

wwPDB X-ray Structure Validation Summary Report (i)

Jan 22, 2024 – 08:11 PM JST

PDB ID	:	8WBK
Title	:	Crystal structure of cis-Epoxysuccinate Hydrolases RhCESH[L]
Authors	:	Dong, S.; Xuan, J.S.; Feng, Y.G.; Cui, Q.
Deposited on	:	2023-09-10
Resolution	:	2.15 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 (i) 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 (1)) were used in the production of this report:

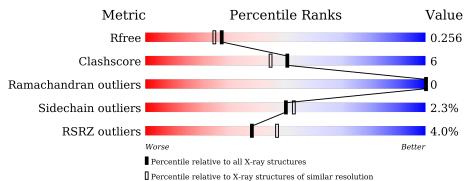
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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 <=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	А	264	2%	12%	10%
1	В	264	78%	11%	10%



8WBK

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3899 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	А	237	Total	C	11	0	S	4	2	0
-		201	1870	1187	322	357	4	1	_	Ŭ
1	В	237	Total	С	Ν	Ο	\mathbf{S}	0	2	0
1	D	231	1870	1187	322	357	4	0		0

A-9GLY-expression tagUNP Q1KLR5A-8SER-expression tagUNP Q1KLR5A-7SER-expression tagUNP Q1KLR5A-6HIS-expression tagUNP Q1KLR5A-5HIS-expression tagUNP Q1KLR5A-4HIS-expression tagUNP Q1KLR5A-3HIS-expression tagUNP Q1KLR5A-2HIS-expression tagUNP Q1KLR5A-1HIS-expression tagUNP Q1KLR5A0SER-expression tagUNP Q1KLR5A1SER-expression tagUNP Q1KLR5A1SER-expression tagUNP Q1KLR5A2GLY-expression tagUNP Q1KLR5A3LEU-expression tagUNP Q1KLR5A4VAL-expression tagUNP Q1KLR5A5PRO-expression tagUNP Q1KLR5A6ARG-expression tagUNP Q1KLR5A8SER-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5B-10MET-expression tag	Chain	Residue	Modelled	Actual	Comment	Reference
A-8SER-expression tagUNP Q1KLR5A-7SER-expression tagUNP Q1KLR5A-6HIS-expression tagUNP Q1KLR5A-5HIS-expression tagUNP Q1KLR5A-4HIS-expression tagUNP Q1KLR5A-4HIS-expression tagUNP Q1KLR5A-3HIS-expression tagUNP Q1KLR5A-2HIS-expression tagUNP Q1KLR5A-1HIS-expression tagUNP Q1KLR5A0SER-expression tagUNP Q1KLR5A1SER-expression tagUNP Q1KLR5A1SER-expression tagUNP Q1KLR5A3LEU-expression tagUNP Q1KLR5A4VAL-expression tagUNP Q1KLR5A5PRO-expression tagUNP Q1KLR5A6ARG-expression tagUNP Q1KLR5A8SER-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A10MET-expression tagUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-9GLY-expression tag <t< td=""><td>А</td><td>-10</td><td>MET</td><td colspan="2">- initiating methionine</td><td>UNP Q1KLR5</td></t<>	А	-10	MET	- initiating methionine		UNP Q1KLR5
A-7SER-expression tagUNP Q1KLR5A-6HIS-expression tagUNP Q1KLR5A-5HIS-expression tagUNP Q1KLR5A-4HIS-expression tagUNP Q1KLR5A-3HIS-expression tagUNP Q1KLR5A-2HIS-expression tagUNP Q1KLR5A-2HIS-expression tagUNP Q1KLR5A-1HIS-expression tagUNP Q1KLR5A0SER-expression tagUNP Q1KLR5A0SER-expression tagUNP Q1KLR5A1SER-expression tagUNP Q1KLR5A1SER-expression tagUNP Q1KLR5A2GLY-expression tagUNP Q1KLR5A3LEU-expression tagUNP Q1KLR5A4VAL-expression tagUNP Q1KLR5A5PRO-expression tagUNP Q1KLR5A6ARG-expression tagUNP Q1KLR5A8SER-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A10MET-expression tagUNP	А	-9	GLY	- expression tag		UNP Q1KLR5
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A-2HIS-expression tagUNP Q1KLRSA-1HIS-expression tagUNP Q1KLRSA0SER-expression tagUNP Q1KLRSA1SER-expression tagUNP Q1KLRSA1SER-expression tagUNP Q1KLRSA2GLY-expression tagUNP Q1KLRSA3LEU-expression tagUNP Q1KLRSA4VAL-expression tagUNP Q1KLRSA5PRO-expression tagUNP Q1KLRSA6ARG-expression tagUNP Q1KLRSA6ARG-expression tagUNP Q1KLRSA7GLY-expression tagUNP Q1KLRSA9HIS-expression tagUNP Q1KLRSA9HIS-expression tagUNP Q1KLRSA9HIS-expression tagUNP Q1KLRSB-10MET-initiating methionineUNP Q1KLRSB-8SER-expression tagUNP Q1KLRSB-8SER-expression tagUNP Q1KLRS	А	-4	HIS	-	expression tag	UNP Q1KLR5
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A4VAL-expression tagUNP Q1KLR5A5PRO-expression tagUNP Q1KLR5A6ARG-expression tagUNP Q1KLR5A7GLY-expression tagUNP Q1KLR5A8SER-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A10MET-expression tagUNP Q1KLR5B-10MET-initiating methionineUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-8SER-expression tagUNP Q1KLR5	A	2	GLY	-	expression tag	UNP Q1KLR5
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A7GLY-expression tagUNP Q1KLR5A8SER-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A10MET-expression tagUNP Q1KLR5B-10MET-initiating methionineUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-8SER-expression tagUNP Q1KLR5	A		PRO	-	expression tag	UNP Q1KLR5
A8SER-expression tagUNP Q1KLR5A9HIS-expression tagUNP Q1KLR5A10MET-expression tagUNP Q1KLR5B-10MET-initiating methionineUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-8SER-expression tagUNP Q1KLR5	A	6	ARG	-	expression tag	UNP Q1KLR5
A9HIS-expression tagUNP Q1KLR5A10MET-expression tagUNP Q1KLR5B-10MET-initiating methionineUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-8SER-expression tagUNP Q1KLR5	A	7	GLY	-	expression tag	UNP Q1KLR5
A10MET-expression tagUNP Q1KLR5B-10MET-initiating methionineUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-8SER-expression tagUNP Q1KLR5	А	8	SER	-	expression tag	UNP Q1KLR5
B-10MET-initiating methionineUNP Q1KLR5B-9GLY-expression tagUNP Q1KLR5B-8SER-expression tagUNP Q1KLR5	А	9	HIS	-	expression tag	UNP Q1KLR5
B-9GLY-expression tagUNP Q1KLR5B-8SER-expression tagUNP Q1KLR5	А	10	MET	-	expression tag	UNP Q1KLR5
B -8 SER - expression tag UNP Q1KLR5	В	-10	MET	-	initiating methionine	UNP Q1KLR5
	В	-9	GLY	-	expression tag	UNP Q1KLR5
	В	-8	SER	-	expression tag	UNP Q1KLR5
B - C SEK - expression tag UNP QIKLRS	В	-7	SER	-	expression tag	UNP Q1KLR5

There are 42 discrepancies between the modelled and reference sequences:

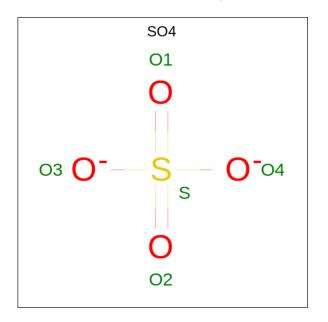
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Chain	Residue	Modelled	Actual Comment		Reference
В	-6	HIS	-	expression tag	UNP Q1KLR5
В	-5	HIS	-	expression tag	UNP Q1KLR5
В	-4	HIS	-	expression tag	UNP Q1KLR5
В	-3	HIS	-	expression tag	UNP Q1KLR5
В	-2	HIS	-	expression tag	UNP Q1KLR5
В	-1	HIS	-	expression tag	UNP Q1KLR5
В	0	SER	-	expression tag	UNP Q1KLR5
В	1	SER	-	expression tag	UNP Q1KLR5
В	2	GLY	-	expression tag	UNP Q1KLR5
В	3	LEU	-	expression tag	UNP Q1KLR5
В	4	VAL	-	expression tag	UNP Q1KLR5
В	5	PRO	-	expression tag	UNP Q1KLR5
В	6	ARG	-	expression tag	UNP Q1KLR5
В	7	GLY	-	expression tag	UNP Q1KLR5
В	8	SER	_	expression tag	UNP Q1KLR5
В	9	HIS	-	expression tag	UNP Q1KLR5
В	10	MET	-	expression tag	UNP Q1KLR5

Continued from previous page...

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	В	1	Total 5	0 4	S 1	0	0

• Molecule 3 is water.

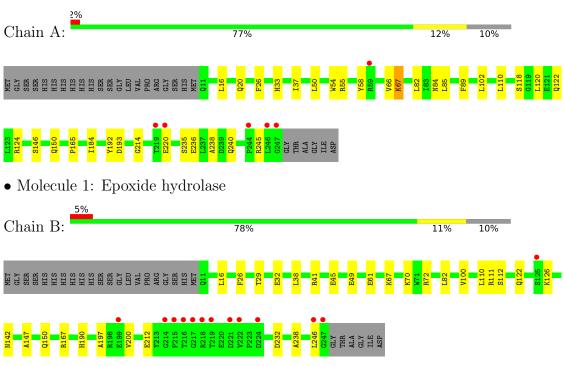


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	77	Total O 77 77	0	0
3	В	77	Total O 77 77	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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	P 1	Depositor
Cell constants	42.13Å 55.62Å 64.20Å	Depositor
a, b, c, α , β , γ	67.34° 75.80° 75.80°	Depositor
Resolution (Å)	34.46 - 2.15	Depositor
Resolution (A)	58.40 - 2.15	EDS
% Data completeness	95.3 (34.46-2.15)	Depositor
(in resolution range)	88.1 (58.40-2.15)	EDS
R _{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.65 (at 2.14 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.205 , 0.258	Depositor
II, II, <i>free</i>	0.210 , 0.256	DCC
R_{free} test set	2000 reflections $(7.48%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	25.6	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39 , 48.2	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3899	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.74% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: $\mathrm{SO4}$

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		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	0/1915	0.66	0/2602	
1	В	0.42	0/1915	0.62	0/2602	
All	All	0.45	0/3830	0.64	0/5204	

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 (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	А	1870	0	1834	23	0
1	В	1870	0	1834	22	0
2	В	5	0	0	0	0
3	А	77	0	0	6	0
3	В	77	0	0	3	0
All	All	3899	0	3668	42	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 6.

The worst 5 of 42 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:50:LEU:HD11	1:A:85:LEU:HB3	1.61	0.81
1:B:167:ARG:HG2	1:B:200[A]:VAL:HG12	1.63	0.80
1:A:26:PHE:HA	1:A:110:LEU:HD22	1.65	0.78
1:B:167:ARG:HG2	1:B:200[B]:VAL:HG22	1.80	0.63
1:B:167:ARG:HG2	1:B:200[B]:VAL:CG2	2.30	0.62

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	Perce	entiles
1	А	237/264~(90%)	236 (100%)	1 (0%)	0	100	100
1	В	237/264~(90%)	236 (100%)	1 (0%)	0	100	100
All	All	474/528~(90%)	472 (100%)	2~(0%)	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 side chain 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		Percentiles
1	А	197/218~(90%)	192~(98%)	5(2%)	47 49
1	В	197/218~(90%)	193 (98%)	4 (2%)	55 59
All	All	394/436~(90%)	385~(98%)	9~(2%)	50 53



5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	В	126	LYS
1	В	232	ASP
1	А	220	GLU
1	А	235	SER
1	В	70	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	33	HIS
1	А	150	GLN
1	А	166	HIS

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 (i)

1 ligand is 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	Dec	Tiple	B	ond leng	gths	В	ond ang	gles
IVIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SO4	В	301	-	4,4,4	0.19	0	$6,\!6,\!6$	0.29	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.

No monomer is involved in short contacts.

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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	237/264~(89%)	0.32	6 (2%) 57 65	24, 36, 64, 99	0
1	В	237/264~(89%)	0.43	13 (5%) 25 34	24, 42, 80, 124	0
All	All	474/528~(89%)	0.37	19 (4%) 38 47	24, 39, 72, 124	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	215	PRO	8.9
1	В	247	GLY	8.8
1	В	219	THR	6.5
1	А	247	GLY	6.1
1	А	219	THR	4.9

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, 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SO4	В	301	5/5	0.88	0.19	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.

