



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 12:30 pm BST

PDB ID : 1CQZ
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE.
Authors : Argiriadi, M.A.; Morisseau, C.; Hammock, B.D.; Christianson, D.W.
Deposited on : 1999-08-12
Resolution : 2.80 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

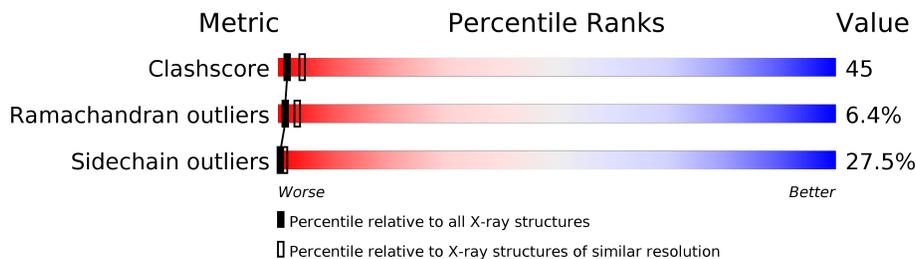
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	
1	B	554	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8218 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
			Total	C	N	O	S			
1	A	487	3879	2501	648	701	29	61	0	0
1	B	541	4299	2766	719	783	31	71	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total 18	O 18	0	0
2	B	22	Total 22	O 22	0	0

SER	G480	F415	R349	A278	T266	M139
VAL	R481	I416	V350	L279	A207	D68
THR	K482	A417	R351	A280	S208	E69
SER	I483	V418	A352	Q281	G	S70
LYS	L484	H419	V353	R265	R211	Y71
ILE	L488	K420	A354	R286	E212	R72
	M489	A421	S355	L287	L213	K73
		T422	L356	E214	F147	S74
		E423	N357	K215	S75	
		I424	T358	V216	K76	
		G425	P359	T217	A77	
		G426	F360	G218	C78	
		I427	M361	T219	G79	
		L428	P362	Q220	A80	
		V429	P363	F221	N81	
		M430	D364	P222	L82	
		T431	V367	E223	P83	
		P432	S368	E224	E84	
		E433	P369	P225	N85	
		D434	M370	G	N85	
		P435	K371	V228	I91	
		L437	V372	P229	K160	
		S438	G	C230	F92	
		K439	S375	N231	S93	
		L440	I376	P232	Q94	
		T441	P377	M233	A95	
		G	V378	D234	A96	
		E444	F379	V235	S100	
		E445	N380	S236	I101	
		I446	G	K243	N102	
		P447	L383	P244	R103	
		F448	F384	G	P104	
		Y449	F385	R247	M105	
		I450	Q386	L248	L106	
		Q451	E387	L249	Q107	
		K455	P388	M253	G	
		T456	E392	G254	I110	
		F458	A393	S255	A111	
		G	L394	G256	L112	
		P461	L395	G	K113	
		L462	E396	L259	G116	
		M463	K397	L261	F117	
		W464	N398	C262	T118	
		Y465	G	H263	T119	
		R466	R401	G264	C120	
		T467	T402	F265	K121	
		T468	F403	P266	I121	
		E469	K404	E267	V122	
		R470	S405	S268	T123	
		W471	P406	G	M124	
		K472	F407	W269	M125	
		K473	R408	F270	W126	
		W474	F409	S271	L127	
		G	A409	W272	M198	
		K477	S410	R273	V199	
		G478	D411	Y274	T200	
		L479	B412	Q275	D129	
			T413	I276	G130	
			G414	E348	D131	
					K132	
					R133	
					N205	

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.90Å 143.00Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	94.6 (20.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.214 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8218	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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	0.66	0/3981	0.87	6/5397 (0.1%)
1	B	0.68	0/4413	0.86	8/5984 (0.1%)
All	All	0.67	0/8394	0.87	14/11381 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASN	C-N-CD	-15.19	87.18	120.60
1	A	231	ASN	C-N-CA	8.88	159.29	122.00
1	B	231	ASN	C-N-CD	-8.27	102.40	120.60
1	B	231	ASN	N-CA-C	5.43	125.67	111.00
1	B	231	ASN	C-N-CA	5.36	144.53	122.00

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	A	3879	0	3863	335	0
1	B	4299	0	4270	398	0
2	A	18	0	0	4	0
2	B	22	0	0	1	0
All	All	8218	0	8133	715	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 45.

The worst 5 of 715 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:B:122:VAL:HG12	1:B:151:ILE:HG13	1.26	1.17
1:A:348:GLU:HA	1:B:133:ARG:HG3	1.33	1.11
1:A:5:VAL:HG22	1:A:118:THR:HB	1.33	1.08
1:B:232:PRO:HD2	1:B:233:ASN:H	1.16	1.03
1:A:58:ILE:HG22	1:A:62:GLN:HG3	1.44	1.00

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	481/554 (87%)	390 (81%)	59 (12%)	32 (7%)	1 3
1	B	539/554 (97%)	438 (81%)	68 (13%)	33 (6%)	1 4
All	All	1020/1108 (92%)	828 (81%)	127 (12%)	65 (6%)	1 3

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	208	SER
1	A	232	PRO
1	A	256	GLY
1	A	415	PHE

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	424/480 (88%)	308 (73%)	116 (27%)	0	1
1	B	468/480 (98%)	339 (72%)	129 (28%)	0	1
All	All	892/960 (93%)	647 (72%)	245 (28%)	0	1

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	525	THR
1	B	101	ILE
1	B	494	LYS
1	A	542	GLN
1	B	50	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	ASN
1	B	125	ASN
1	B	451	GLN
1	B	85	ASN
1	B	107	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.