



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 03:51 pm GMT

PDB ID : 1EK2  
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE  
COMPLEXED WITH CDU INHIBITOR  
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Deposited on : 2000-03-06  
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

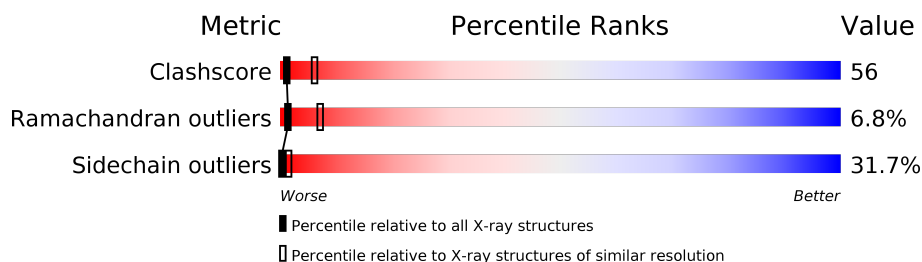
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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 [i](#)

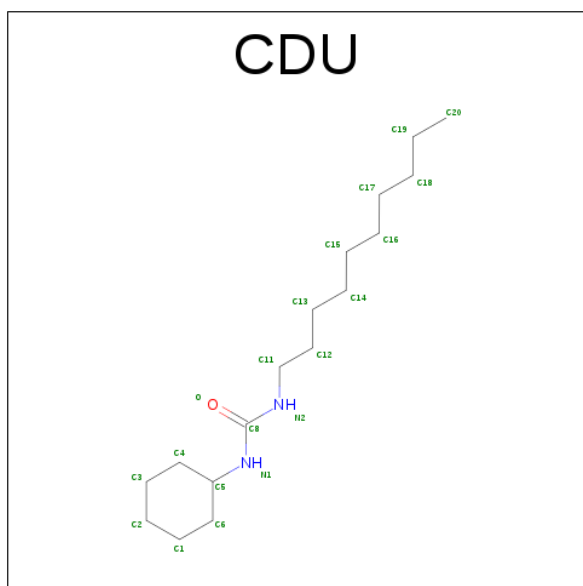
There are 3 unique types of molecules in this entry. The entry contains 8237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-CYCLOHEXYL-N'-DECYLUREA (three-letter code: CDU) (formula:  $C_{17}H_{34}N_2O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	17	2	1		
2	B	1	Total	C	N	O	0	0
			20	17	2	1		

- Molecule 3 is water.

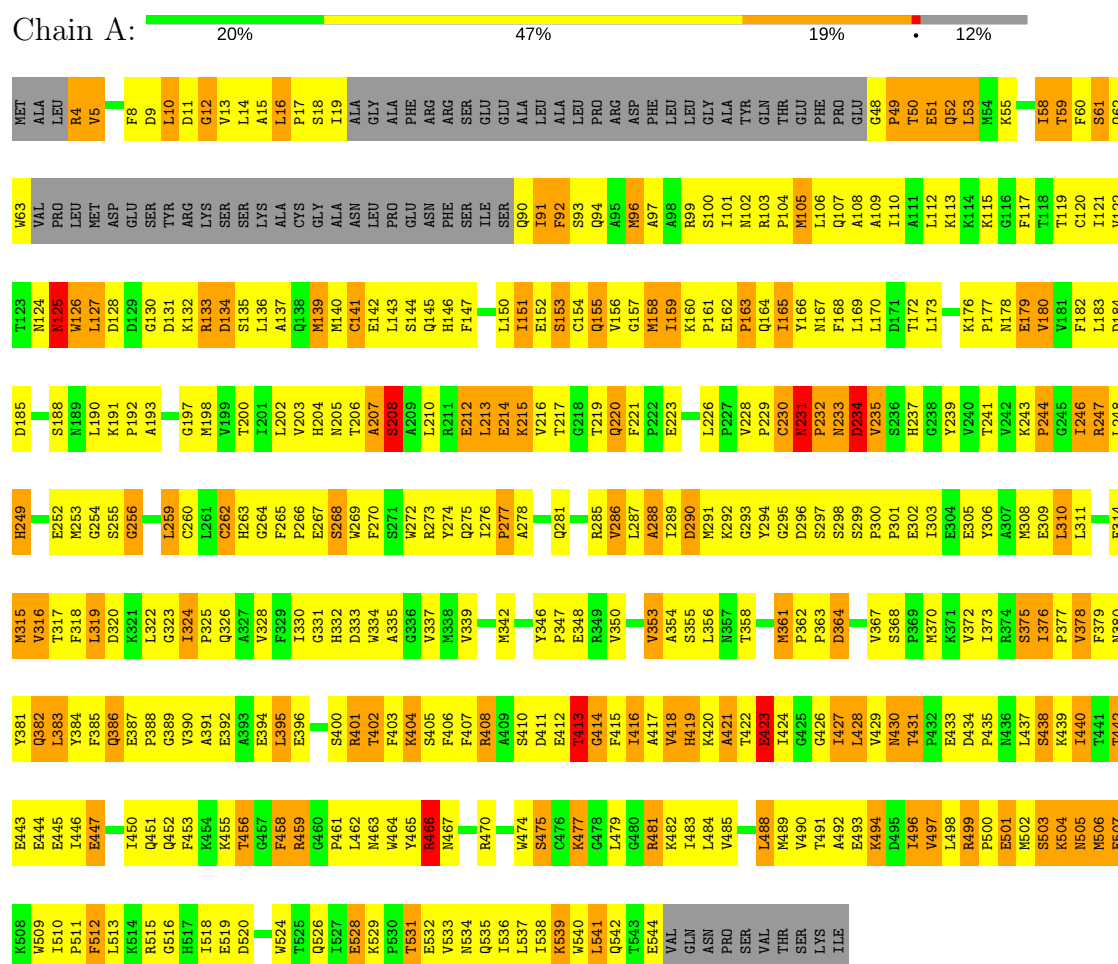
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	9	Total 9	O 9	0	0

### 3 Residue-property plots

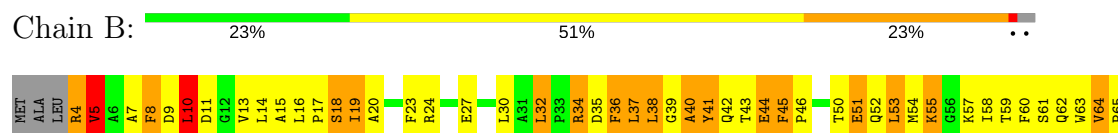
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: EPOXIDE HYDROLASE



#### • Molecule 1: EPOXIDE HYDROLASE



E519	K455	G389	G323	L259	P192	Q130	L66
D520	T456	V390	I324	C260	G197	D131	H67
H523	G457	A391	P325	L261	M198	R132	D68
H524	F458	E392	Q326	C262	G199	R133	E69
T525	R459	L395	A327	H263	T200	D134	S70
Q526	G460	E396	F328	Q264	L201	S135	Y71
I527	P461	S400	I330	F265	L202	L136	R72
E528	L462	R401	G331	P266	G203	A137	K73
K529	M463	T402	H332	E267	N204	Q138	S74
F530	Y464	F403	D333	S268	N205	M139	S75
T531	Y465	R404	K334	W269	T206	K76	A77
E532	R466	K404	F335	F270	A207	L143	C78
E533	M467	S405	A336	S271	S208	S144	
N534	R470	F406	G336	W272	A209	Q145	
Q535	L474	F407	V337	R273	L210	H146	L82
I536	Y475	R408	K338	Y274	R211	P83	P83
I537	S476	A409	V339	Q275	E212	D148	E84
I538	C476	S410	K342	I276	L213	F149	N85
K539	K477	D411		P277	L150	L150	F86
W540	G478	E412	Y346	A278	I151	I151	S87
L541	L479	T413	P347	Q281	E152	E152	I88
Q542	G480	G414	E348	V216	S153	S153	S89
T543	R481	F415	K349	T217	C154	Q90	Q90
E544	K482	I416	V350	R285	G218	Y155	I91
VAL	L483	A417		V286	T219	V156	
GLN	L484	V418	V353	L287	Q220	G157	Q84
ASN	Y485	H419	A354	A288	F221	M158	A95
PRO		K420	S355	I289	P222	I159	N96
SER	L488	A421	L356	D290		K160	
VAL	M489	T422	K357	M291	P225	P161	R99
THR	V490	E423	T358	K292	L226	E162	S100
SER	T491	I424		Q293	P227	P163	I101
LYS	A492	G425	K361	G295	Y228	Q164	N102
ILE	E493	G426	P362	D296	P229	I165	R103
	K494	I427	P363	S297	C230	Y166	P104
	D495	L428	D364	S298	N231	M167	M105
	L496	V429		P232	P231	F168	L106
	V497	M430	V367	S299	N233	L169	Q107
	L498	T431	S368	P300	D234	L170	A108
	R499	P432	P369	P301	V235	D171	A109
	P500	E433	K370	E302	S236	T172	I110
	E501	L437	K371	I303	H237	L173	A111
	M502		V372	E304	G238	K174	L112
	S503	S438	I373	E305	Y239	A176	K113
	K504	K439	K374	Y306	V240	K176	K114
	N505	I440	S375	A307	T241	P177	K115
	M506	T441	I376	M308	V242	N178	G116
	E507	T442	V377	E309	E179	E179	F117
	V508	E443	V378	L310	P244	V180	T118
	W509	E444	F379	L311	G245	V181	T119
	I510	E445	N380		I246	F182	C120
	P511	I446	Y381	E314	R247	L183	I121
	F512	E447	Q382	M315	L248	D184	V122
	L513		L383	V316	H249	D185	T123
	V514	I450	Y384	T317		F186	N124
	R515	Q451	F385	F318	W253	G187	N125
	G516	Q452	Q386	L319	G254	S188	V126
	H517	F453	E387	D320	S255	M189	L127
	I518	K454	P388	K321	G256	L190	D128
				L322		D129	

## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	151.90Å 143.00Å 60.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.211 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

## 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: CDU

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	0.43	0/3981	0.64	0/5397
1	B	0.42	0/4413	0.61	0/5984
All	All	0.42	0/8394	0.62	0/11381

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	A	3879	0	3863	431	0
1	B	4299	0	4270	485	0
2	A	20	0	34	5	0
2	B	20	0	34	1	0
3	A	10	0	0	0	0
3	B	9	0	0	1	0
All	All	8237	0	8201	893	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 56.

The worst 5 of 893 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:16:LEU:HG	1:B:17:PRO:HA	1.29	1.10
1:A:484:LEU:HD13	1:B:61:SER:HB2	1.37	1.06
1:A:348:GLU:HA	1:B:133:ARG:HG3	1.37	1.01
1:A:122:VAL:HG22	1:A:151:ILE:HG13	1.44	1.00
1:B:122:VAL:HG22	1:B:151:ILE:HG13	1.46	0.95

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%)	350 (73%)	98 (20%)	33 (7%)	1	7
1	B	539/554 (97%)	393 (73%)	110 (20%)	36 (7%)	1	7
All	All	1020/1108 (92%)	743 (73%)	208 (20%)	69 (7%)	1	7

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	61	SER
1	A	207	ALA
1	A	231	ASN
1	A	232	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	424/480 (88%)	293 (69%)	131 (31%)	0	1
1	B	468/480 (98%)	316 (68%)	152 (32%)	0	1
All	All	892/960 (93%)	609 (68%)	283 (32%)	0	1

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	541	LEU
1	B	96	MET
1	B	481	ARG
1	B	4	ARG
1	B	53	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	517	HIS
1	B	107	GLN
1	B	419	HIS
1	B	85	ASN
1	B	146	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	CDU	A	1100	-	20,20,20	1.79	7 (35%)	22,22,22	2.08	4 (18%)
2	CDU	B	1200	-	20,20,20	1.79	7 (35%)	22,22,22	2.09	4 (18%)

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	CDU	A	1100	-	-	0/15/23/23	0/1/1/1
2	CDU	B	1200	-	-	0/15/23/23	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CDU	C3-C2	2.01	1.59	1.51
2	A	1100	CDU	C3-C2	2.02	1.59	1.51
2	A	1100	CDU	C2-C1	2.06	1.59	1.51
2	B	1200	CDU	C2-C1	2.07	1.59	1.51
2	B	1200	CDU	C1-C6	2.50	1.59	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	CDU	O-C8-N2	-4.27	114.84	122.62
2	A	1100	CDU	O-C8-N2	-4.27	114.84	122.62
2	B	1200	CDU	O-C8-N1	-3.57	115.77	122.61
2	A	1100	CDU	O-C8-N1	-3.53	115.84	122.61
2	A	1100	CDU	C5-N1-C8	4.83	131.85	123.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CDU	5	0
2	B	1200	CDU	1	0

## 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.