



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2014 – 02:02 PM EDT

PDB ID : 4C4X
Title : Crystal structure of human bifunctional epoxide hydroxylase 2 complexed with C9
Authors : Pilger, J.; Mazur, A.; Monecke, P.; Schreuder, H.; Elshorst, B.; Langer, T.; Schiffer, A.; Krimm, I.; Wegstroth, M.; Lee, D.; Hessler, G.; Wendt, K.-U.; Becker, S.; Griesinger, C.
Deposited on : 2013-09-09
Resolution : 2.17 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>

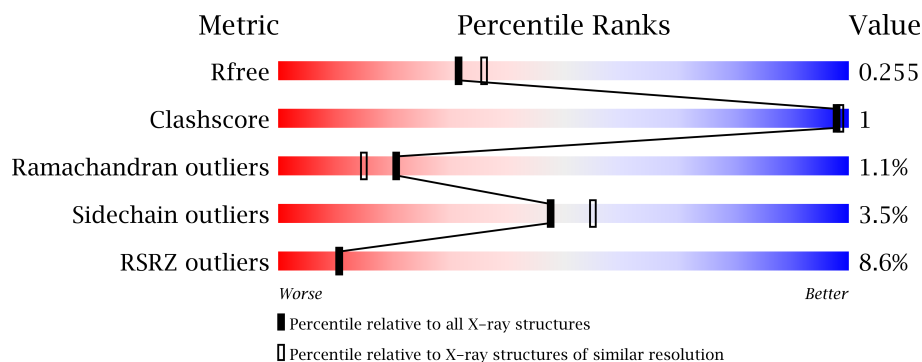
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
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) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 2.17 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	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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	326	
1	B	326	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	W9M	B	1548[A]	-	X
2	W9M	B	1548[B]	-	X

2 Entry composition i

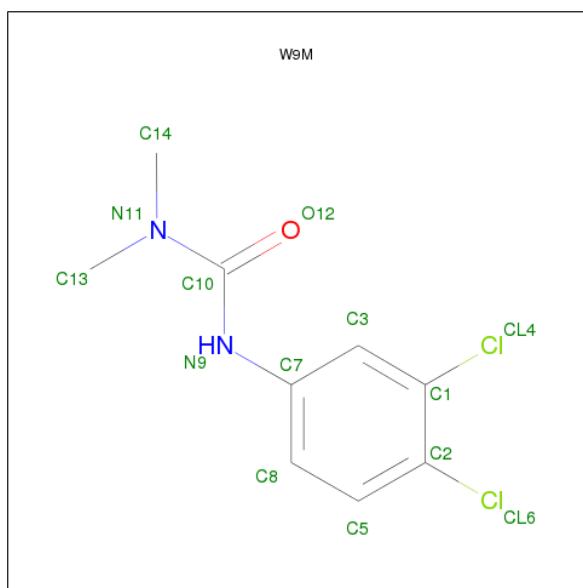
There are 3 unique types of molecules in this entry. The entry contains 5562 atoms, of which 0 are hydrogen and 0 are deuterium.

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 BIFUNCTIONAL EPOXIDE HYDROLASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2528	1626	425	455	22			
1	B	314	Total	C	N	O	S	0	0	0
			2533	1629	426	456	22			

- Molecule 2 is 3-(3,4-DICHLOROPHENYL)-1,1-DIMETHYL-UREA (three-letter code: W9M) (formula: C₉H₁₀Cl₂N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	1
			28	18	4	4	2		
2	B	1	Total	C	Cl	N	O	0	1
			28	18	4	4	2		

- Molecule 3 is water.

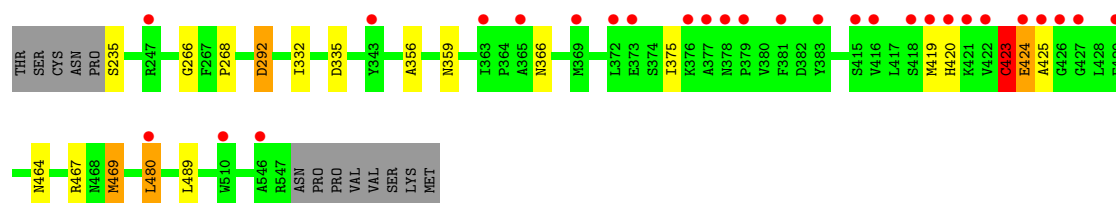
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total 232	O 232	0	0
3	B	213	Total 213	O 213	0	0

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 errors 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.

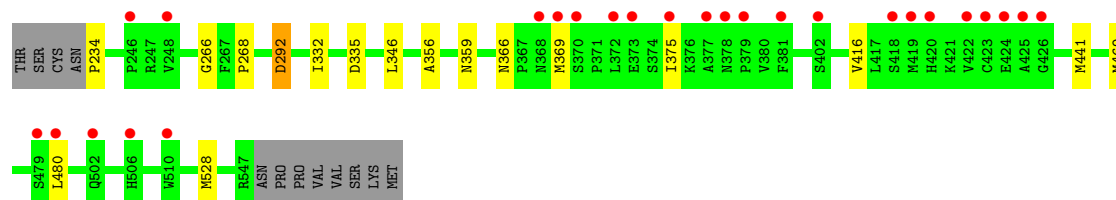
• Molecule 1: BIFUNCTIONAL EPOXIDE HYDROLASE 2

Chain A:



• Molecule 1: BIFUNCTIONAL EPOXIDE HYDROLASE 2

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.69Å 79.87Å 88.61Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	29.63 – 2.17 44.30 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.63-2.17) 98.5 (44.30-2.17)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.211 , 0.242 0.219 , 0.255	Depositor DCC
R_{free} test set	2528 reflections (7.77%)	DCC
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.8	EDS
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35057 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5562	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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: W9M

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	0.37	0/2603	0.60	2/3529 (0.1%)
1	B	0.37	0/2608	0.59	2/3536 (0.1%)
All	All	0.37	0/5211	0.60	4/7065 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	PRO	N-CA-CB	5.91	110.39	103.30
1	A	423	CYS	C-N-CA	5.75	136.07	121.70
1	B	292	ASP	N-CA-C	-5.35	96.56	111.00
1	A	292	ASP	N-CA-C	-5.32	96.64	111.00

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	2528	0	2461	5	0
1	B	2533	0	2463	2	0
2	A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	0	0	0
3	A	232	0	0	0	0
3	B	213	0	0	0	0
All	All	5562	0	4924	7	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 1.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:266:GLY:HA3	1:B:335:ASP:HB3	1.75	0.68
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.81	0.61
1:A:332:ILE:HG12	1:A:356:ALA:HB3	1.89	0.54
1:B:332:ILE:HG12	1:B:356:ALA:HB3	1.91	0.52
1:A:464:ASN:HA	1:A:467:ARG:HD2	2.01	0.42
1:A:423:CYS:HA	1:A:424:GLU:O	2.20	0.42
1:A:375:ILE:HD11	1:A:469:MET:HG2	2.01	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	311/326 (95%)	293 (94%)	13 (4%)	5 (2%)	14	9
1	B	312/326 (96%)	296 (95%)	14 (4%)	2 (1%)	33	31
All	All	623/652 (96%)	589 (94%)	27 (4%)	7 (1%)	21	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	GLU

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Mol	Chain	Res	Type
1	A	425	ALA
1	A	480	LEU
1	B	480	LEU
1	A	423	CYS
1	A	268	PRO
1	B	268	PRO

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	274/287 (96%)	265 (97%)	9 (3%)	50	58
1	B	274/287 (96%)	264 (96%)	10 (4%)	47	53
All	All	548/574 (96%)	529 (96%)	19 (4%)	48	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	SER
1	A	292	ASP
1	A	359	ASN
1	A	366	ASN
1	A	419	MET
1	A	420	HIS
1	A	469	MET
1	A	480	LEU
1	A	489	LEU
1	B	292	ASP
1	B	346	LEU
1	B	359	ASN
1	B	366	ASN
1	B	369	MET
1	B	375	ILE
1	B	416	VAL
1	B	441	MET
1	B	469	MET
1	B	528	MET

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	366	ASN
1	A	518	HIS
1	B	366	ASN
1	B	505	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 ⓘ

4 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	W9M	A	1548[A]	-	14,14,14	1.61	1 (7%)	19,19,19	0.80	2 (10%)
2	W9M	A	1548[B]	-	14,14,14	1.61	1 (7%)	19,19,19	0.99	2 (10%)
2	W9M	B	1548[A]	-	14,14,14	1.63	1 (7%)	19,19,19	0.79	2 (10%)
2	W9M	B	1548[B]	-	14,14,14	1.63	1 (7%)	19,19,19	0.90	2 (10%)

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	W9M	A	1548[A]	-	-	0/8/8/8	0/1/1/1
2	W9M	A	1548[B]	-	-	0/8/8/8	0/1/1/1
2	W9M	B	1548[A]	-	-	0/8/8/8	0/1/1/1
2	W9M	B	1548[B]	-	-	0/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1548[B]	W9M	C10-N11	6.09	1.46	1.36
2	B	1548[A]	W9M	C10-N11	6.07	1.46	1.36
2	A	1548[B]	W9M	C10-N11	6.00	1.46	1.36
2	A	1548[A]	W9M	C10-N11	5.99	1.46	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1548[B]	W9M	N9-C10-N11	2.99	119.03	115.74
2	A	1548[B]	W9M	O12-C10-N11	-2.89	117.09	122.27
2	B	1548[B]	W9M	O12-C10-N11	-2.70	117.42	122.27
2	B	1548[B]	W9M	N9-C10-N11	2.62	118.61	115.74
2	A	1548[A]	W9M	O12-C10-N11	-2.53	117.75	122.27
2	B	1548[A]	W9M	O12-C10-N11	-2.51	117.78	122.27
2	A	1548[A]	W9M	N9-C10-N11	2.05	117.99	115.74
2	B	1548[A]	W9M	N9-C10-N11	2.00	117.94	115.74

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	313/326 (96%)	0.56	28 (8%)	10 10	20, 33, 71, 88	0
1	B	314/326 (96%)	0.50	26 (8%)	11 12	19, 33, 70, 87	0
All	All	627/652 (96%)	0.53	54 (8%)	11 11	19, 33, 71, 88	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	MET	8.3
1	A	372	LEU	5.3
1	B	369	MET	5.0
1	A	418	SER	4.9
1	B	418	SER	4.9
1	A	416	VAL	4.7
1	B	368	ASN	4.6
1	A	426	GLY	4.5
1	A	510	TRP	4.4
1	B	370	SER	4.4
1	A	424	GLU	4.2
1	B	377	ALA	4.2
1	B	372	LEU	4.1
1	A	373	GLU	4.1
1	B	426	GLY	4.1
1	B	378	ASN	3.8
1	B	375	ILE	3.7
1	A	383	TYR	3.6
1	B	419	MET	3.5
1	A	247	ARG	3.4
1	B	373	GLU	3.4
1	B	379	PRO	3.4
1	A	378	ASN	3.3
1	A	381	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	376	LYS	3.1
1	B	510	TRP	3.0
1	B	480	LEU	3.0
1	A	425	ALA	3.0
1	B	424	GLU	3.0
1	B	502	GLN	3.0
1	B	506	HIS	2.8
1	A	379	PRO	2.8
1	B	425	ALA	2.7
1	B	381	PHE	2.7
1	B	420	HIS	2.7
1	A	369	MET	2.7
1	A	415	SER	2.7
1	A	429	PHE	2.6
1	A	365	ALA	2.5
1	A	363	ILE	2.5
1	A	546	ALA	2.5
1	A	343	TYR	2.4
1	A	421	LYS	2.4
1	B	423	CYS	2.3
1	A	377	ALA	2.2
1	B	246	PRO	2.2
1	A	422	VAL	2.2
1	A	420	HIS	2.2
1	B	248	VAL	2.1
1	A	427	GLY	2.1
1	B	422	VAL	2.1
1	A	480	LEU	2.0
1	B	479	SER	2.0
1	B	402	SER	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	W9M	B	1548[B]	14/14	0.30	5.62	76,76,76,76	14
2	W9M	B	1548[A]	14/14	0.30	2.77	69,70,70,71	14
2	W9M	A	1548[B]	14/14	0.25	0.58	72,73,73,73	14
2	W9M	A	1548[A]	14/14	0.25	0.51	62,62,63,63	14

6.5 Other polymers ⓘ

There are no such residues in this entry.