



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:50 PM GMT

PDB ID : 1CQZ  
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE.  
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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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

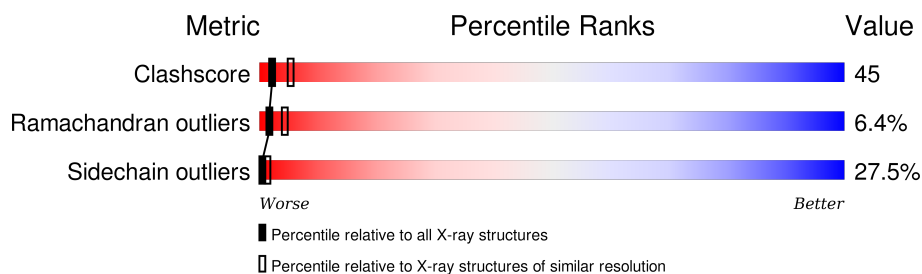
# 1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

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
1	A	487	Total	C	N	O	S	61	0	0
			3879	2501	648	701	29			
1	B	541	Total	C	N	O	S	71	0	0
			4299	2766	719	783	31			

- Molecule 2 is water.

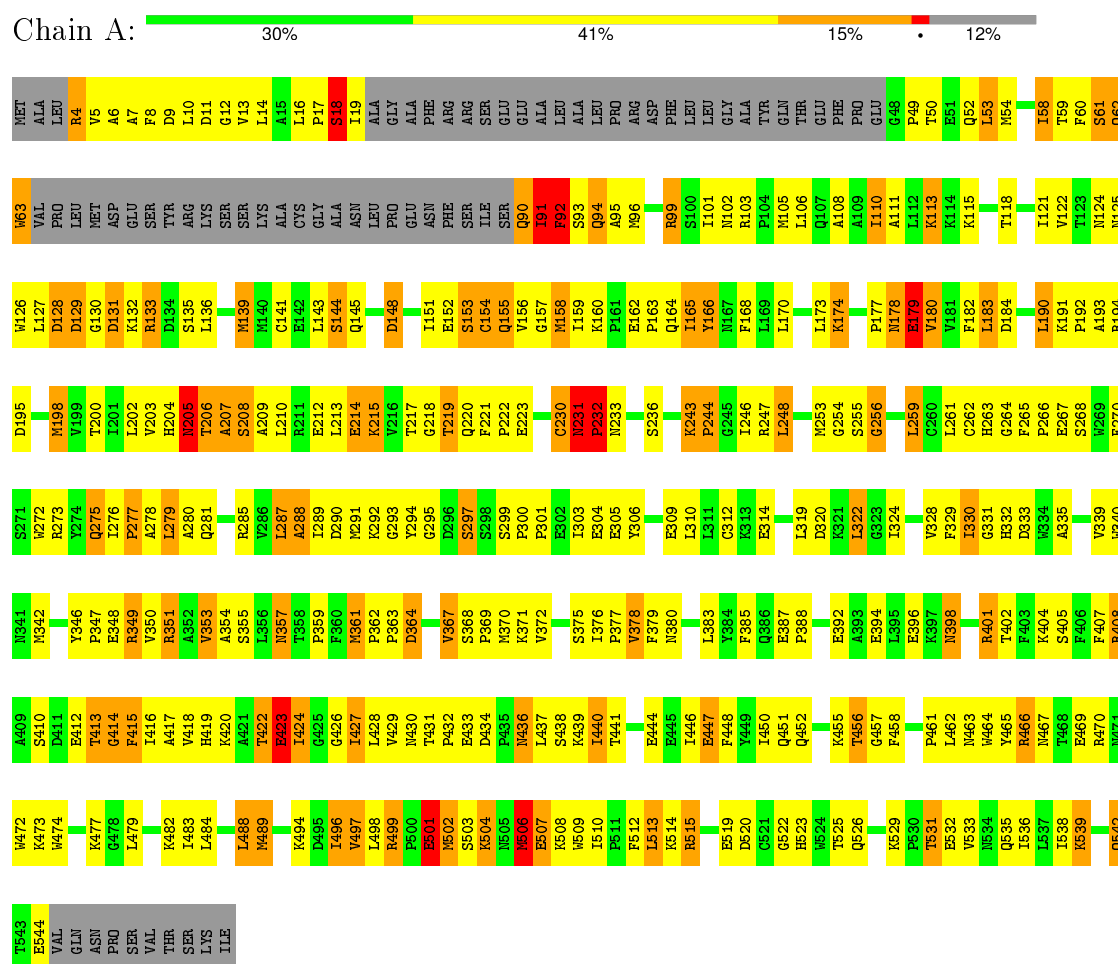
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		
2	B	22	Total	O	0	0
			22	22		

### 3 Residue-property plots

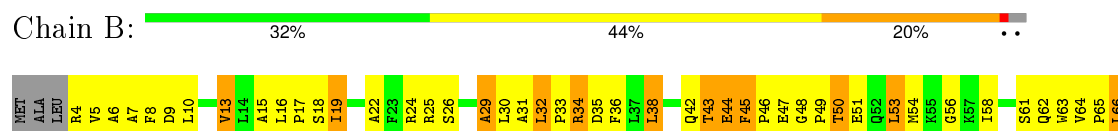
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: EPOXIDE HYDROLASE



#### • Molecule 1: EPOXIDE HYDROLASE



SER	G480	F415	R349	A278	M139	M67
VAL	L481	I416	V350	L279	A207	D68
THR	K482	A417	R351	A280	C141	S70
SER	L483	V418	A352	Q281	E142	R71
LYS	L484	H419	V363		L143	R72
ILE		K420	A354	R285	E112	
	L488	A421	S355	V286	L213	K73
	M489	T422	L356	L287	E214	S74
		E423	R357	A288	K215	S75
	K494	I424	T358	T289	V216	K76
	D495	G425	D290	D290	T217	A77
I496	G426	F360	M291	G216	L150	C78
I497	I427	R361	K292	T219	I151	G79
L498	L428	F428	G293	G220	E152	A80
L499	V429	F363	V294	F221	S153	N81
	M500	D364	G295	P222	C154	L82
	F501	T431	D296	E223	Q155	P83
	M502	P432	S297	A234	E84	N95
	S503	E433	S298	P225	M158	
	K504	D434	S299	V228	I159	I91
	N505	P435	P300	P229	P161	P92
	M506	A436	K371	P301	C330	S93
	E507	L437	V372	E302	E162	Q94
	K508	S438	I303	I303	P163	A95
	M509	K439	E304	P232	Q164	N96
	I510	L440	R376	E305	I165	
	P511	T441	P377	D234	Y166	
	F512	F378	V379	V235		S100
	I513	E444	F379	S236	L169	I101
	K514	E445	N380	L310	L170	N102
	R515	L446		L311		R103
		E447	L383	C312	L173	
	E519	F448	V384	K313		M105
	D520	Y449	F385	E314	P177	L106
	C521	I450	G386		N178	Q107
	G522	Q451	E387	F318	E179	
	H523		F388	L319	V180	I110
	M524	K455		D320	V181	A111
	T525	T456	E392	K321	F182	L112
	Q526	G457	A393	L322	L183	K113
		F458	E394	G323	D184	
	K529		L395	I324	D185	G116
	P530	P461	E396		C260	F117
	T531	L462	K397	V328	L261	T118
	S532	N463	N398	F329	C262	C119
	V533	W464		H330	H263	T120
	N534	Y465	B401	G331	G264	I121
	Q535	A466	T402	H332	P265	V122
	I536	N467	F403	D333	P266	T123
	L537	T468	K404	W334	E267	R194
	I538	E469	S405	A335	S268	N125
	K539	R470	F406		W269	L126
		M471	F407	V339	P270	L127
		W472	R408	N340	S271	D128
	Q542	K473	A409	N342	W272	D129
	E544	W474	S410	R341	R273	G130
			D411		Y274	D131
	VAL	K477	E412	Y346	Q275	V203
GLN		G478	T413	P347	L276	H204
ASN		L479	T414	E249	D277	R133
ASP						

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.90 Å   143.00 Å   60.00 Å 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.	Xtriage
Total number of atoms	8218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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	4
1	B	539/554 (97%)	438 (81%)	68 (13%)	33 (6%)	2	5
All	All	1020/1108 (92%)	828 (81%)	127 (12%)	65 (6%)	2	4

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 ⓘ

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 ⓘ

There are no RNA molecules 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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.