318[B]:VAL:HG22	1:A:319:PRO:HD3	1.93	0.51
1:B:238:ILE:HD11	1:B:353:PRO:HD3	1.95	0.49
1:A:40:ILE:HD13	1:A:62[B]:THR:HG22	1.94	0.49
1:A:115:HIS:HD2	1:A:116:GLY:O	1.97	0.48
1:B:241[B]:MET:HG2	1:B:350:VAL:HG12	1.97	0.46
1:A:120:SER:OG	1:A:122[B]:VAL:HG12	2.16	0.45
1:B:251:TYR:CG	1:B:252:ALA:N	2.86	0.43
1:B:166:LEU:HD13	1:B:196:PHE:CD2	2.53	0.43
1:B:115:HIS:HD2	1:B:116:GLY:O	2.01	0.43
1:A:241[B]:MET:HG2	1:A:350:VAL:HG12	1.99	0.43
1:A:284:TRP:CG	1:A:349:LEU:HD21	2.54	0.43
1:B:284:TRP:CG	1:B:349:LEU:HD21	2.54	0.43
1:A:115:HIS:CE1	1:A:149:LEU:H	2.36	0.42
1:A:38[B]:SER:OG	1:A:271:ILE:HG13	2.18	0.42
1:B:249:TYR:HE2	1:B:318[A]:VAL:HG13	1.84	0.42
1:A:115:HIS:HE1	1:A:149:LEU:H	1.67	0.42
1:A:251:TYR:CG	1:A:252:ALA:N	2.88	0.41
1:B:159:PRO:HG2	1:B:162:LYS:HZ2	1.85	0.41

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	397/408 (97%)	391 (98%)	6 (2%)	0	100	100
1	B	388/408 (95%)	382 (98%)	5 (1%)	1 (0%)	50	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	785/816 (96%)	773 (98%)	11 (1%)	1 (0%)	59	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	ALA

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	348/350 (99%)	347 (100%)	1 (0%)	96	88
1	B	342/350 (98%)	340 (99%)	2 (1%)	92	80
All	All	690/700 (99%)	687 (100%)	3 (0%)	94	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	B	17	ASN
1	B	189	GLN

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

Mol	Chain	Res	Type
1	A	115	HIS
1	A	217	ASN
1	B	17	ASN
1	B	115	HIS
1	B	394	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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	$\# Z > 2$
2	FMT	A	408	-	2,2,2	0.61	0	1,1,1	0.39	0
2	FMT	A	409	-	2,2,2	0.63	0	1,1,1	0.27	0
2	FMT	B	408	-	2,2,2	0.67	0	1,1,1	0.34	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
2	FMT	A	408	-	-	0/0/0/0	0/0/0/0
2	FMT	A	409	-	-	0/0/0/0	0/0/0/0
2	FMT	B	408	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	387/408 (94%)	0.27	16 (4%)	35 39	5, 14, 22, 31	0
1	B	380/408 (93%)	0.25	12 (3%)	45 49	5, 13, 24, 31	0
All	All	767/816 (93%)	0.26	28 (3%)	41 43	5, 13, 23, 31	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	5.4
1	A	328	THR	4.7
1	B	222	PRO	4.6
1	B	3	LYS	4.2
1	B	40[A]	ILE	3.8
1	A	222	PRO	3.6
1	A	3	LYS	3.5
1	A	223	GLU	3.5
1	A	106	GLU	3.3
1	A	320	THR	3.1
1	A	224	GLY	3.0
1	B	219	SER	3.0
1	A	368[A]	ASP	2.9
1	B	106	GLU	2.8
1	A	319	PRO	2.7
1	B	328	THR	2.7
1	B	220	ALA	2.6
1	B	10	SER	2.4
1	A	246	THR	2.4
1	B	15	SER	2.4
1	A	219	SER	2.3
1	A	71	GLU	2.1
1	A	70[A]	SER	2.1
1	A	227	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	2.1
1	A	26	GLU	2.1
1	B	26	GLU	2.1
1	B	4	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FMT	B	408	3/3	0.10	1.25	6,6,7,7	0
2	FMT	A	408	3/3	0.10	0.44	8,8,8,8	0
2	FMT	A	409	3/3	0.08	-1.65	17,17,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.