



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:01 pm GMT

PDB ID : 1CR6
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE
COMPLEXED WITH CPU INHIBITOR
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Deposited on : 1999-08-13
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

<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	:	1.7.2 (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

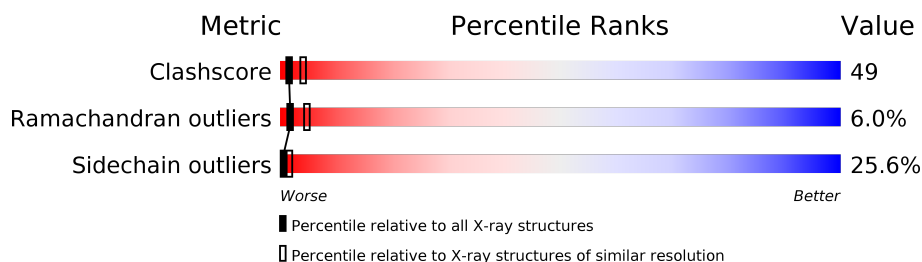
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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. 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](#)

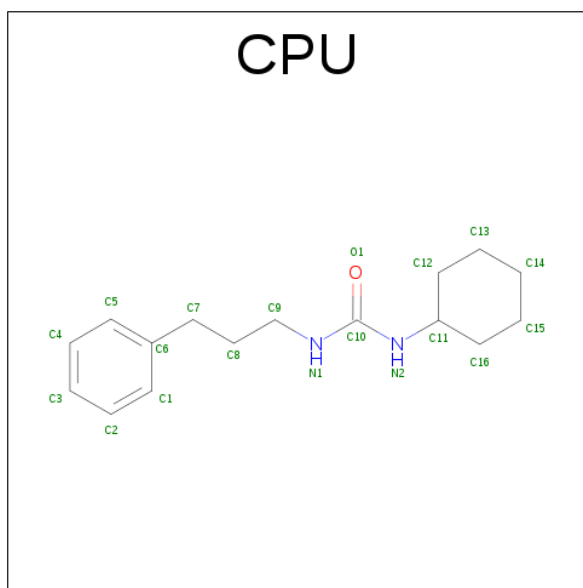
There are 3 unique types of molecules in this entry. The entry contains 8237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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'-(PROPYL)PHENYL UREA (three-letter code: CPU) (formula: $C_{16}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	16	2	1		
2	B	1	Total	C	N	O	0	0
			19	16	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	9	Total 9	O 9	0	0

Q535	W471	T402	G323	L259	L190	N125	W63
I536	W472	F403	I324	L259	K191	N126	P64
L537	K473	F404	P325	G262	P192	L127	P65
I538	W474	K404	V328	H263	A193	D128	L66
K639	W475	S405	F329	G264	K194	D129	M67
	G476	F406		P265	B195	G130	D68
	K477	R407		P266	M196	D131	E69
	G478	R408		H332	G197	L132	S70
	L479	F409		D333	M198	R133	Y71
	G480	E412		W334	V199	D134	R72
	R481	T413		V337	T200	S135	K73
	K482	G414		V337	L201	L136	S74
	L483	F415		M338	S271	A137	S75
	L484	L416		V339	W272	W203	K76
	V485	A417		R273	H204	Q138	A77
		V418		M342	N205	M139	C78
		H419		G274	T206	M140	G79
	L488	K420		Q275	A207		A80
	K489	K420		L276	S208		N81
	V490	A421		P277	A209	Q145	L82
	T491	T422		A278	S209	H146	P83
		E423		L279	L210	D147	E84
	K494	I424		V350	R211	D148	
	G495	G425		G281	E212	F149	N85
	L496	G426			L213	L150	F86
	V497	I427		P284	E214	I151	S87
	L498	L428		R285	K215	E152	I88
	R499	V429		L286	V216	S153	S89
	F500	N430		L356	T217	Q154	Q90
	E501	T431		N357	G218	Q155	I91
	M502	P432		T358	L289	V156	F92
	S503	E433		P360	D290	G157	S93
	K504	D434		M361	F221	M158	Q94
	N505	P435		P362	K292	I159	A95
				P363	E223	K160	M96
				D364	E294	P163	
	S438			G295	A294	E162	R99
	K439			D296	P225	P163	S100
	L440			P366		P163	I101
	T441			S367	V228	Q164	N102
				S368	P229	I165	R103
	L446			P369	S299	V166	P104
	E447			M370	C230	N167	M105
	F448			K371	P232		L106
	H515			E302	D233	L170	Q107
	G516			I373	D234	D171	A108
	H517			E304	V235	T172	I109
				S375	E305	L173	I110
	T456			V376	H237	K174	I111
	G457			A307	G238	A175	L112
	F458			M308		K176	
	W524			E309	K243	P177	K115
	T525			F379	L310	P244	G116
	Q526			N380	L311	G245	F117
	L527			V381	L312	L246	I181
	E528			Q382	K312	R247	T118
				L383	K313	F182	I119
	M529			E314	L248	L183	C120
				M315	H249		I121
	F530				F250	F186	I122
	T531			D320	G170	G187	V121
	E532			E396	K370	S188	T123
	V533			K397	L371	S255	N124
	N534			N398	L372	G256	

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, 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)	91.0 (20.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.201 , 0.312	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8237	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: CPU

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	0.60	0/3981	0.79	1/5397 (0.0%)
1	B	0.60	0/4413	0.80	3/5984 (0.1%)
All	All	0.60	0/8394	0.80	4/11381 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ASN	C-N-CD	-11.76	94.72	120.60
1	B	231	ASN	C-N-CA	7.25	152.46	122.00
1	A	488	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	488	LEU	CA-CB-CG	5.32	127.53	115.30

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	370	0
1	B	4299	0	4270	434	0
2	A	19	0	24	5	0
2	B	19	0	24	5	0
3	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	0	0	0
All	All	8237	0	8181	786	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 49.

The worst 5 of 786 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:232:PRO:HD2	1:B:233:ASN:H	1.11	1.11
1:B:5:VAL:HG21	1:B:173:LEU:HD21	1.35	1.08
1:A:101:ILE:HG21	1:A:106:LEU:HD12	1.38	1.06
1:B:300:PRO:HG2	1:B:305:GLU:HG2	1.36	1.05
1:B:496:ILE:H	1:B:496:ILE:HD12	1.19	1.04

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%)	392 (82%)	59 (12%)	30 (6%)	2	4
1	B	539/554 (97%)	431 (80%)	77 (14%)	31 (6%)	2	5
All	All	1020/1108 (92%)	823 (81%)	136 (13%)	61 (6%)	2	5

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	207	ALA
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	244	PRO
1	A	256	GLY

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%)	322 (76%)	102 (24%)	1	2
1	B	468/480 (98%)	342 (73%)	126 (27%)	0	1
All	All	892/960 (93%)	664 (74%)	228 (26%)	0	2

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	VAL
1	B	78	CYS
1	B	475	SER
1	B	13	VAL
1	B	43	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	ASN
1	B	90	GLN
1	B	281	GLN
1	A	517	HIS
1	A	146	HIS

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	CPU	A	1100	-	20,20,20	1.78	8 (40%)	23,24,24	1.40	3 (13%)
2	CPU	B	1200	-	20,20,20	1.94	10 (50%)	23,24,24	1.69	5 (21%)

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	CPU	A	1100	-	-	0/11/19/19	0/2/2/2
2	CPU	B	1200	-	-	0/11/19/19	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CPU	C15-C16	2.03	1.58	1.53
2	A	1100	CPU	C14-C13	2.05	1.59	1.51
2	B	1200	CPU	C5-C6	2.07	1.43	1.38
2	A	1100	CPU	C4-C3	2.08	1.43	1.38
2	B	1200	CPU	C3-C2	2.10	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	CPU	O1-C10-N1	-3.88	115.55	122.62
2	A	1100	CPU	O1-C10-N1	-3.60	116.06	122.62
2	B	1200	CPU	N1-C10-N2	2.03	121.07	115.83
2	B	1200	CPU	C8-C7-C6	2.18	121.85	113.67
2	A	1100	CPU	N1-C10-N2	2.25	121.64	115.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	CPU	5	0
2	B	1200	CPU	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 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.