



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:55 PM UTC

PDB ID : 1CR6 / pdb_00001cr6
Title : CRYSTAL STRUCTURE OF MURINE SOLUBLE EPOXIDE HYDROLASE
COMPLEXED WITH CPU INHIBITOR
Authors : Argiriadi, M.A.; Morisseau, C.; Hammock, B.D.; Christianson, D.W.
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

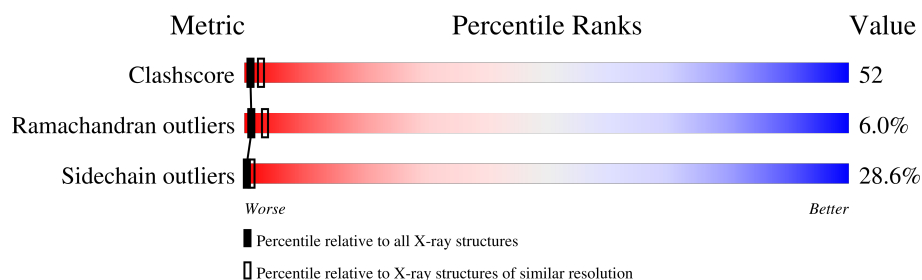
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

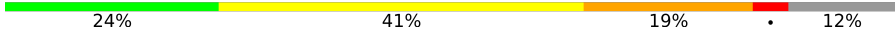
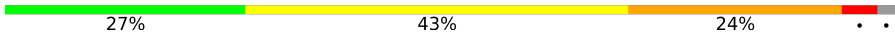
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of 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 [i](#)

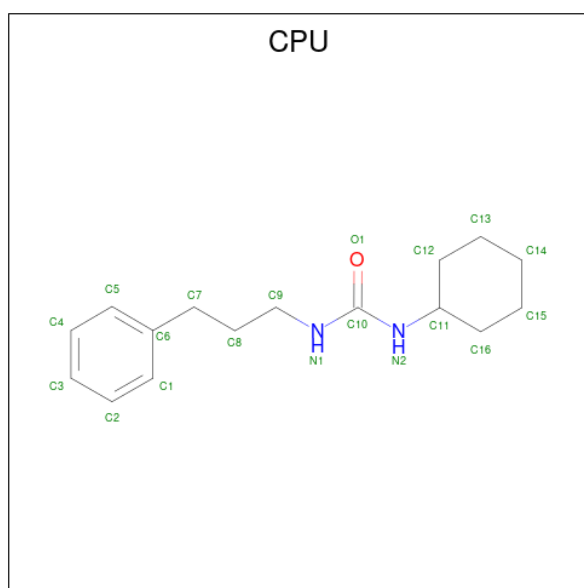
There are 3 unique types of molecules in this entry. The entry contains 8237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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.

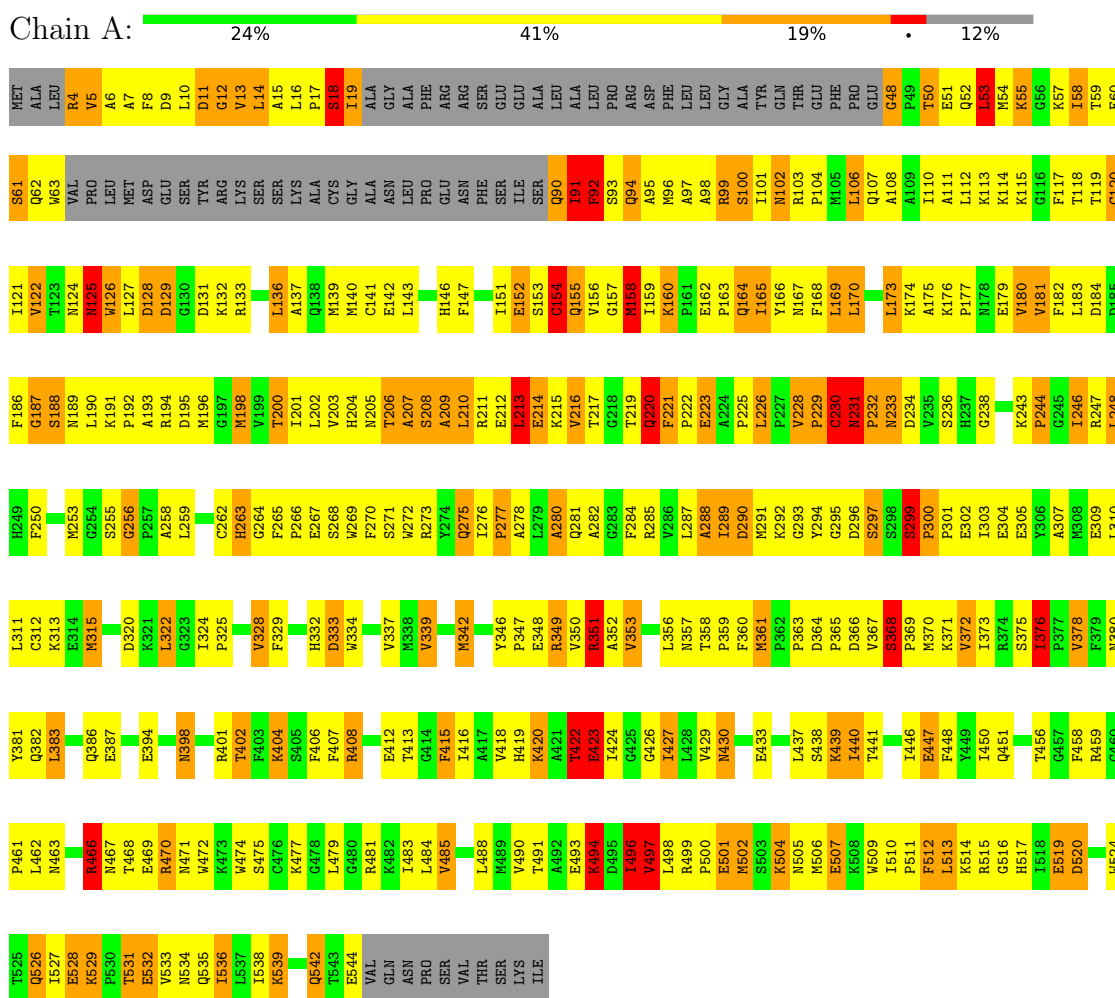
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	9	Total 9	O 9	0	0

3 Residue-property plots

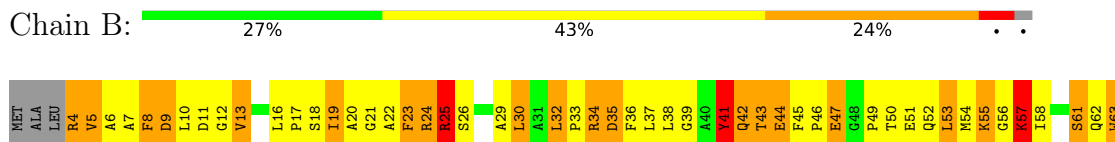
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



W524	R459	G460	P461	L462	N463	R466	N467	T468	E469	R470	N471	W472	K473	W474	S475	C476	K477	G478	L479	L488	M489	V490	T491	K494	D495	T496	Y497	L498	P499	P500	E501	M502	S503	K504	N505	M506	E507	W509	T510	P511	F512	L513	K514	R515	G516	H517	T518	E519	D520															
	Q382	L383	Q386	E387	E396	K397	N398	R401	T402	F403	K404	S405	F406	F407	R408	E412	T413	G414	F415	T416	A417	V418	H419	K420	G421	A422	T423	E424	G425	G426	T427	L428	V429	M430	T431	P432	E433	D434	P435	M436	L437	S438	K439	T440	T441	I446	E447	F448	Y449	I450	Q451	T456	G457	F458										
	C312	K313	E314	N315	D320	K321	L322	G323	I324	P325	V328	F329	H332	D333	W334	V337	N338	V339	M342	Y346	F347	E348	R349	V350	K351	A352	V353	L356	N357	T358	P359	F360	M361	P362	P363	D364	P365	D366	V367	P368	P369	M370	K371	V372	I373	R374	S375	K376	P377	Q378	T456	N380	Y381											
	F250	M253	G254	S255	G256	P257	A258	L259	C262	H263	G264	P265	P266	E267	S268	W269	F270	S271	W272	R273	Y274	Q275	E276	P277	A278	L279	K280	Q281	V282	G283	F284	R285	V286	L287	A288	I289	D290	M291	K292	G293	Y294	G295	D296	S297	S298	S299	P300	P301	E302	I303	E304	E305	Y306	A307	K308	E309	L310	L311						
	G187	S188	N189	L190	K191	G192	A193	R194	D195	M196	G197	M198	V199	T200	I201	L202	V203	H204	N205	T206	A207	S208	A209	L210	E211	E212	L213	E214	S215	V216	T217	G218	T219	Q220	F221	P222	E223	A224	P225	L226	V227	V228	P229	C230	N231	P232	V233	D234	V235	S236	H237	G238	K243	P244	G245	I246	R247	L248	H249					
	N125	W126	L127	D128	D129	G130	D131	K132	R133	D134	S135	L136	A137	Q138	M139	M140	C141	E142	L143	S144	Q145	H146	F147	D148	F149	L150	I151	E152	S153	C154	Q155	V156	G157	M158	I159	K160	P161	E162	P163	I164	M165	Y166	N167	F168	L169	L170	D171	L172	L173	K174	A175	K176	P177	T178	T179	V180	G181	F182	L183	F186				
	V64	P65	L66	M67	D68	E69	S70	Y71	R72	K73	S74	S75	K76	A77	G78	G79	A80	N81	L82	P83	E84	N85	F86	S87	I88	S89	Q90	I91	F92	S93	Q94	A95	M96	R99	S100	I101	N102	R103	P104	M105	L106	Q107	A108	A109	I110	A111	L112	K113	K114	K115	G116	F117	T118	C120	I121	V122	T123	N124						
	W524	R459	G460	P461	L462	N463	R466	N467	T468	E469	R470	N471	W472	K473	W474	S475	C476	K477	G478	L479	L488	M489	V490	T491	K494	D495	T496	Y497	L498	P499	P500	E501	M502	S503	K504	N505	M506	E507	W509	T510	P511	F512	L513	K514	R515	G516	H517	T518	E519	D520														
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C312		K313	E314	N315	D320	K321	L322	G323	I324	P325	V328	F329	H332	D333	W334	V337	N338	V339	M342	Y346	F347	E348	R349	V350	K351	A352	V353	L356	N357	T358	P359	F360	M361	P362	P363	D364	P365	D366	V367	P368	P369	M370	K371	V372	I373	R374	S375	K376	P377	Q378	T456	N380	Y381											
F250		M253	G254	S255	G256	P257	A258	L259	C262	H263	G264	P265	P266	E267	S268	W269	F270	S271	W272	R273	Y274	Q275	E276	P277	A278	L279	K280	Q281	V282	G283	F284	R285	V286	L287	A288	I289	D290	M291	K292	G293	Y294	G295	D296	S297	S298	S299	P300	P301	E302	I303	E304	E305	Y306	A307	K308	E309	L310	L311						
G187		S188	N189	L190	K191	G192	A193	R194	D195	M196	G197	M198	V199	T200	I201	L202	V203	H204	N205	T206	A207	S208	A209	L210	E211	E212	L213	E214	S215	V216	T217	G218	T219	Q220	F221	P222	E223	A224	P225	L226	V227	V228	P229	C230	N231	P232	V233	D234	V235	S236	H237	G238	K243	P244	G245	I246	R247	L248	H249					
N125		W126	L127	D128	D129	G130	D131	K132	R133	D134	S135	L136	A137	Q138	M139	M140	C141	E142	L143	S144	Q145	H146	F147	D148	F149	L150	I151	E152	S153	C154	Q155	V156	G157	M158	I159	K160	P161	E162	P163	I164	M165	Y166	N167	F168	L169	L170	D171	L172	L173	K174	A175	K176	P177	T178	T179	V180	G181	F182	L183	F186				
V64		P65	L66	M67	D68	E69	S70	Y71	R72	K73	S74	S75	K76	A77	G78	G79	A80	N81	L82	P83	E84	N85	F86	S87	I88	S89	Q90	I91	F92	S93	Q94	A95	M96	R99	S100	I101	N102	R103	P104	M105	L106	Q107	A108	A109	I110	A111	L112	K113	K114	K115	G116	F117	T118	C120	I121	V122	T123	N124						
W524		R459	G460	P461	L462	N463	R466	N467	T468	E469	R470	N471	W472	K473	W474	S475	C476	K477	G478	L479	L488	M489	V490	T491	K494	D495	T496	Y497	L498	P499	P500	E501	M502	S503	K504	N505	M506	E507	W509	T510	P511	F512	L513	K514	R515	G516	H517	T518	E519	D520														
		Q382	L383	Q386	E387	E396	K397	N398	R401	T402	F403	K404	S405	F406	F407	R408	E412	T413	G414	F415	T416	A417	V418	H419	K420	G421	A422	T423	E424	G425	G426	T427	L428	V429	M430	T431	P432	E433	D434	P435	M436	L437	S438	K439	T440	T441	I446	E447	F448	Y449	I450	Q451	T456	G457	F458									
	C312	K313	E314	N315	D320	K321	L322	G323	I324	P325	V328	F329	H332	D333	W334	V337	N338	V339	M342	Y346	F347	E348	R349	V350	K351	A352	V353	L356	N357	T358	P359	F360	M361	P362	P363	D364	P365	D366	V367	P368	P369	M370	K371	V372	I373	R374	S375	K376	P377	Q378	T456	N380	Y381											
	F250	M253	G254	S255	G256	P257	A258	L259	C262	H263	G264	P265	P266	E267	S268	W269	F270	S271	W272	R273	Y274	Q275	E276	P277	A278	L279	K280	Q281	V282	G283	F284	R285	V286	L287	A288	I289	D290	M291	K292	G293	Y294	G295	D296	S297	S298	S299	P300	P301	E302	I303	E304	E305	Y306	A307	K308	E309	L310	L311						
	G187	S188	N189	L190	K191	G192	A193	R194	D195	M196	G197	M198	V199	T200	I201	L202	V203	H204	N205	T206	A207	S208	A209	L210	E211	E212	L213	E214	S215	V216	T217	G218	T219	Q220	F221	P222	E223	A224	P225	L226	V227	V228	P229	C230	N231	P232	V233	D234	V235	S236	H237	G238	K243	P244	G245	I246	R247	L248	H249					
	N125	W126	L127	D128	D129	G130	D131	K132	R133	D134	S135	L136	A137	Q138	M139	M140	C141	E142	L143	S144	Q145	H146	F147	D148	F149	L150	I151	E152	S153	C154	Q155	V156	G157	M158	I159	K160	P161	E162	P163	I164	M165	Y166	N167	F168	L169	L170	D171	L172	L173	K174	A175	K176	P177	T178	T179	V180	G181	F182	L183	F186				
	V64	P65	L66	M67	D68	E69	S70	Y71	R72	K73	S74	S75	K76	A77	G78	G79	A80	N81	L82	P83	E84	N85	F86	S87	I88	S89	Q90	I91	F92	S93	Q94	A95	M96	R99	S100	I101	N102	R103	P104	M105	L106	Q107	A108	A109	I110	A111	L112	K113	K114	K115	G116	F117	T118	C120	I121	V122	T123	N124						
	W524	R459	G460	P461	L462	N463	R466	N467	T468	E469	R470	N471	W472	K473	W474	S475	C476	K477	G478	L479	L488	M489	V490	T491	K494	D495	T496	Y497	L498	P499	P500	E501	M502	S503	K504	N505	M506	E507	W509	T510	P511	F512	L513	K514	R515	G516	H517	T518	E519	D520														
		Q382	L383	Q386	E387	E396	K397	N398	R401	T402	F403	K404	S405	F406	F407	R408	E412	T413	G414	F415	T416	A417	V418	H419	K420	G421	A422	T423	E424	G425	G426	T427	L428	V429	M430	T431	P432	E433	D434	P435	M436	L437	S438	K439	T440	T441	I446	E447	F448	Y449	I450	Q451	T456	G457	F458									
C312		K313	E314	N315	D320	K321	L322	G323	I324	P325	V328	F329	H332	D333	W334	V337	N338	V339	M342	Y346	F347	E348	R349	V350	K351	A352	V353	L356	N357	T358	P359	F360	M361	P362	P363	D364	P365	D366	V367	P368	P369	M370	K371	V372	I373	R374	S375	K376	P377	Q378	T456	N380	Y381											
F250		M253	G254	S255	G256	P257	A258	L259	C262	H263	G264	P265	P266	E267	S268	W269	F270	S271	W272	R273	Y274	Q275	E276	P277	A278	L279	K280	Q281	V282	G283	F284	R285	V286	L287	A288	I289	D290	M291	K292	G293	Y294	G295	D296	S297	S298	S299	P300	P301	E302	I303	E304	E305	Y306	A307	K308	E309	L310	L311						
G187		S188	N189	L190	K191	G192	A193	R194	D195	M196	G197	M198	V199	T200	I201	L202	V203	H204	N205	T206	A207	S208	A209	L210	E211	E212	L213	E214	S215	V216	T217	G218	T219	Q220	F221	P222	E223	A224	P225	L226	V227	V228	P229	C230	N231	P232	V233	D234	V235	S236	H237	G238	K243	P244	G245	I246	R247	L248	H249					
N125		W126	L127	D128	D129	G130	D131	K132	R133	D134	S135	L136	A137	Q138	M139	M140	C141	E142	L143	S144	Q145	H146	F147	D148	F149	L150	I151	E152	S153	C154	Q155	V156	G157	M158	I159	K160	P161	E162	P163	I164	M165	Y166	N167	F168	L169	L170	D171	L172	L173	K174	A175	K176	P177	T178	T179	V180	G181	F182	L183	F186				
V64		P65	L66	M67	D68	E69	S70	Y71	R72	K73	S74	S75	K76	A77	G7																																																	

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	0.72	0/3981	1.27	60/5397 (1.1%)
1	B	0.70	0/4413	1.25	62/5984 (1.0%)
All	All	0.71	0/8394	1.26	122/11381 (1.1%)

There are no bond length outliers.

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	GLU	CA-C-N	12.31	133.10	119.93
1	A	387	GLU	C-N-CA	12.31	133.10	119.93
1	B	231	ASN	C-N-CD	-11.76	94.72	120.60
1	B	231	ASN	CA-C-N	10.61	152.46	127.00
1	B	231	ASN	C-N-CA	10.61	152.46	127.00

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	397	0
1	B	4299	0	4270	460	0
2	A	19	0	24	5	0
2	B	19	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	0	0	0
3	B	9	0	0	0	0
All	All	8237	0	8181	839	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 52.

The worst 5 of 839 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%)	1	3
1	B	539/554 (97%)	431 (80%)	77 (14%)	31 (6%)	1	4
All	All	1020/1108 (92%)	823 (81%)	136 (13%)	61 (6%)	1	3

5 of 61 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	A	231	ASN
1	A	244	PRO
1	A	256	GLY

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%)	309 (73%)	115 (27%)	0	1
1	B	468/480 (98%)	328 (70%)	140 (30%)	0	1
All	All	892/960 (93%)	637 (71%)	255 (29%)	0	1

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	ARG
1	B	422	THR
1	B	85	ASN
1	B	412	GLU
1	B	485	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	517	HIS
1	B	517	HIS
1	B	102	ASN
1	B	281	GLN
1	B	90	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 oligosaccharides 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	1.89	10 (50%)	24,24,24	1.95	4 (16%)
2	CPU	B	1200	-	20,20,20	2.04	12 (60%)	24,24,24	1.99	6 (25%)

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	-	-	5/11/19/19	0/2/2/2
2	CPU	B	1200	-	-	3/11/19/19	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CPU	C1-C6	3.91	1.46	1.38
2	A	1100	CPU	C1-C6	3.39	1.45	1.38
2	A	1100	CPU	C4-C5	3.20	1.44	1.38
2	B	1200	CPU	C4-C3	2.98	1.44	1.38
2	B	1200	CPU	C12-C11	2.57	1.57	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1100	CPU	C9-C8-C7	-6.75	100.41	113.10
2	B	1200	CPU	C9-C8-C7	-5.90	102.02	113.10
2	B	1200	CPU	O1-C10-N1	-4.03	115.55	122.47
2	A	1100	CPU	O1-C10-N1	-3.73	116.06	122.47
2	B	1200	CPU	C11-N2-C10	3.03	129.44	122.92

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

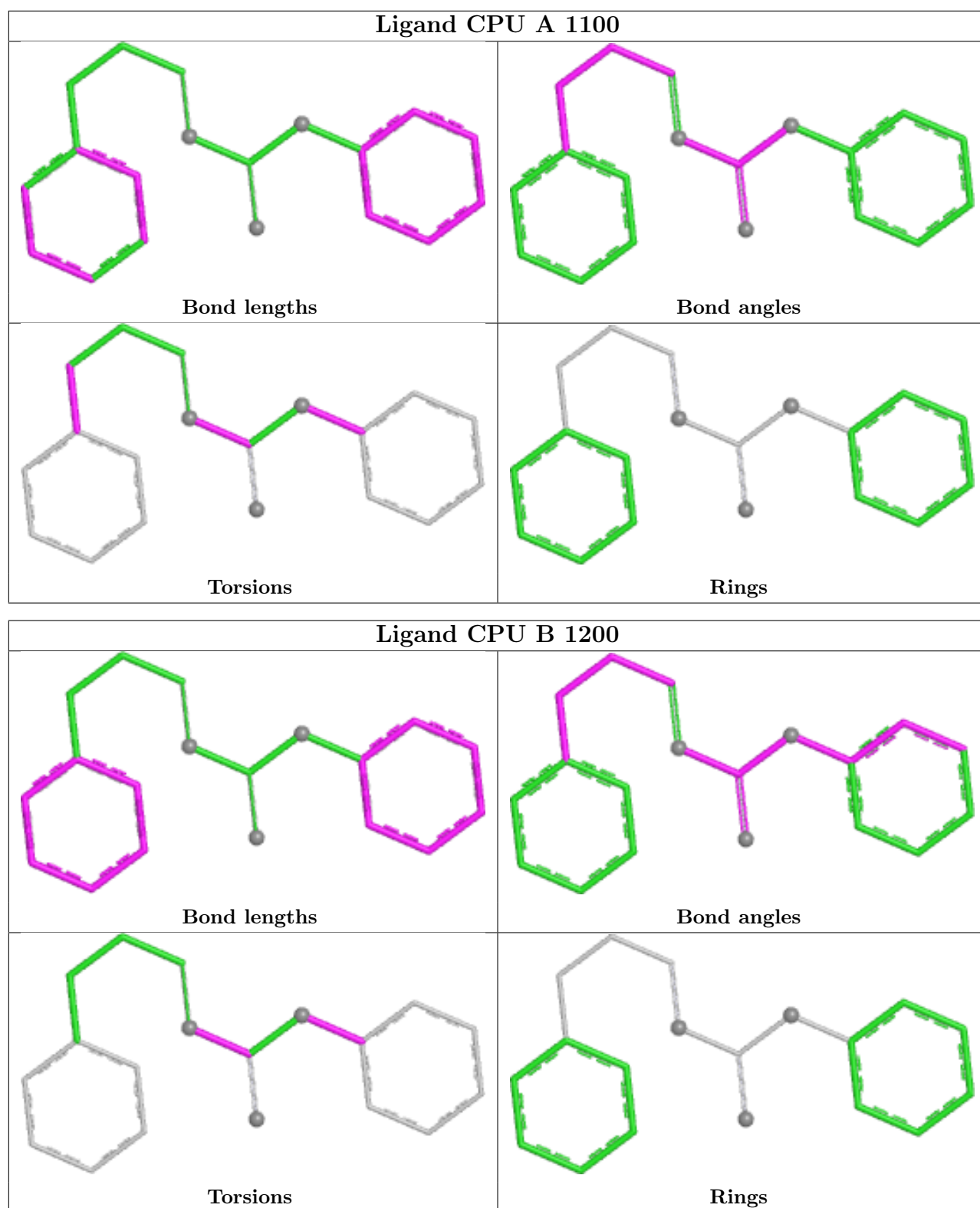
Mol	Chain	Res	Type	Atoms
2	B	1200	CPU	C16-C11-N2-C10
2	A	1100	CPU	C16-C11-N2-C10
2	A	1100	CPU	O1-C10-N1-C9
2	B	1200	CPU	O1-C10-N1-C9
2	A	1100	CPU	N2-C10-N1-C9

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.