wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 06:01 pm BST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

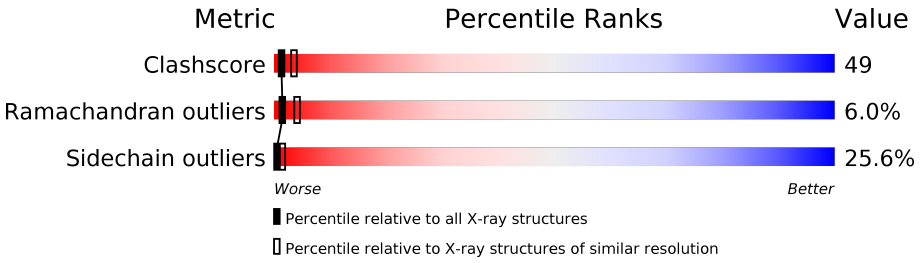
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	29% 43% 15% • 12%
1	B	554	31% 46% 20% • •

2 Entry composition

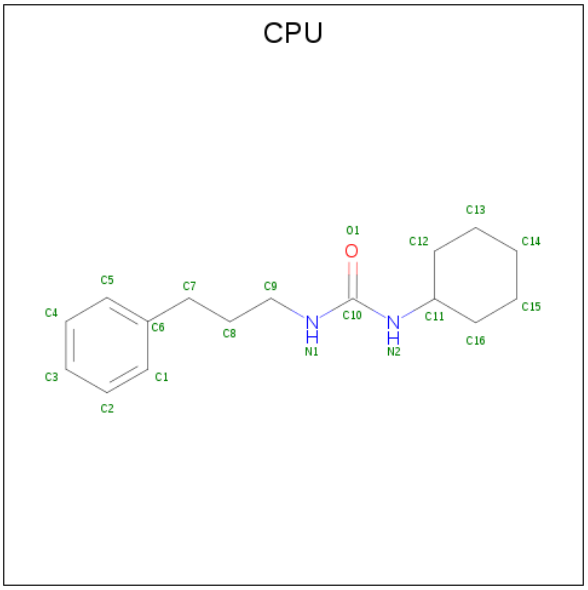
There are 3 unique types of molecules in this entry. The entry contains 8237 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O 12 12	0	0
3	B	9	Total O 9 9	0	0

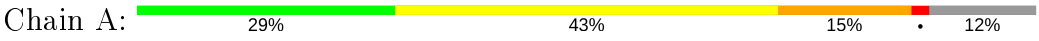
3 Residue-property plots (i)

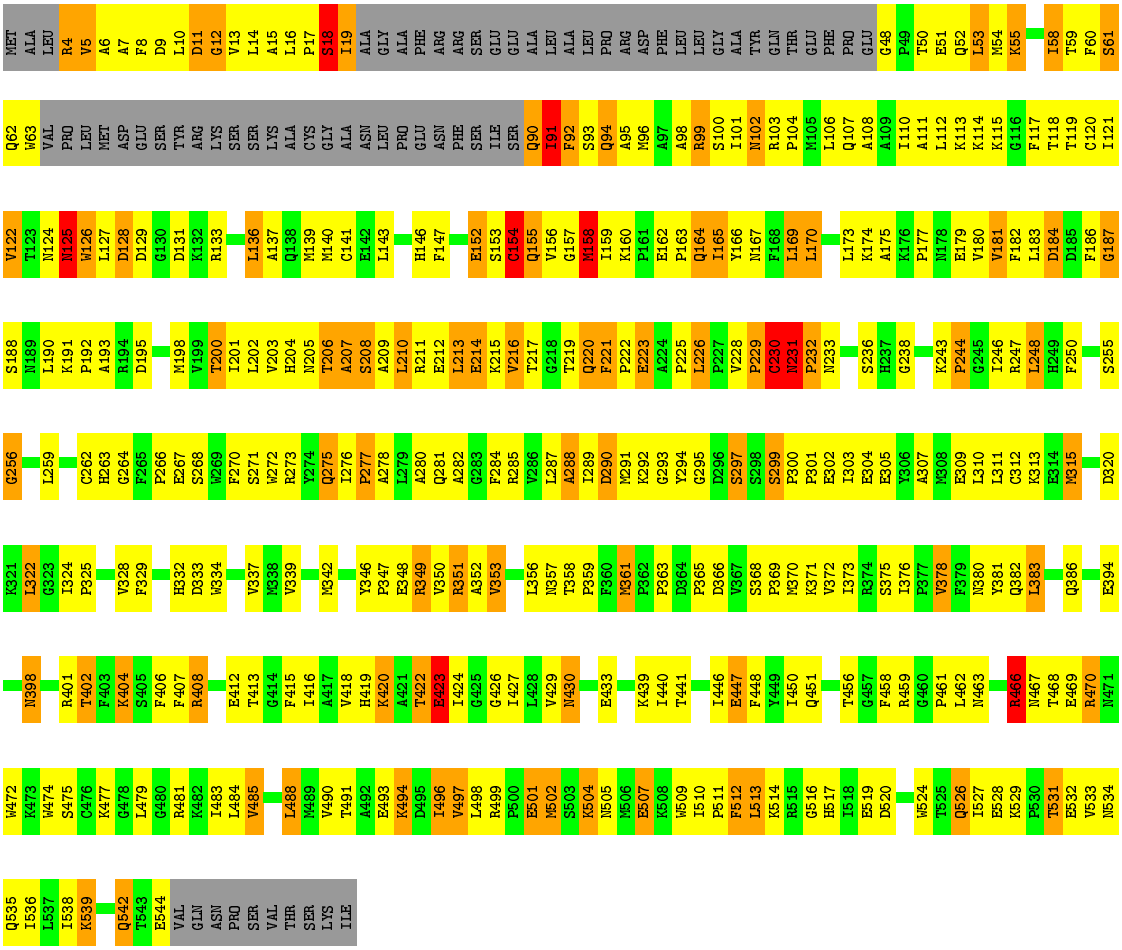
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

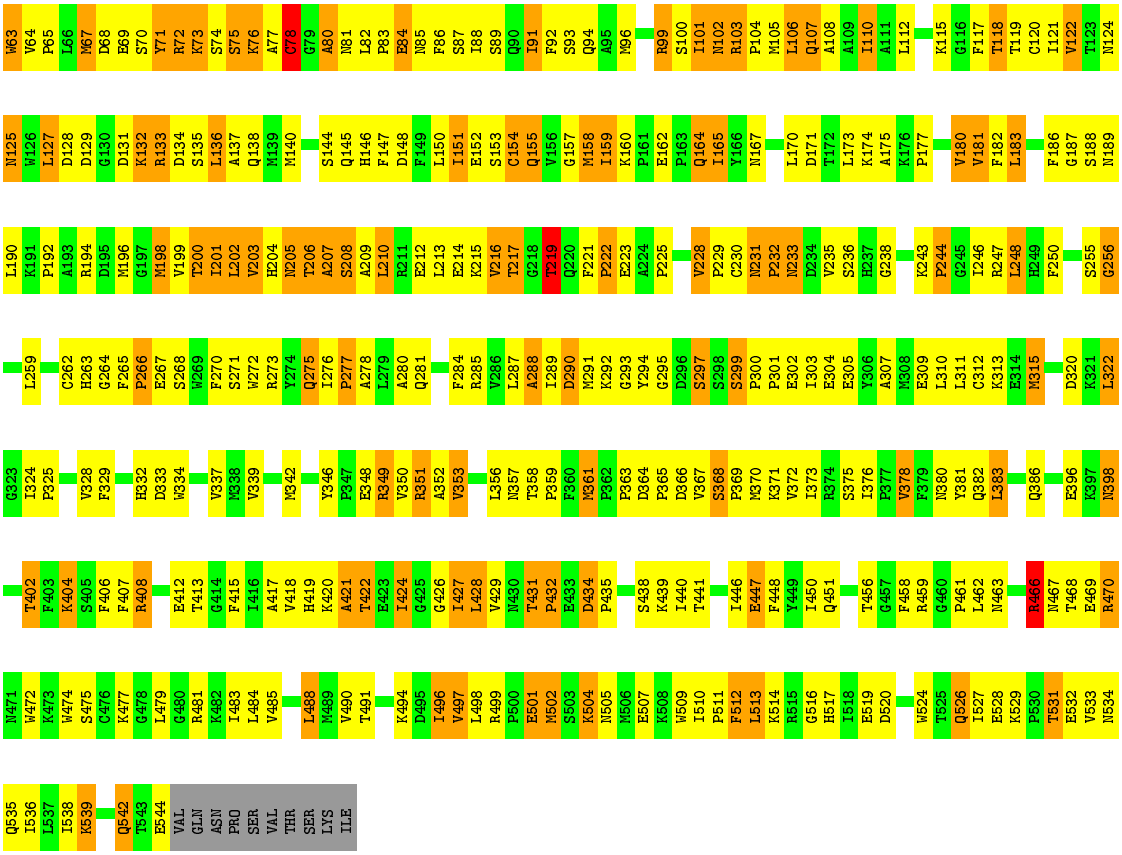
Chain A:





- Molecule 1: EPOXIDE HYDROLASE

Chain B:


W63 V64 P65 L66 M67 D68 E69 S70 Y71 R72 K73 S74 S75 K76 A77 C78 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 K115 G116 F117 T118 T119 C120 I121 V122 T123 N124
N125 W126 L127 D128 D129 G130 D131 K132 R133 D134 S135 L136 A137 Q138 M139 M140 S144 Q145 H146 F147 D148 F149 L150 I151 E152 S153 C154 Q155 Y156 G157 M158 I159 K160 P161 E162 P163 Q164 I165 Y166 N167 L170 D171 T172 L173 K174 A175 K176 P177 V180 V181 F182 L183 F186 G187 S188 N189
L190 K191 P192 A193 R194 D195 M196 G197 M198 V199 T200 I201 L202 V203 H204 N205 T206 A207 S208 A209 L210 R211 E212 L213 E214 K215 V216 T217 G218 T219 Q220 F221 P222 E223 A224 P225 V228 P229 C230 N231 P232 N233 D234 V235 S236 H237 G238 K243 P244 G245 I246 R247 L248 H249 F250 S255 G256
L259 C262 H263 G264 F265 P266 E267 S268 W269 F270 S271 W272 R273 Y274 Q275 I276 P277 A278 L279 A280 Q281 F284 R285 V286 L287 A288 I289 D290 M291 K292 G293 Y294 G295 D296 S297 S298 S299 P300 P301 E302 I303 E304 E305 Y306 A307 M308 E309 L310 L311 C312 K313 E314 M315 D320 K321 L322
G323 I324 P325 V328 F329 H332 D333 W334 V337 N338 V339 M342 Y346 P347 E348 R349 V350 R351 A352 V353 L356 N357 T358 P359 F360 M361 P362 P363 D364 P365 D366 V367 S368 P369 M370 K371 V372 I373 R374 S375 I376 P377 V378 F379 N380 Y381 Q382 L383 Q386 E396 K397 N398
T402 F403 K404 S405 F406 F407 R408 E412 T413 G414 F415 I416 A417 V418 H419 K420 A421 T422 E423 I424 G425 G426 I427 L428 V429 N430 T431 P432 E433 D434 P435 S438 K439 I440 T441 I446 E447 F448 Y449 I450 Q451 T456 G457 F458 R459 G460 P461 L462 N463 R466 N467 T468 E469 R470
N471 W472 K473 W474 S475 C476 K477 G478 L479 G480 R481 K482 I483 L484 V485 L488 M489 V490 T491 K494 D495 I496 V497 L498 R499 P500 E501 M502 S503 K504 N505 M506 E507 K508 W509 I510 P511 F512 L513 K514 R515 G516 H517 I518 E519 D520 W524 T525 Q526 I527 E528 K529 P530 T531 E532 V533 N534
Q535 I536 L537 I538 K539 Q542 T543 E544 VAL GLN ASN PRO SER VAL THR SER LYS ILE

4 Data and refinement statistics (i)

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

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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%)	1 4
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 4

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

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 (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 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	B	1200	-	20,20,20	1.90	8 (40%)	24,24,24	2.01	6 (25%)
2	CPU	A	1100	-	20,20,20	1.74	8 (40%)	24,24,24	1.97	4 (16%)

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	B	1200	-	-	3/11/19/19	0/2/2/2
2	CPU	A	1100	-	-	5/11/19/19	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	CPU	C1-C6	3.61	1.46	1.38
2	A	1100	CPU	C1-C6	3.14	1.45	1.38
2	A	1100	CPU	C4-C5	2.59	1.44	1.38
2	B	1200	CPU	C4-C3	2.56	1.44	1.38
2	B	1200	CPU	C12-C11	2.52	1.57	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1100	CPU	C9-C8-C7	-7.04	100.41	112.95
2	B	1200	CPU	C9-C8-C7	-6.14	102.02	112.95
2	B	1200	CPU	O1-C10-N1	-3.99	115.55	122.50
2	A	1100	CPU	O1-C10-N1	-3.70	116.06	122.50
2	B	1200	CPU	C11-N2-C10	3.04	129.44	123.02

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	B	1200	CPU	O1-C10-N1-C9
2	A	1100	CPU	O1-C10-N1-C9
2	B	1200	CPU	N2-C10-N1-C9

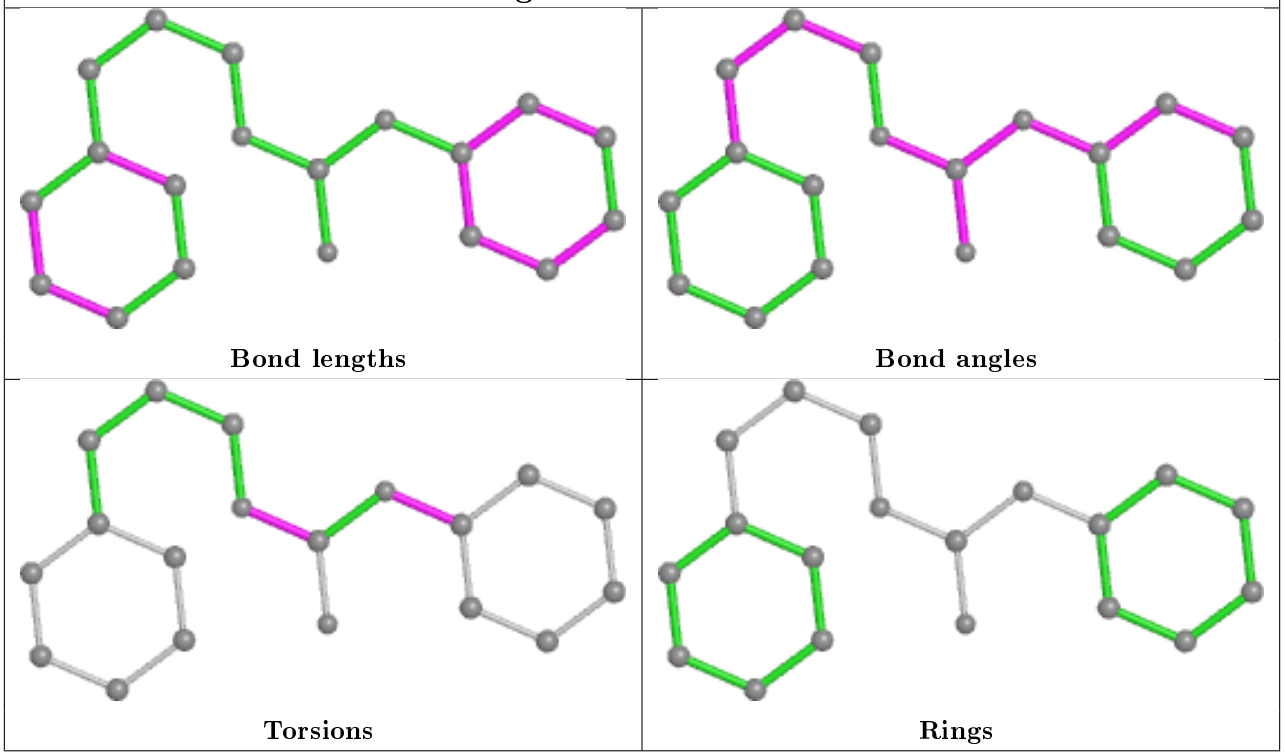
There are no ring outliers.

2 monomers are involved in 10 short contacts:

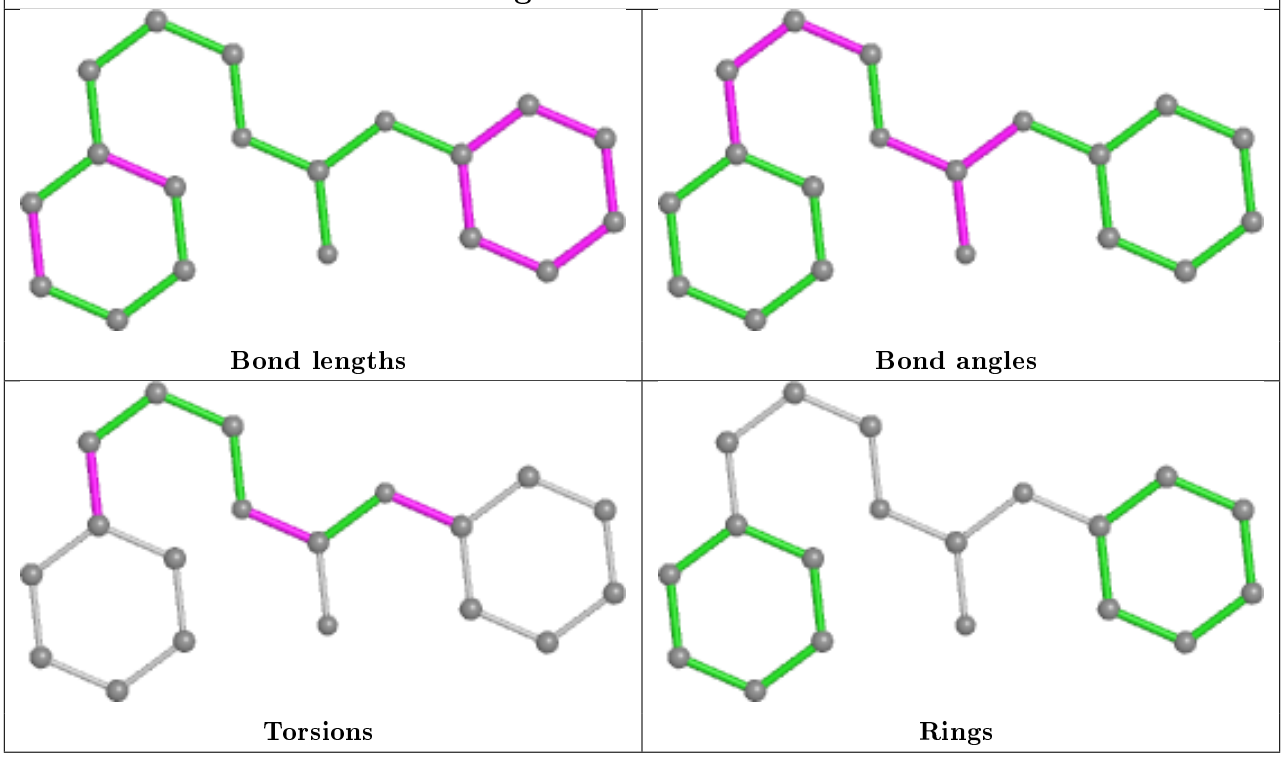
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1200	CPU	5	0
2	A	1100	CPU	5	0

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 then 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.

Ligand CPU B 1200



Ligand CPU A 1100



5.7 Other polymers (i)

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

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.