



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:13 PM GMT

PDB ID : 1EK1
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE
COMPLEXED WITH CIU INHIBITOR
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Deposited on : 2000-03-06
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/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
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

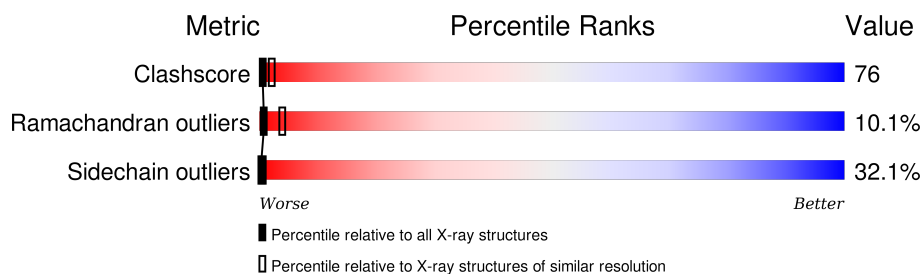
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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. 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](#)

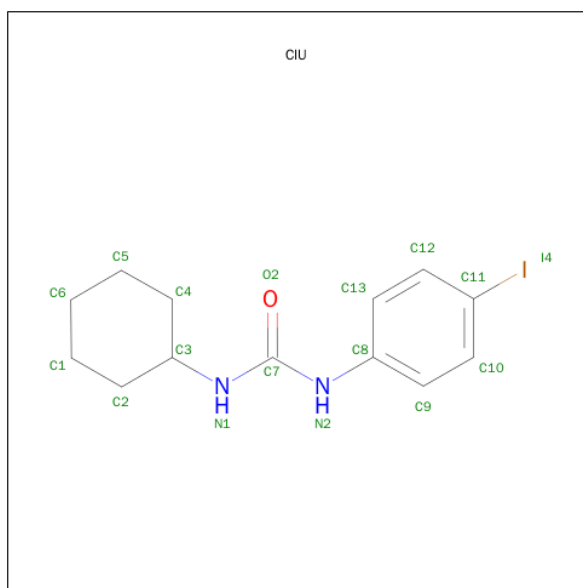
There are 3 unique types of molecules in this entry. The entry contains 8255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	490	Total	C	N	O	S	61	0	0
			3901	2517	651	704	29			
1	B	541	Total	C	N	O	S	71	0	0
			4299	2766	719	783	31			

- Molecule 2 is N-CYCLOHEXYL-N'-(4-IODOPHENYL)UREA (three-letter code: CIU) (formula: C₁₃H₁₇IN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	0	0
			17	13	1	2	1		
2	B	1	Total	C	I	N	O	0	0
			17	13	1	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	17	Total 17	O 17	0	0

D495	P432	P369	A307	P244	D184	T123	K62
I496	E433	M370	P508	G245	D185	M124	M63
Y497	D434	K371	E309	I246	F186	M125	V64
L498	P435	V372	L310	R247	G187	L126	P65
R499	M436	I373	L311	L248	S188	L127	L66
P500	L437	K374	G312	H249	N189	D128	M67
E501	S438	S375	R313	F250	L190	D129	D68
M502	K439	I376	E314	V251	K191	G130	E69
S503	T440	P377	K315	E252	P192	D131	S70
K504	T441	V378	V316	M253	A193	K132	Y71
M505	T442	F379	T317	G254	R194	R133	K72
M506		N360	F318	S255	D195	D134	K73
E507	E445	Y381	L319	G256	M196	S135	S74
K508	I446	Q382	D320		G197	L136	S75
M509	E447	L383	K321	L299	M198	A137	K76
L510	F448	Y384	L322		Y199	Q138	A77
P511	Y449	F385	G323	H263	T200	M139	G78
F512	L450	Q386	L324	G264	T201	M140	G79
Q451	Q451	E387	P325	F265	L202	C141	A80
L513	Q452	P388	Q326	P266	V203	E142	L82
K514	F453	G389	A327	E267	H204	L143	P83
M515	K454	V390	F328	S268	T205	Q144	E84
G516	K455		V329	W269	T206	Q145	P85
			I330	F270	A207	H146	N85
G521	T456	L395	G331	S271	S208	F147	F86
G522	G457	E396	H332	W272	A209	D148	S87
H523	P458	K397	D333	R273	L210	F149	I88
W524	R459	N398	L334	Y274	R211	L150	S89
T525	G460	M399	G336	Q275	E212	I151	Q90
Q526	P461	S400	A335	I276	L213	E152	I91
I527	L462	R401	G336	P277	E214	S153	F92
E528	M463	T402	V337	A278	K215	C154	S93
K529	W464	F403	G338	L279	V216	Q155	Q94
P530	T465	K404	V339	A280	T217	V156	
T531	R466	F406	K340	Q281	G218	G157	Y96
E532	M467	F407	K341	A282	T219	M158	
V533	T468	R408	A343	G283	Q220	I159	R99
N534	E469	A409	K345	F284	F221	K160	S100
Q535	R470	S410	L344	R285	P222	P161	I101
I536	M471	D411		V286	E223	E162	M102
L537	W472	E412	P347	L287	A224	P163	R103
F538	K473	E413	E348	A288	P225	Q164	P104
K539	W474	G414	K349	I289	L226	I165	M105
S475	S475	G415	V350	D290	P227	L166	L106
C476	K477	I416	A352	M291	V228	M167	Q107
K478	G478	A417	V353	K292	P229	F168	A108
E544	L479	H418	A354	G293	C230	L169	A109
	G480	H419	S355	Y294	N231	I110	I110
VAL	R481	K420	L356	G295	P232	A111	A111
GLN	K482	A421	N357	D296	N233	L112	L112
ASN	L483	T422	T358	S297	D234	K174	K113
PRO	I484	E423	P359	S298	V235	A175	K114
SER		I424	F360	S299	S236	K176	K115
VAL		G425	P361	P300	H237	P177	G116
THR	L488	G426	P362	F301	G238	N178	F117
SER	M489	I427	P363	E302	Y239	E179	T118
LYS	W490	L428	B364	I303	V240	V180	T119
ILE	T491	V429		E304	T241	F181	C120
	A492	N430	V367	E305	V242	F182	C121
	E493	T431	S368		Y306	L183	V122

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, α , β , γ	151.90 Å 143.00 Å 60.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8255	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CIU

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	0.77	1/4004 (0.0%)	0.95	11/5430 (0.2%)
1	B	0.77	0/4413	0.96	11/5984 (0.2%)
All	All	0.77	1/8417 (0.0%)	0.96	22/11414 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	CYS	CB-SG	5.35	1.91	1.82

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ASN	C-N-CD	-12.52	93.07	120.60
1	B	231	ASN	C-N-CA	7.61	153.97	122.00
1	A	218	GLY	N-CA-C	-6.85	95.98	113.10
1	B	66	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	231	ASN	N-CA-C	5.82	126.72	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3901	0	3890	581	0
1	B	4299	0	4270	676	0
2	A	17	0	17	2	0
2	B	17	0	17	5	0
3	A	4	0	0	0	0
3	B	17	0	0	5	0
All	All	8255	0	8194	1220	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 76.

The worst 5 of 1220 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:293:GLY:HA2	1:A:299:SER:HB2	1.33	1.10
1:B:141:CYS:O	1:B:144:SER:HB3	1.52	1.10
1:B:61:SER:O	1:B:64:VAL:HG23	1.51	1.09
1:B:223:GLU:H	1:B:223:GLU:CD	1.53	1.08
1:B:183:LEU:HD23	1:B:201:ILE:HD12	1.31	1.08

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	484/554 (87%)	345 (71%)	90 (19%)	49 (10%)	1	4
1	B	539/554 (97%)	384 (71%)	101 (19%)	54 (10%)	1	4
All	All	1023/1108 (92%)	729 (71%)	191 (19%)	103 (10%)	1	4

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	18	SER
1	A	63	TRP
1	A	65	PRO
1	A	91	ILE

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	427/480 (89%)	291 (68%)	136 (32%)	0	0
1	B	468/480 (98%)	317 (68%)	151 (32%)	0	0
All	All	895/960 (93%)	608 (68%)	287 (32%)	0	0

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	ARG
1	B	73	LYS
1	B	459	ARG
1	A	531	THR
1	B	43	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	B	146	HIS
1	B	463	ASN
1	A	526	GLN
1	B	94	GLN

5.3.3 RNA ⓘ

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](#)

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	CIU	A	1100	-	18,18,18	2.71	10 (55%)	23,23,23	1.83	4 (17%)
2	CIU	B	1200	-	18,18,18	2.72	11 (61%)	23,23,23	1.83	4 (17%)

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	CIU	A	1100	-	-	0/8/16/16	0/2/2/2
2	CIU	B	1200	-	-	0/8/16/16	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CIU	C7-N2	-2.44	1.33	1.37
2	A	1100	CIU	C7-N2	-2.43	1.33	1.37
2	B	1200	CIU	C7-N1	-2.01	1.30	1.35
2	B	1200	CIU	C10-C11	2.29	1.44	1.38
2	A	1100	CIU	C10-C11	2.32	1.44	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1100	CIU	O2-C7-N1	-3.39	114.34	122.76
2	B	1200	CIU	O2-C7-N1	-3.37	114.38	122.76
2	B	1200	CIU	C3-N1-C7	2.32	129.24	123.28
2	A	1100	CIU	C3-N1-C7	2.33	129.27	123.28
2	A	1100	CIU	N2-C7-N1	4.67	121.24	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CIU	2	0
2	B	1200	CIU	5	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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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