



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 11:10 AM JST

PDB ID : 8ZR5
EMDB ID : EMD-60392
Title : Cryo-EM Structure of GPR119-Gs-Firuglipel complex
Authors : Wong, T.S.; Zeng, Z.C.; Xiong, T.T.; Gan, S.Y.; Qiu, C.; Du, Y.
Deposited on : 2024-06-04
Resolution : 3.31 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

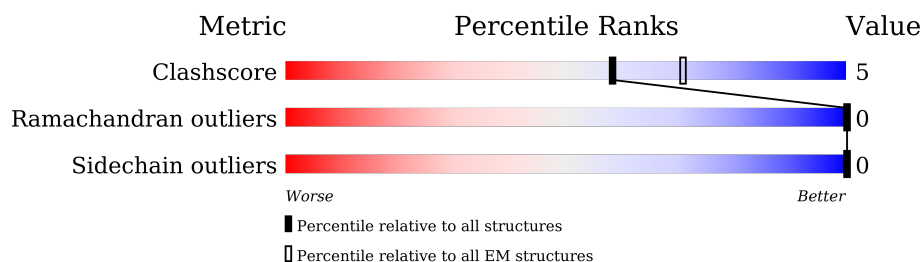
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 3.31 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	394	
2	B	373	
3	G	71	
4	N	157	
5	C	358	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16221 atoms, of which 8069 are hydrogens and 0 are deuteriums.

In the tables below, 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	237	Total	C	H	N	O	S	0	0
			3903	1235	1943	356	362	7		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	conflict	UNP P63092
A	226	ALA	GLY	conflict	UNP P63092
A	268	ALA	GLU	conflict	UNP P63092
A	271	LYS	ASN	conflict	UNP P63092
A	274	ASP	LYS	conflict	UNP P63092
A	280	LYS	ARG	conflict	UNP P63092
A	284	ASP	THR	conflict	UNP P63092
A	285	THR	ILE	conflict	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	338	Total	C	H	N	O	S	0	0
			5098	1604	2500	467	506	21		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP P62873
B	-20	HIS	-	expression tag	UNP P62873
B	-19	HIS	-	expression tag	UNP P62873
B	-18	HIS	-	expression tag	UNP P62873
B	-17	HIS	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	VAL	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	GLY	-	expression tag	UNP P62873
B	344	TRP	-	expression tag	UNP P62873
B	345	ARG	-	expression tag	UNP P62873
B	346	LEU	-	expression tag	UNP P62873
B	347	PHE	-	expression tag	UNP P62873
B	348	LYS	-	expression tag	UNP P62873
B	349	LYS	-	expression tag	UNP P62873
B	350	ILE	-	expression tag	UNP P62873
B	351	SER	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	57	Total	C	H	N	O	S	0	0
			885	273	449	77	83	3		

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	128	Total	C	H	N	O	S	0	0
			1910	605	937	170	192	6		

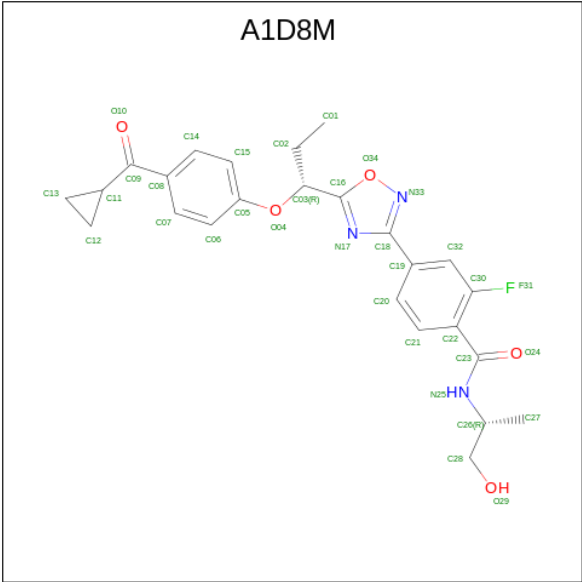
- Molecule 5 is a protein called Glucose-dependent insulintropic receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	C	284	Total	C	H	N	O	S	0	0
			4365	1429	2214	344	360	18		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	ASP	-	expression tag	UNP Q8TDV5
C	-14	TYR	-	expression tag	UNP Q8TDV5
C	-13	LYS	-	expression tag	UNP Q8TDV5
C	-12	ASP	-	expression tag	UNP Q8TDV5
C	-11	ASP	-	expression tag	UNP Q8TDV5
C	-10	ASP	-	expression tag	UNP Q8TDV5
C	-9	ASP	-	expression tag	UNP Q8TDV5
C	-8	LYS	-	expression tag	UNP Q8TDV5
C	-7	LEU	-	expression tag	UNP Q8TDV5
C	-6	GLU	-	expression tag	UNP Q8TDV5
C	-5	VAL	-	expression tag	UNP Q8TDV5
C	-4	LEU	-	expression tag	UNP Q8TDV5
C	-3	PHE	-	expression tag	UNP Q8TDV5
C	-2	GLN	-	expression tag	UNP Q8TDV5
C	-1	GLY	-	expression tag	UNP Q8TDV5
C	0	PRO	-	expression tag	UNP Q8TDV5
C	336	HIS	-	expression tag	UNP Q8TDV5
C	337	HIS	-	expression tag	UNP Q8TDV5
C	338	HIS	-	expression tag	UNP Q8TDV5
C	339	HIS	-	expression tag	UNP Q8TDV5
C	340	HIS	-	expression tag	UNP Q8TDV5
C	341	HIS	-	expression tag	UNP Q8TDV5
C	342	HIS	-	expression tag	UNP Q8TDV5

- Molecule 6 is 4-[5-[(1 {R})-1-(4-cyclopropylcarbonylphenoxy)propyl]-1,2,4-oxadiazol-3-yl]-2-fluoranyl- {N}-[(2 {R})-1-oxidanylpropan-2-yl]benzamide (three-letter code: A1D8M) (formula: C₂₅H₂₆FN₃O₅) (labeled as "Ligand of Interest" by depositor).

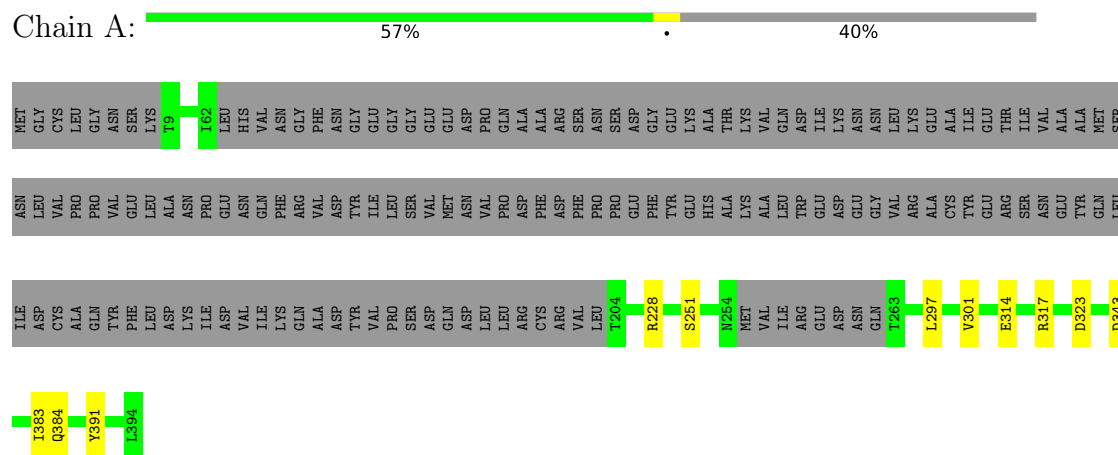


Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
6	C	1	60	25	1	26	3	5	0

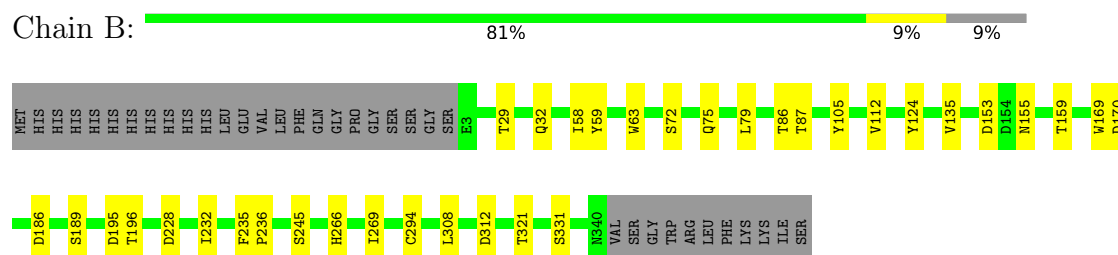
3 Residue-property plots

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.

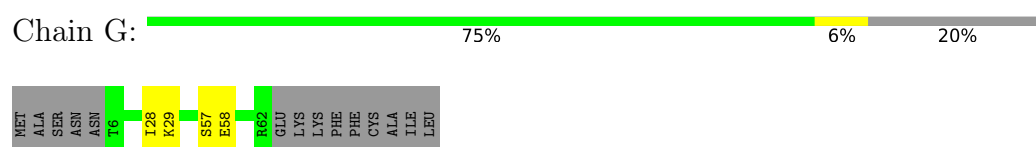
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



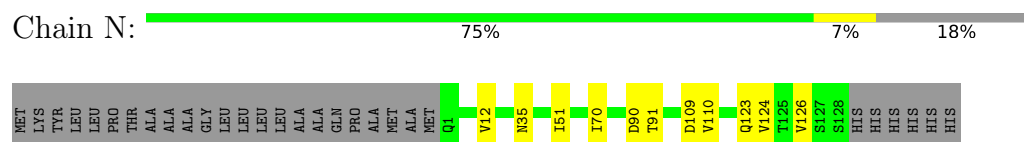
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



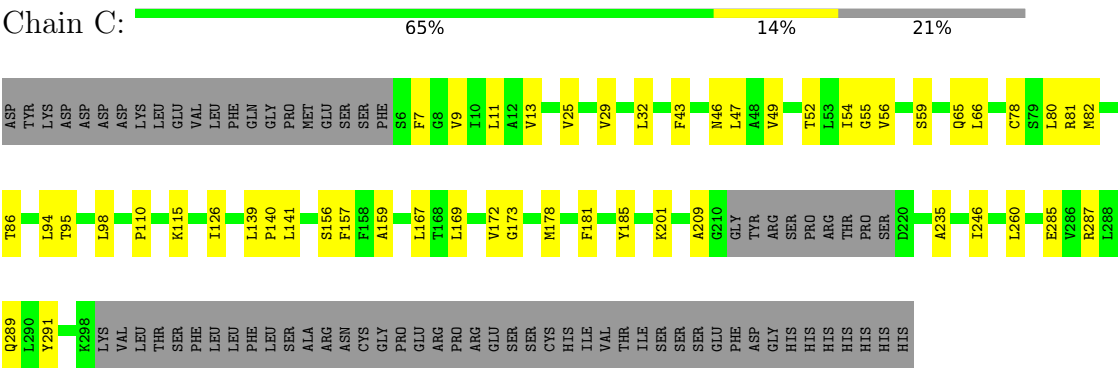
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: Nanobody 35



● Molecule 5: Glucose-dependent insulintropic receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	383236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: A1D8M

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	0.29	0/1996	0.52	0/2683
2	B	0.28	0/2645	0.55	0/3587
3	G	0.24	0/442	0.47	0/597
4	N	0.27	0/993	0.51	0/1345
5	C	0.38	0/2201	0.51	0/2997
All	All	0.31	0/8277	0.52	0/11209

There are no bond length outliers.

There are no bond angle outliers.

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	1960	1943	1940	9	0
2	B	2598	2500	2499	23	0
3	G	436	449	448	3	0
4	N	973	937	940	8	0
5	C	2151	2214	2214	34	0
6	C	34	26	0	1	0
All	All	8152	8069	8041	73	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.

The worst 5 of 73 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)
2:B:228:ASP:O	2:B:245:SER:HB2	1.99	0.63
5:C:25:VAL:O	5:C:29:VAL:HG23	1.97	0.63
5:C:43:PHE:CE1	5:C:98:LEU:HD21	2.35	0.62
1:A:228:ARG:NH1	2:B:186:ASP:OD1	2.35	0.59
1:A:314:GLU:OE1	1:A:317:ARG:NH2	2.35	0.59

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 PDB entries followed by that with respect to all EM entries.

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	231/394 (59%)	224 (97%)	7 (3%)	0	100	100
2	B	336/373 (90%)	323 (96%)	13 (4%)	0	100	100
3	G	55/71 (78%)	54 (98%)	1 (2%)	0	100	100
4	N	126/157 (80%)	122 (97%)	4 (3%)	0	100	100
5	C	280/358 (78%)	274 (98%)	6 (2%)	0	100	100
All	All	1028/1353 (76%)	997 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	211/349 (60%)	211 (100%)	0	100	100
2	B	279/312 (89%)	279 (100%)	0	100	100
3	G	46/58 (79%)	46 (100%)	0	100	100
4	N	106/127 (84%)	106 (100%)	0	100	100
5	C	228/307 (74%)	228 (100%)	0	100	100
All	All	870/1153 (76%)	870 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

1 ligand is 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
6	A1D8M	C	401	-	33,37,37	1.02	1 (3%)	43,52,52	1.37	5 (11%)

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
6	A1D8M	C	401	-	-	4/28/34/34	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	401	A1D8M	C22-C30	2.08	1.41	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	401	A1D8M	C18-N17-C16	-4.82	100.77	103.79
6	C	401	A1D8M	C32-C30-C22	-3.19	120.13	123.53
6	C	401	A1D8M	C05-O04-C03	2.46	120.26	118.62
6	C	401	A1D8M	C19-C32-C30	2.42	121.65	119.59
6	C	401	A1D8M	C19-C18-N33	2.29	122.10	119.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	401	A1D8M	C27-C26-C28-O29
6	C	401	A1D8M	C08-C09-C11-C12
6	C	401	A1D8M	O10-C09-C11-C12
6	C	401	A1D8M	N25-C26-C28-O29

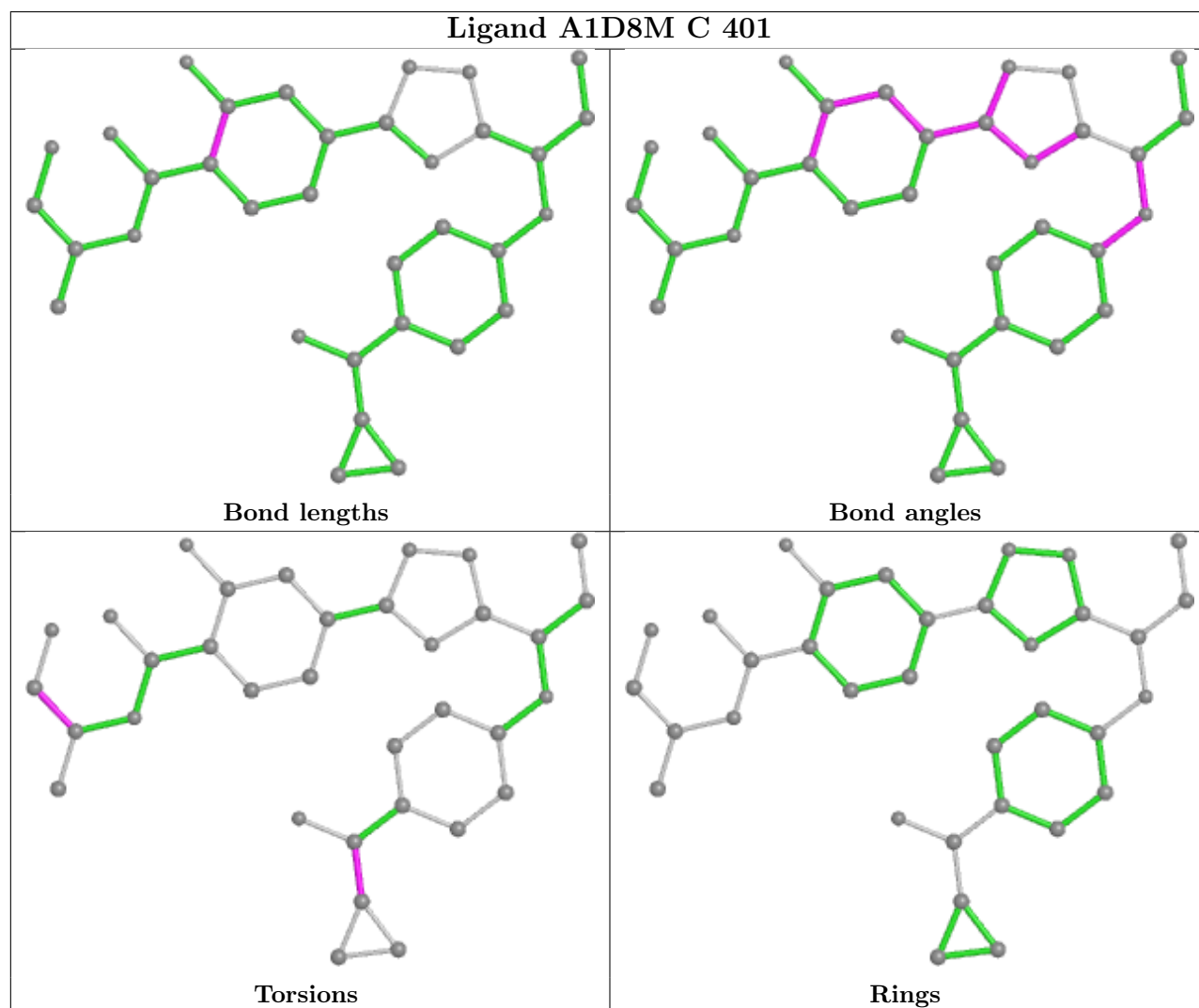
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	A1D8M	1	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.