Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 06:15 am GMT

PDB ID	:	2CNE
Title	:	Structural Insights into the Design of Nonpeptidic Isothiazolidinone- Containing Inhibitors of Protein Tyrosine Phosphatase 1B
Authors	:	Ala, P.J.; Gonneville, L.; Hillman, M.; Becker-Pasha, M.; Yue, E.W.; Douty, B.; Wayland, B.; Polam, P.; Crawley, M.L.; McLaughlin, E.; Sparks, R.B.; Glass, B.; Takvorian, A.; Combs, A.P.; Burn, T.C.; Hollis, G.F.; Wynn, R.
Deposited on	:	2006-05-21
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

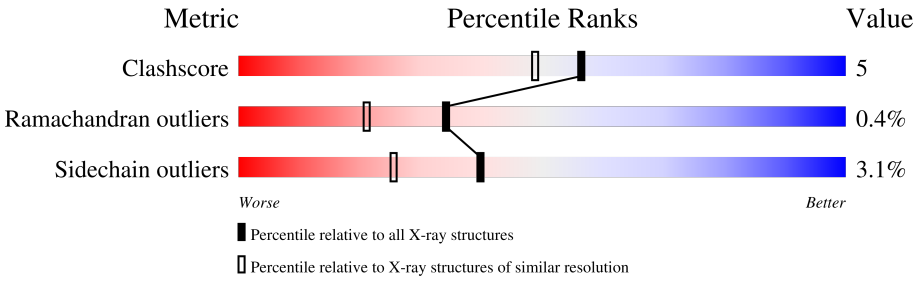
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	81% 13% • 6%

2 Entry composition (i)

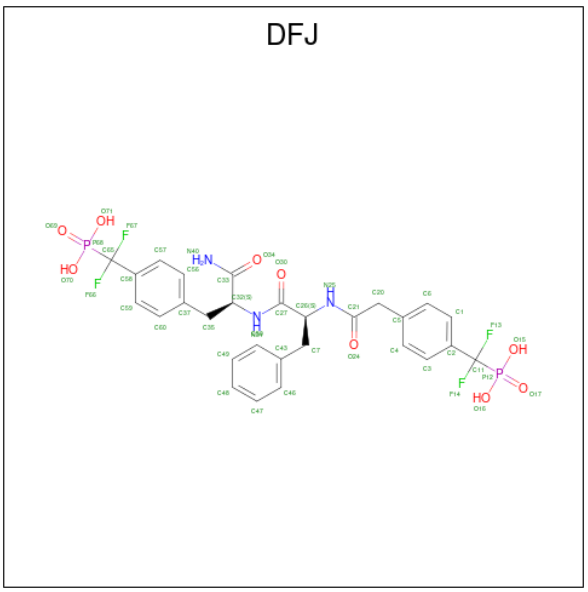
There are 5 unique types of molecules in this entry. The entry contains 2665 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TYROSINE-PROTEIN PHOSPHATASE NON-RECEPTOR TYPE 1.

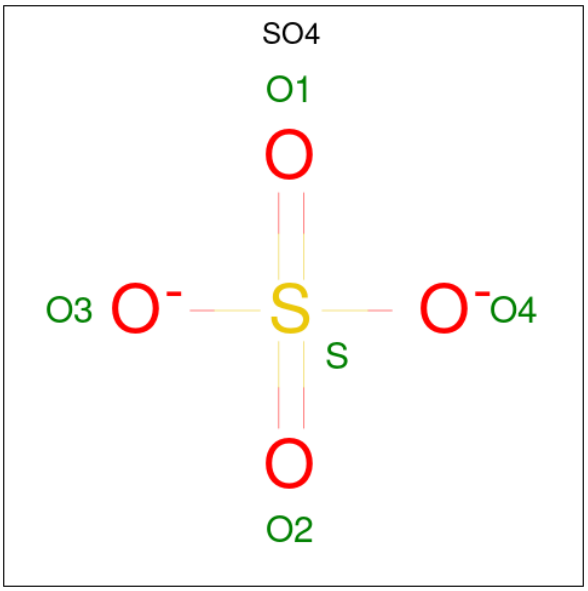
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	287	2349	1488	414	431	16	0	0	1

- Molecule 2 is N-({4-[DIFLUORO(PHOSPHONO)METHYL]PHENYL}ACETYL)-L-PHENYLALANYL-4-[DIFLUORO(PHOSPHONO)METHYL]-L-PHENYLALANINAMIDE (three-letter code: DFJ) (formula: $C_{28}H_{29}F_4N_3O_9P_2$).



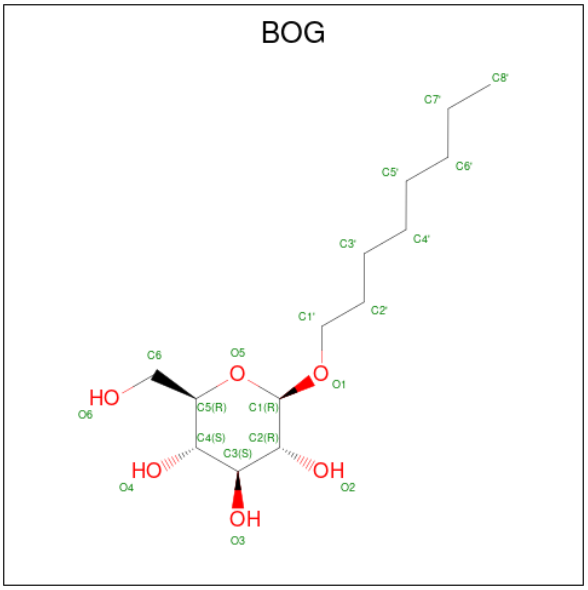
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
2	A	1	46	28	4	3	9	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 14 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	240	240	240	0	0

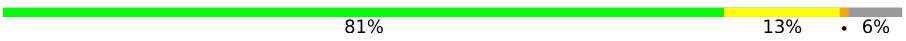
3 Residue-property plots (i)

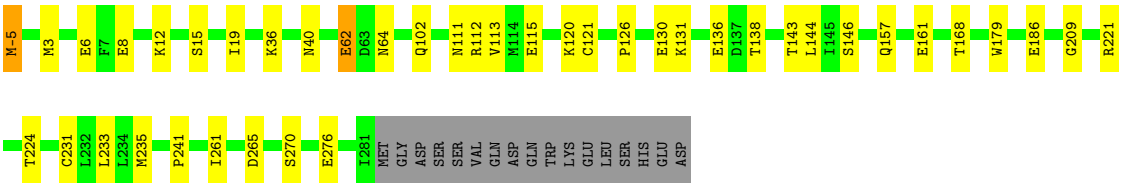
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: TYROSINE-PROTEIN PHOSPHATASE NON-RECEPTOR TYPE 1

Chain A:





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	62.11Å 70.98Å 83.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.197 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2665	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: BOG, DFJ, SO4

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	0.46	0/2407	0.68	1/3245 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	2349	0	2307	24	0
2	A	46	0	25	0	0
3	A	10	0	0	0	0
4	A	20	0	28	0	0
5	A	240	0	0	3	0
All	All	2665	0	2360	24	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 5.

All (24) 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:62:GLU:H	1:A:62:GLU:CD	1.91	0.74
1:A:130:GLU:HG3	5:A:2146:HOH:O	1.91	0.71
1:A:231:CYS:O	1:A:235:MET:HG3	2.02	0.60
1:A:111:ASN:HD21	1:A:121:CYS:HB2	1.69	0.57
1:A:40:ASN:ND2	1:A:64:ASN:HD21	2.03	0.55
1:A:40:ASN:HD21	1:A:64:ASN:HD21	1.56	0.54
1:A:126:PRO:HG2	1:A:144:LEU:HB2	1.89	0.53
1:A:-5:MET:HE3	1:A:3:MET:HE3	1.91	0.52
1:A:115:GLU:HB2	1:A:120:LYS:HG3	1.92	0.51
1:A:113:VAL:HG13	1:A:121:CYS:O	2.17	0.45
1:A:161:GLU:HG3	1:A:168:THR:HG22	1.99	0.44
1:A:36:LYS:HA	1:A:36:LYS:HD3	1.85	0.44
1:A:102:GLN:O	1:A:209:GLY:HA3	2.18	0.44
1:A:224:THR:HG23	1:A:270:SER:OG	2.17	0.44
1:A:-5:MET:HE3	1:A:3:MET:CE	2.48	0.43
1:A:235:MET:HE2	1:A:241:PRO:O	2.18	0.43
1:A:8:GLU:O	1:A:12:LYS:HG2	2.19	0.43
1:A:179:TRP:CE2	1:A:221:ARG:HG2	2.55	0.42
1:A:120:LYS:HA	1:A:120:LYS:HD3	1.83	0.41
1:A:146:SER:OG	1:A:157:GLN:HG3	2.20	0.41
1:A:6:GLU:CG	5:A:2226:HOH:O	2.69	0.41
1:A:131:LYS:O	1:A:143:THR:HA	2.21	0.41
1:A:6:GLU:HG2	5:A:2226:HOH:O	2.20	0.40
1:A:15:SER:O	1:A:19:ILE:HG12	2.21	0.40

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	285/304 (94%)	279 (98%)	5 (2%)	1 (0%)	34 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ILE

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	260/277 (94%)	252 (97%)	8 (3%)	40 25

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	MET
1	A	62	GLU
1	A	136	GLU
1	A	138	THR
1	A	186	GLU
1	A	233	LEU
1	A	265	ASP
1	A	276	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-4	HIS
1	A	1	HIS
1	A	21	GLN
1	A	25	HIS
1	A	40	ASN
1	A	78	GLN
1	A	157	GLN

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Mol	Chain	Res	Type
1	A	193	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)

4 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	$\#\|Z\| > 2$
4	BOG	A	1284	-	20,20,20	1.14	3 (15%)	25,25,25	0.64	0
3	SO4	A	1282	-	4,4,4	0.16	0	6,6,6	0.19	0
3	SO4	A	1283	-	4,4,4	0.21	0	6,6,6	0.12	0
2	DFJ	A	1281	-	42,48,48	5.51	26 (61%)	62,72,72	2.67	31 (50%)

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
4	BOG	A	1284	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DFJ	A	1281	-	-	2/48/58/58	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1281	DFJ	P12-O17	16.40	1.76	1.50
2	A	1281	DFJ	P12-O15	13.58	1.79	1.54
2	A	1281	DFJ	P12-O16	12.03	1.76	1.54
2	A	1281	DFJ	P68-O69	11.74	1.68	1.50
2	A	1281	DFJ	P68-O71	9.60	1.72	1.54
2	A	1281	DFJ	P68-O70	7.95	1.69	1.54
2	A	1281	DFJ	C65-C58	-5.62	1.46	1.50
2	A	1281	DFJ	C3-C2	5.51	1.48	1.39
2	A	1281	DFJ	C59-C58	5.20	1.47	1.39
2	A	1281	DFJ	C57-C58	5.18	1.47	1.39
2	A	1281	DFJ	C1-C2	5.14	1.47	1.39
2	A	1281	DFJ	C4-C3	4.45	1.46	1.38
2	A	1281	DFJ	C57-C56	4.33	1.46	1.38
2	A	1281	DFJ	C6-C1	4.33	1.46	1.38
2	A	1281	DFJ	C11-C2	-4.31	1.47	1.50
2	A	1281	DFJ	C50-C43	4.20	1.47	1.38
2	A	1281	DFJ	C47-C46	4.18	1.47	1.38
2	A	1281	DFJ	C49-C50	4.03	1.47	1.38
2	A	1281	DFJ	C4-C5	3.94	1.47	1.38
2	A	1281	DFJ	C60-C59	3.88	1.45	1.38
2	A	1281	DFJ	C46-C43	3.86	1.47	1.38
2	A	1281	DFJ	C6-C5	3.82	1.47	1.38
2	A	1281	DFJ	C56-C37	3.68	1.46	1.38
2	A	1281	DFJ	C60-C37	3.63	1.46	1.38
2	A	1281	DFJ	C49-C48	3.58	1.47	1.38
2	A	1281	DFJ	C48-C47	3.55	1.47	1.38
4	A	1284	BOG	O5-C1	3.00	1.49	1.41
4	A	1284	BOG	C4-C5	2.23	1.57	1.53
4	A	1284	BOG	O1-C1	2.13	1.43	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1281	DFJ	C6-C5-C4	6.42	128.25	118.17
2	A	1281	DFJ	C60-C37-C56	5.78	127.25	118.17
2	A	1281	DFJ	F14-C11-F13	-5.15	100.22	106.73
2	A	1281	DFJ	F14-C11-C2	4.69	116.53	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1281	DFJ	C50-C43-C46	4.55	125.32	118.17
2	A	1281	DFJ	C59-C58-C57	4.51	124.68	117.97
2	A	1281	DFJ	C3-C4-C5	-4.44	114.92	121.03
2	A	1281	DFJ	F13-C11-C2	4.37	116.12	110.49
2	A	1281	DFJ	C57-C58-C65	-4.33	115.93	119.84
2	A	1281	DFJ	C1-C6-C5	-4.27	115.16	121.03
2	A	1281	DFJ	C20-C5-C6	-4.20	114.88	120.89
2	A	1281	DFJ	C3-C2-C1	3.86	123.72	117.97
2	A	1281	DFJ	P12-C11-C2	3.70	120.06	108.95
2	A	1281	DFJ	C57-C56-C37	-3.66	115.99	121.03
2	A	1281	DFJ	C59-C60-C37	-3.52	116.19	121.03
2	A	1281	DFJ	P68-C65-C58	3.20	118.55	108.95
2	A	1281	DFJ	F67-C65-F66	3.05	110.58	106.73
2	A	1281	DFJ	C1-C2-C11	-2.94	117.19	119.84
2	A	1281	DFJ	C20-C5-C4	-2.81	116.87	120.89
2	A	1281	DFJ	C49-C50-C43	-2.70	116.49	120.63
2	A	1281	DFJ	O71-P68-O70	2.63	115.40	107.99
2	A	1281	DFJ	O16-P12-O17	2.59	118.87	113.06
2	A	1281	DFJ	C56-C57-C58	-2.51	117.86	121.22
2	A	1281	DFJ	C35-C37-C60	-2.48	115.98	120.91
2	A	1281	DFJ	O15-P12-O17	2.47	118.61	113.06
2	A	1281	DFJ	C47-C46-C43	-2.43	116.90	120.63
2	A	1281	DFJ	C60-C59-C58	-2.38	118.03	121.22
2	A	1281	DFJ	C26-N25-C21	-2.22	115.94	121.65
2	A	1281	DFJ	C35-C37-C56	-2.08	116.78	120.91
2	A	1281	DFJ	C7-C43-C46	-2.03	116.88	120.91
2	A	1281	DFJ	C20-C21-N25	2.02	119.13	115.88

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1281	DFJ	N31-C32-C33-O34
2	A	1281	DFJ	N31-C32-C33-N40

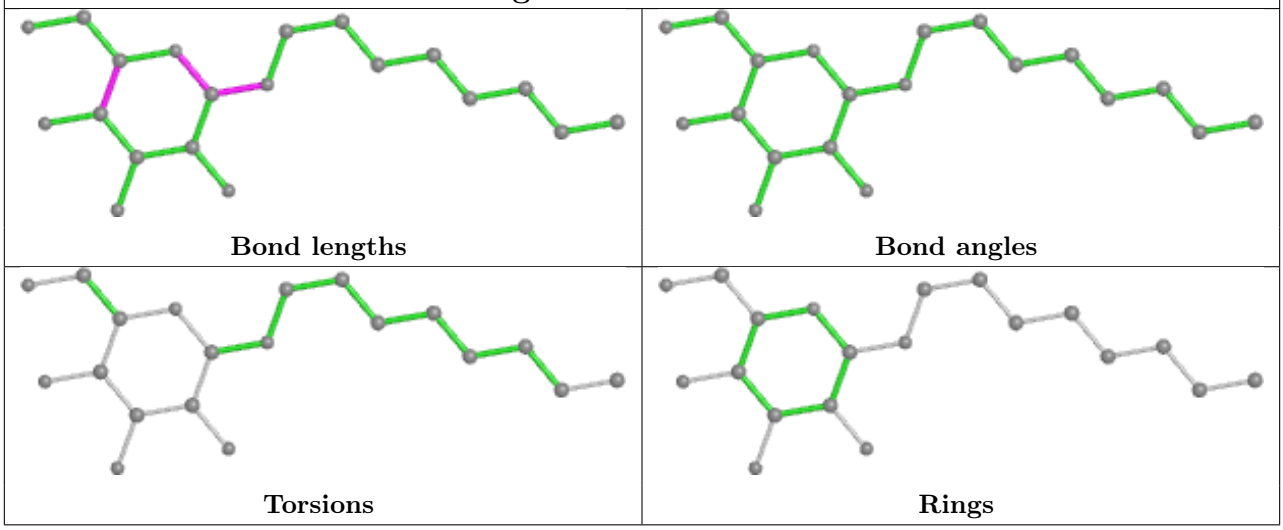
There are no ring outliers.

No monomer is involved in short contacts.

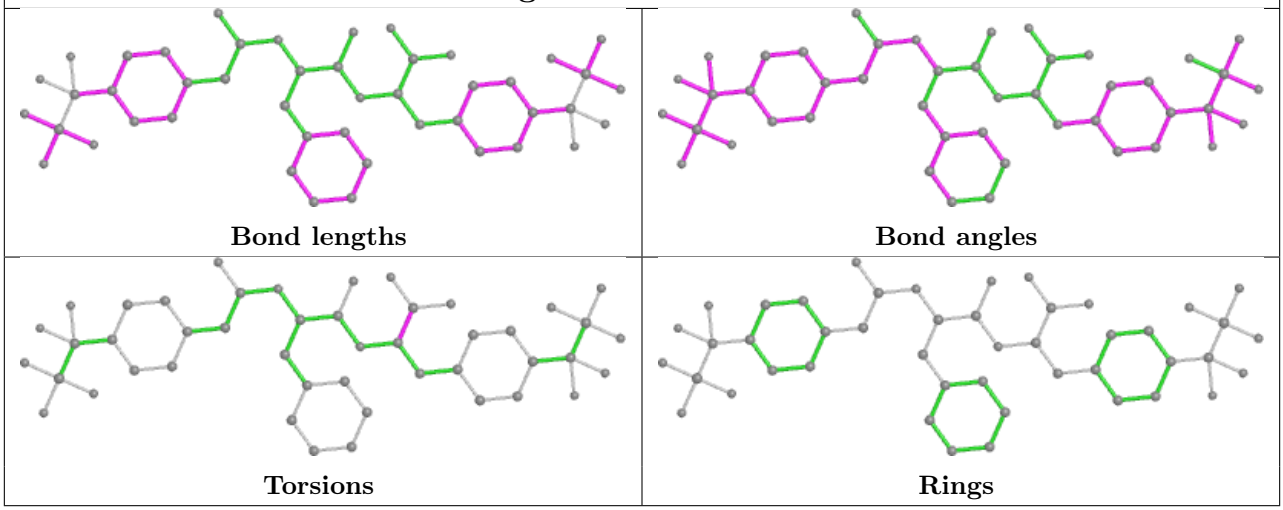
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 BOG A 1284



Ligand DFJ A 1281



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.