wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 10:00 PM EDT

PDB ID	:	1FR6
Title	:	REFINED CRYSTAL STRUCTURE OF BETA-LACTAMASE FROM CITROBACTER FREUNDII INDICATES A MECHANISM FOR BETA-LACTAM HYDROLYSIS
Authors	:	Oefner, C.; D'Arcy, A.; Daly, J.J.; Winkler, F.K.
Deposited on	:	2000-09-07
Resolution	:	2.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

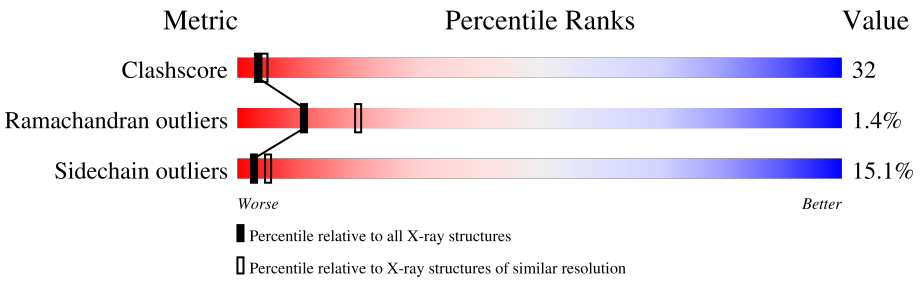
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	361	39% 45% 13% •
1	B	361	39% 44% 14% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AZR	B	362	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6038 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.

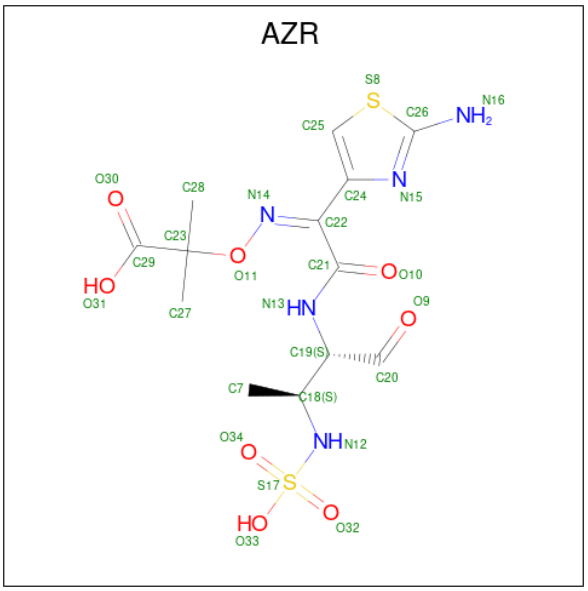
- Molecule 1 is a protein called BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2806	1801	479	517	9	0	0	0
1	B	361	2806	1801	479	517	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	SER	THR	SEE REMARK 999	UNP Q46041
A	176	LYS	THR	SEE REMARK 999	UNP Q46041
A	180	HIS	GLN	SEE REMARK 999	UNP Q46041
A	228	ILE	VAL	SEE REMARK 999	UNP Q46041
A	253	GLU	LYS	SEE REMARK 999	UNP Q46041
A	278	VAL	LEU	SEE REMARK 999	UNP Q46041
A	285	SER	ASN	SEE REMARK 999	UNP Q46041
A	348	VAL	ALA	SEE REMARK 999	UNP Q46041
B	175	SER	THR	SEE REMARK 999	UNP Q46041
B	176	LYS	THR	SEE REMARK 999	UNP Q46041
B	180	HIS	GLN	SEE REMARK 999	UNP Q46041
B	228	ILE	VAL	SEE REMARK 999	UNP Q46041
B	253	GLU	LYS	SEE REMARK 999	UNP Q46041
B	278	VAL	LEU	SEE REMARK 999	UNP Q46041
B	285	SER	ASN	SEE REMARK 999	UNP Q46041
B	348	VAL	ALA	SEE REMARK 999	UNP Q46041

- Molecule 2 is 2-({[(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-oxo-2-{[(2S,3S)-1-oxo-3-(sulfoamino)butan-2-yl]amino}ethylidene]amino}oxy)-2-methylpropanoic acid (three-letter code: AZR) (formula: $C_{13}H_{19}N_5O_8S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	28	13	5	8	2	0	0
			Total	C	N	O	S		
2	B	1	28	13	5	8	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	189	189	189	0	0
			Total	O		
3	B	181	181	181	0	0

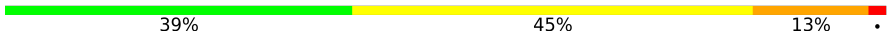
3 Residue-property plots (i)

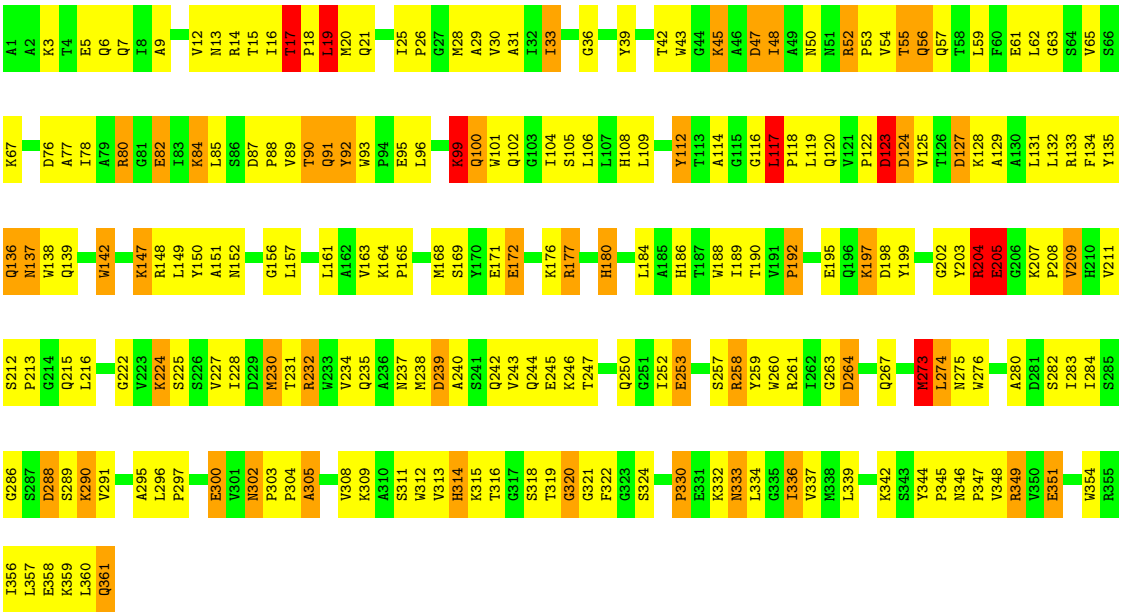
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

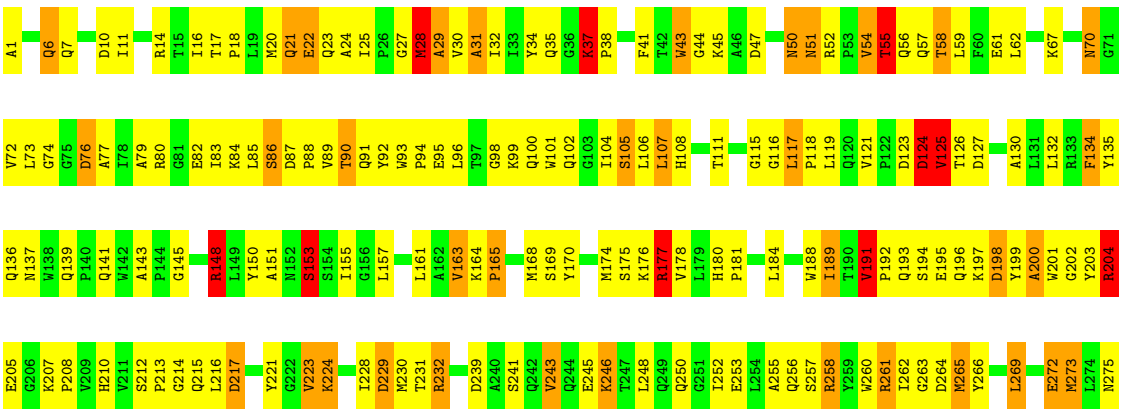
Chain A:





• Molecule 1: BETA-LACTAMASE

Chain B:



K279
A280
D281
S282
I283
I284
S285
G286
S287
D288
S289
K290
V291
A292
L293
A294
A295
L296
N302
P303
P304
A305
K309
H314
K315
S318
T319
G320
G321
F322
Y325
V326
A327
F328
L334
G335
I336
V337
N341
Y344
P345
V348
R349
V350
E351
A352
A353
W354
R355
I356
L357
E358
K359
L360
Q361

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 21	Depositor
Cell constants a, b, c, α, β, γ	98.07Å 84.63Å 89.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6038	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: AZR

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	1.18	3/2881 (0.1%)	1.92	66/3925 (1.7%)
1	B	1.23	3/2881 (0.1%)	1.91	80/3925 (2.0%)
All	All	1.20	6/5762 (0.1%)	1.91	146/7850 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	SER	CB-OG	7.83	1.52	1.42
1	A	105	SER	CB-OG	7.58	1.52	1.42
1	B	105	SER	CB-OG	5.96	1.50	1.42
1	B	241	SER	CB-OG	5.76	1.49	1.42
1	A	14	ARG	CD-NE	-5.71	1.36	1.46

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	ARG	CD-NE-CZ	32.96	169.75	123.60
1	B	349	ARG	NE-CZ-NH2	15.77	128.19	120.30
1	A	14	ARG	NE-CZ-NH1	15.06	127.83	120.30
1	A	264	ASP	CB-CG-OD1	13.26	130.24	118.30
1	B	258	ARG	NE-CZ-NH2	-11.86	114.37	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	148	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	204	ARG	Sidechain
1	B	261	ARG	Sidechain
1	B	80	ARG	Sidechain

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	2806	0	2795	194	3
1	B	2806	0	2795	185	6
2	A	28	0	17	5	0
2	B	28	0	17	9	0
3	A	189	0	0	27	2
3	B	181	0	0	14	1
All	All	6038	0	5624	367	6

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 32.

The worst 5 of 367 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:227:VAL:HG23	1:A:339:LEU:HD12	1.38	1.02
1:A:25:ILE:HD13	1:A:28:MET:HE1	1.45	0.97
1:B:258:ARG:NH1	1:B:275:ASN:HD21	1.62	0.95
1:B:55:THR:H	1:B:58:THR:CG2	1.80	0.95
1:B:73:LEU:HD22	1:B:174:MET:HE2	1.46	0.94

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:OE2	3:B:542:HOH:O[2_664]	1.73	0.47
1:A:180:HIS:NE2	1:B:1:ALA:CA[2_664]	1.74	0.46
1:A:180:HIS:NE2	1:B:1:ALA:CB[2_664]	1.81	0.39
1:B:355:ARG:NH1	3:A:549:HOH:O[4_555]	1.92	0.28
1:A:180:HIS:CD2	1:B:1:ALA:CB[2_664]	2.02	0.18

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	359/361 (99%)	323 (90%)	30 (8%)	6 (2%)	9 16
1	B	359/361 (99%)	327 (91%)	28 (8%)	4 (1%)	14 26
All	All	718/722 (99%)	650 (90%)	58 (8%)	10 (1%)	11 20

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	B	98	GLY
1	B	102	GLN
1	A	263	GLY
1	A	320	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	292/292 (100%)	252 (86%)	40 (14%)	3 7
1	B	292/292 (100%)	244 (84%)	48 (16%)	2 4
All	All	584/584 (100%)	496 (85%)	88 (15%)	3 5

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	163	VAL
1	B	253	GLU
1	B	175	SER
1	B	204	ARG
1	B	282	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	141	GLN
1	B	210	HIS
1	B	196	GLN
1	B	244	GLN
1	A	333	ASN

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 monosaccharides 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	AZR	B	362	1	23,28,28	3.95	8 (34%)	22,41,41	2.49	9 (40%)
2	AZR	A	362	1	23,28,28	4.68	4 (17%)	22,41,41	3.49	14 (63%)

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	AZR	B	362	1	-	9/28/35/35	0/1/1/1
2	AZR	A	362	1	-	15/28/35/35	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	362	AZR	O34-S17	14.95	1.59	1.42
2	B	362	AZR	O34-S17	14.26	1.58	1.42
2	A	362	AZR	O32-S17	14.17	1.58	1.42
2	B	362	AZR	O32-S17	9.03	1.52	1.42
2	A	362	AZR	S17-N12	6.86	1.68	1.59

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	362	AZR	O10-C21-C22	9.34	131.12	120.35
2	B	362	AZR	C23-O11-N14	8.03	117.47	110.33
2	A	362	AZR	O11-N14-C22	5.42	120.30	111.87
2	A	362	AZR	O32-S17-O34	-5.32	107.59	120.16
2	A	362	AZR	C23-O11-N14	4.34	114.19	110.33

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	362	AZR	C22-N14-O11-C23
2	A	362	AZR	C27-C23-O11-N14
2	A	362	AZR	C28-C23-O11-N14
2	A	362	AZR	C18-N12-S17-O33
2	A	362	AZR	C18-N12-S17-O34

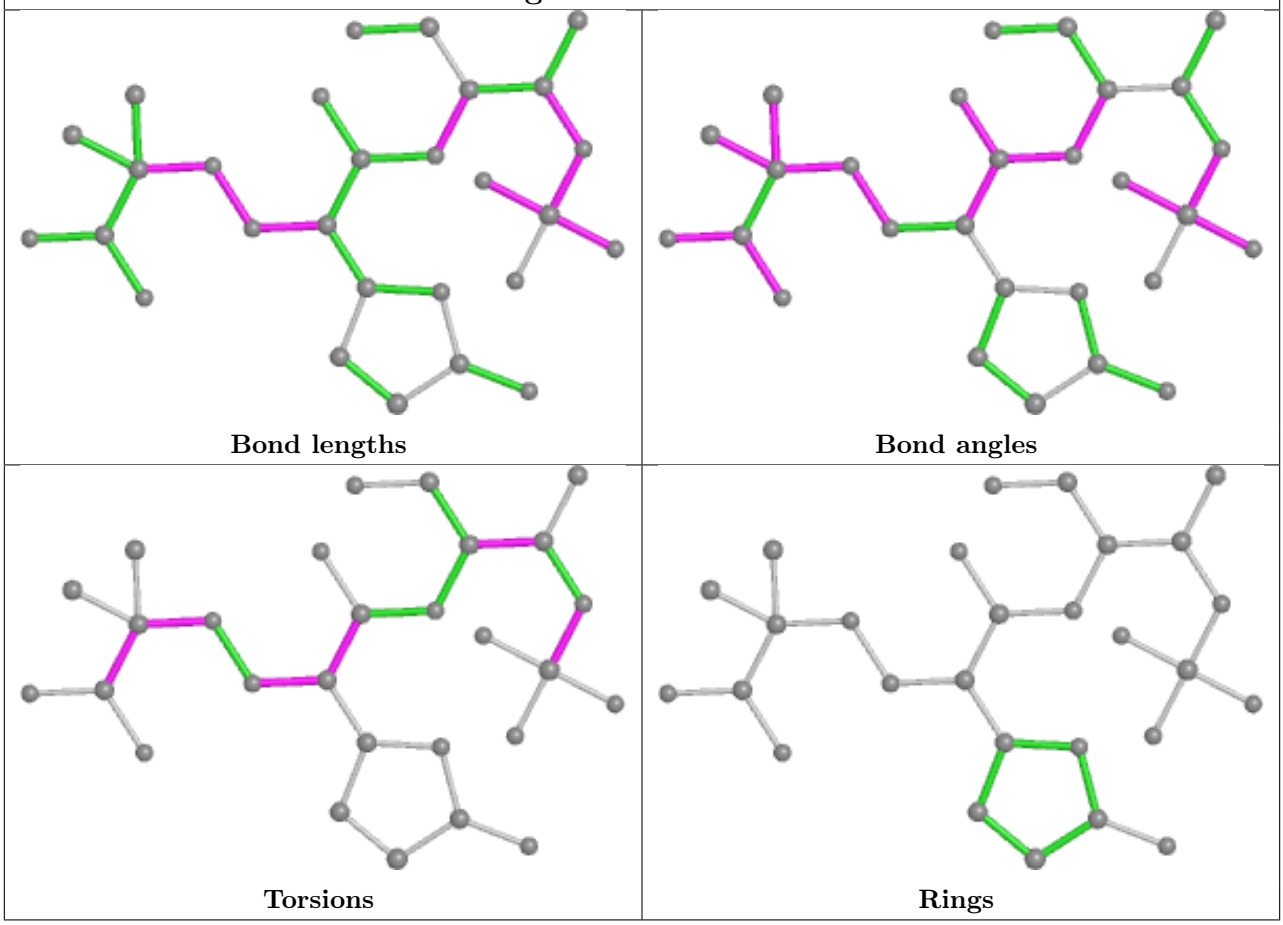
There are no ring outliers.

2 monomers are involved in 14 short contacts:

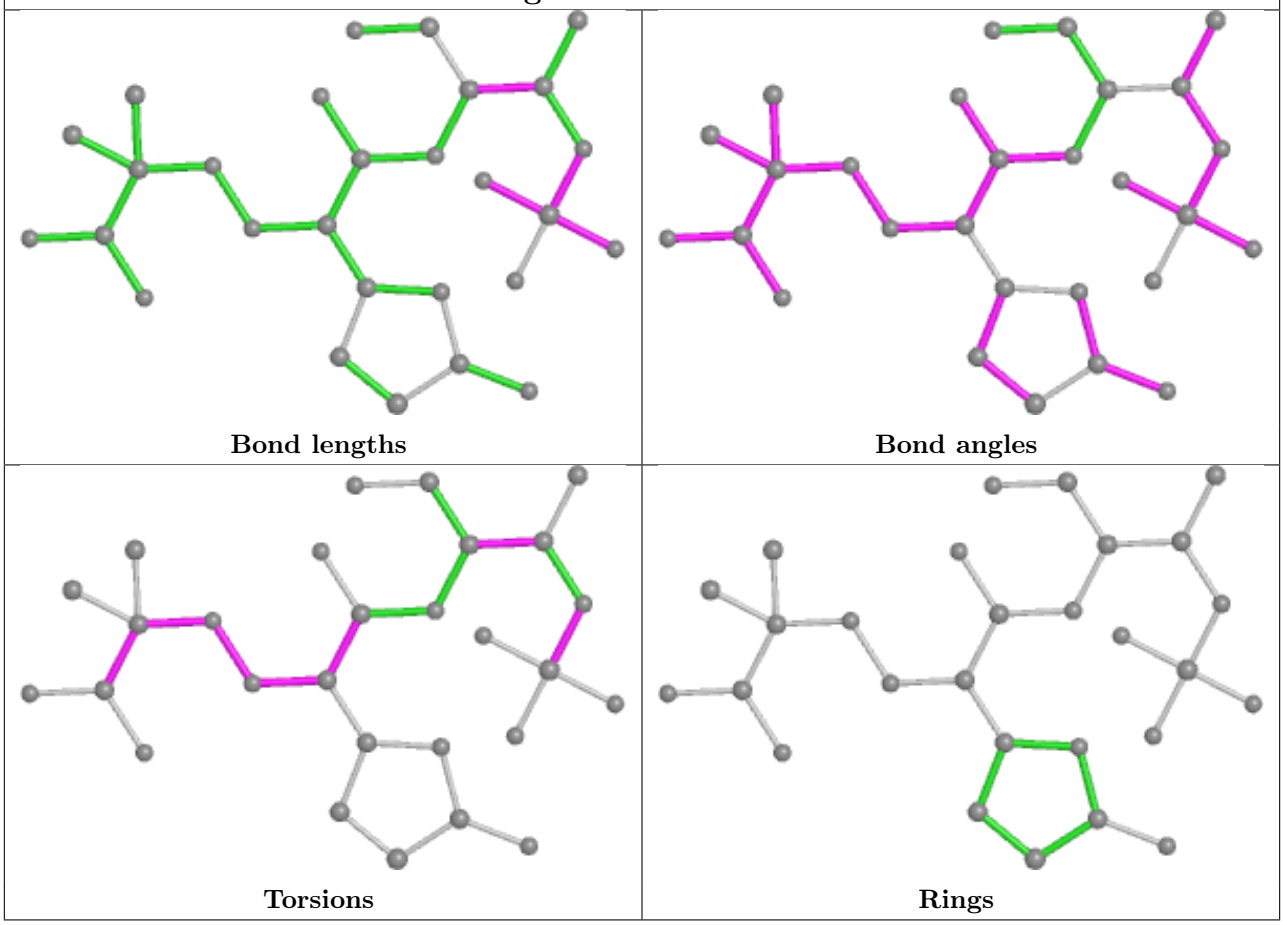
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	362	AZR	9	0
2	A	362	AZR	5	0

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 AZR B 362



Ligand AZR A 362



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 (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.