



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:06 am BST

PDB ID : 6I5E
Title : X-ray structure of apo human soluble Epoxide Hydrolase C-terminal Domain (hsEH CTD)
Authors : Abis, G.; Kopec, J.; Yue, W.W.; Conte, M.R.
Deposited on : 2018-11-13
Resolution : 2.60 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 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 : 2.11
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) : 2.11

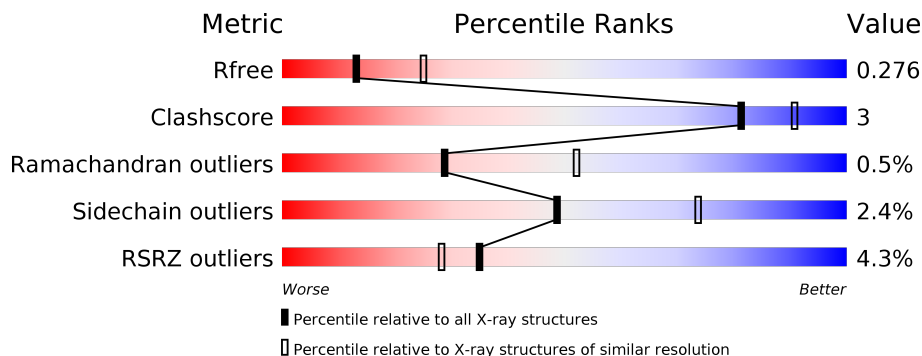
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	344	
1	B	344	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5099 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 Bifunctional epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2543	1635	426	459	23	0	0	0
1	B	316	2543	1635	426	459	23	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	MET	-	initiating methionine	UNP P34913
A	213	HIS	-	expression tag	UNP P34913
A	214	HIS	-	expression tag	UNP P34913
A	215	HIS	-	expression tag	UNP P34913
A	216	HIS	-	expression tag	UNP P34913
A	217	HIS	-	expression tag	UNP P34913
A	218	HIS	-	expression tag	UNP P34913
A	219	SER	-	expression tag	UNP P34913
A	220	THR	-	expression tag	UNP P34913
A	221	GLU	-	expression tag	UNP P34913
A	222	ASN	-	expression tag	UNP P34913
A	223	LEU	-	expression tag	UNP P34913
A	224	TYR	-	expression tag	UNP P34913
A	225	PHE	-	expression tag	UNP P34913
A	226	GLN	-	expression tag	UNP P34913
A	227	GLY	-	expression tag	UNP P34913
A	228	SER	-	expression tag	UNP P34913
A	229	SER	-	expression tag	UNP P34913
B	212	MET	-	initiating methionine	UNP P34913
B	213	HIS	-	expression tag	UNP P34913
B	214	HIS	-	expression tag	UNP P34913
B	215	HIS	-	expression tag	UNP P34913
B	216	HIS	-	expression tag	UNP P34913
B	217	HIS	-	expression tag	UNP P34913
B	218	HIS	-	expression tag	UNP P34913

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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	SER	-	expression tag	UNP P34913
B	220	THR	-	expression tag	UNP P34913
B	221	GLU	-	expression tag	UNP P34913
B	222	ASN	-	expression tag	UNP P34913
B	223	LEU	-	expression tag	UNP P34913
B	224	TYR	-	expression tag	UNP P34913
B	225	PHE	-	expression tag	UNP P34913
B	226	GLN	-	expression tag	UNP P34913
B	227	GLY	-	expression tag	UNP P34913
B	228	SER	-	expression tag	UNP P34913
B	229	SER	-	expression tag	UNP P34913

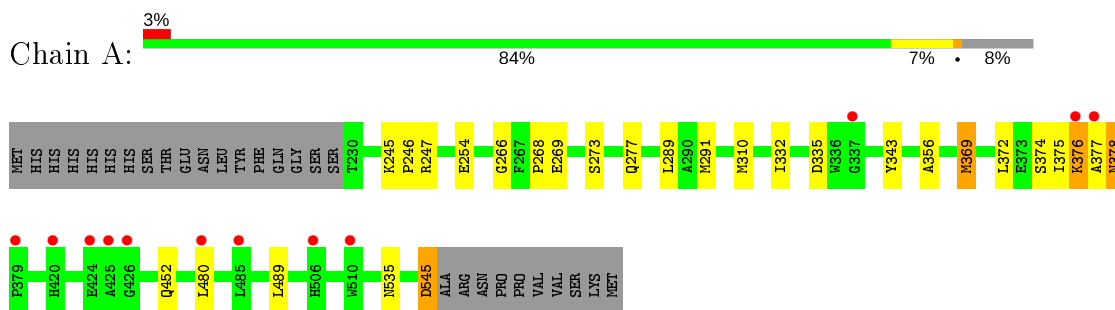
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	4	Total O 4 4	0	0

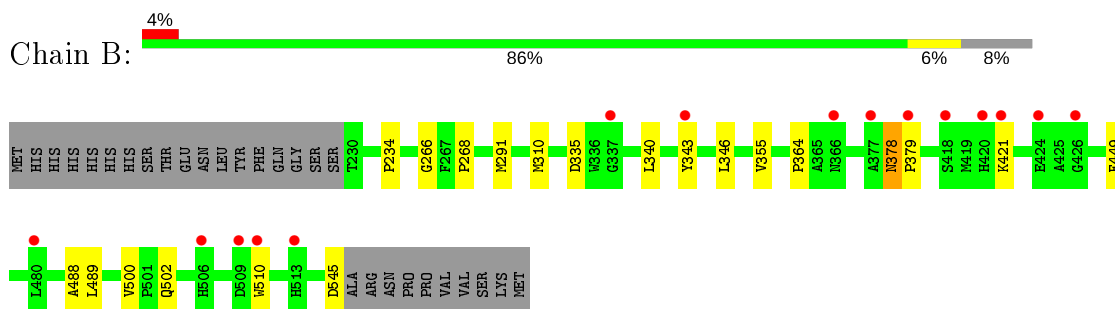
3 Residue-property plots [i](#)

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: Bifunctional epoxide hydrolase 2



- Molecule 1: Bifunctional epoxide hydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.22Å 80.14Å 104.70Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	70.51 – 2.60 29.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.51-2.60) 100.0 (29.60-2.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.246 , 0.277 0.247 , 0.276	Depositor DCC
R_{free} test set	1101 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.818	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5099	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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	0.57	0/2619	0.75	0/3553
1	B	0.55	0/2619	0.74	1/3553 (0.0%)
All	All	0.56	0/5238	0.74	1/7106 (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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	340	LEU	CA-CB-CG	5.64	128.26	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide
1	B	291	MET	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 the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2543	0	2465	18	0
1	B	2543	0	2465	8	0
2	A	9	0	0	0	0
2	B	4	0	0	0	0
All	All	5099	0	4930	26	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.

All (26) 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:A:369:MET:SD	1:A:374:SER:OG	2.27	0.93
1:A:375:ILE:O	1:A:377:ALA:N	2.06	0.89
1:A:375:ILE:C	1:A:377:ALA:H	1.95	0.70
1:A:375:ILE:O	1:A:378:ASN:N	2.23	0.65
1:B:500:VAL:CG1	1:B:502:GLN:HG3	2.29	0.62
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.82	0.60
1:A:375:ILE:C	1:A:377:ALA:N	2.54	0.59
1:B:266:GLY:HA3	1:B:335:ASP:HB3	1.91	0.53
1:B:310:MET:HG2	1:B:343:TYR:CD2	2.45	0.52
1:A:254:GLU:HG3	1:A:289:LEU:HD23	1.93	0.51
1:A:545:ASP:OD1	1:A:545:ASP:N	2.42	0.51
1:A:369:MET:SD	1:A:374:SER:CA	2.99	0.50
1:A:369:MET:SD	1:A:374:SER:CB	3.01	0.48
1:B:364:PRO:HG2	1:B:510:TRP:CE2	2.50	0.46
1:A:332:ILE:HG12	1:A:356:ALA:HB3	2.00	0.44
1:A:245:LYS:HB2	1:A:246:PRO:HD2	2.01	0.43
1:A:310:MET:HG3	1:A:343:TYR:CE2	2.53	0.42
1:B:234:PRO:HG2	1:B:449:PHE:CE1	2.54	0.42
1:A:369:MET:SD	1:A:374:SER:N	2.93	0.42
1:A:375:ILE:O	1:A:376:LYS:C	2.58	0.42
1:A:269:GLU:HB3	1:A:273:SER:OG	2.20	0.42
1:A:277:GLN:HG3	1:A:535:ASN:ND2	2.35	0.42
1:B:500:VAL:HG12	1:B:502:GLN:HG3	2.02	0.41
1:B:355:VAL:O	1:B:488:ALA:HA	2.20	0.41
1:A:369:MET:HG3	1:A:369:MET:O	2.21	0.41
1:B:378:ASN:HD22	1:B:379:PRO:HD2	1.85	0.40

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	314/344 (91%)	302 (96%)	10 (3%)	2 (1%)	25	47
1	B	314/344 (91%)	306 (98%)	7 (2%)	1 (0%)	41	64
All	All	628/688 (91%)	608 (97%)	17 (3%)	3 (0%)	29	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	LYS
1	A	268	PRO
1	B	268	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	276/304 (91%)	268 (97%)	8 (3%)	42	68
1	B	276/304 (91%)	271 (98%)	5 (2%)	59	80
All	All	552/608 (91%)	539 (98%)	13 (2%)	49	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ARG
1	A	369	MET
1	A	372	LEU
1	A	378	ASN
1	A	452	GLN
1	A	480	LEU
1	A	489	LEU
1	A	545	ASP
1	B	346	LEU
1	B	378	ASN
1	B	421	LYS
1	B	489	LEU
1	B	545	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	378	ASN
1	A	384	GLN
1	A	535	ASN
1	B	378	ASN
1	B	452	GLN
1	B	453	GLN
1	B	535	ASN
1	B	536	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](#)

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

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	316/344 (91%)	0.14	12 (3%) 40 33	24, 41, 78, 114	0
1	B	316/344 (91%)	0.20	15 (4%) 31 25	23, 41, 78, 113	0
All	All	632/688 (91%)	0.17	27 (4%) 35 28	23, 41, 78, 114	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	SER	7.9
1	A	376	LYS	4.9
1	B	420	HIS	4.2
1	B	377	ALA	4.1
1	A	420	HIS	3.7
1	B	480	LEU	3.6
1	B	513	HIS	3.1
1	B	506	HIS	3.1
1	A	510	TRP	3.1
1	A	485	LEU	3.0
1	B	510	TRP	2.9
1	B	424	GLU	2.8
1	A	379	PRO	2.8
1	B	337	GLY	2.8
1	B	343	TYR	2.7
1	A	480	LEU	2.7
1	A	377	ALA	2.7
1	B	379	PRO	2.5
1	B	421	LYS	2.5
1	B	366	ASN	2.4
1	A	425	ALA	2.3
1	A	337	GLY	2.3
1	B	426	GLY	2.3
1	A	506	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	509	ASP	2.2
1	A	426	GLY	2.1
1	A	424	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.