



wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:08 PM JST

PDB ID : 8IQ4
EMDB ID : EMD-35657
Title : Cryo-EM structure of Carboprost-bound prostaglandin-F2-alpha receptor-miniGq-Nb35 complex
Authors : Lv, X.; Gao, K.; Nie, J.; Zhang, X.; Zhang, S.; Ren, Y.; Li, Q.; Huang, J.; Liu, L.; Zhang, X.; Sun, X.; Zhang, W.; Liu, X.
Deposited on : 2023-03-15
Resolution : 2.70 Å(reported)

This is a wwPDB EM 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/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

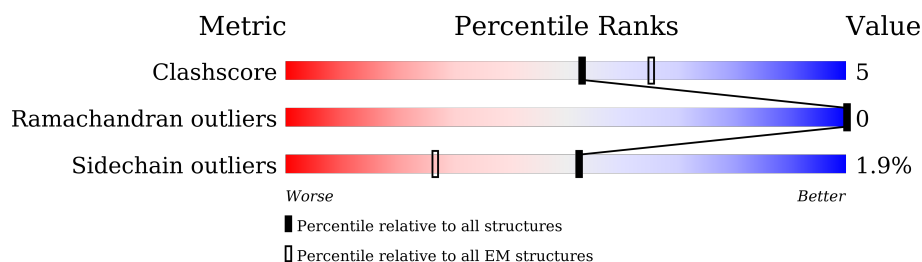
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	R	384	
2	A	245	
3	B	358	
4	G	71	
5	N	134	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7080 atoms, of which 0 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 Prostaglandin F2-alpha receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	274	Total	C	N	O	S	0	0
			2065	1373	339	333	20		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-7	ASP	-	expression tag	UNP P43088
R	-6	TYR	-	expression tag	UNP P43088
R	-5	LYS	-	expression tag	UNP P43088
R	-4	ASP	-	expression tag	UNP P43088
R	-3	ASP	-	expression tag	UNP P43088
R	-2	ASP	-	expression tag	UNP P43088
R	-1	ASP	-	expression tag	UNP P43088
R	0	ALA	-	expression tag	UNP P43088
R	360	HIS	-	expression tag	UNP P43088
R	361	HIS	-	expression tag	UNP P43088
R	362	HIS	-	expression tag	UNP P43088
R	363	HIS	-	expression tag	UNP P43088
R	364	HIS	-	expression tag	UNP P43088
R	365	HIS	-	expression tag	UNP P43088
R	366	GLY	-	expression tag	UNP P43088
R	367	GLY	-	expression tag	UNP P43088
R	368	SER	-	expression tag	UNP P43088
R	369	GLY	-	expression tag	UNP P43088
R	370	GLY	-	expression tag	UNP P43088
R	371	LEU	-	expression tag	UNP P43088
R	372	GLU	-	expression tag	UNP P43088
R	373	VAL	-	expression tag	UNP P43088
R	374	LEU	-	expression tag	UNP P43088
R	375	PHE	-	expression tag	UNP P43088
R	376	GLN	-	expression tag	UNP P43088

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	201	Total 1564	C 1007	N 270	O 281	S 6	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP P63092
A	10	PRO	-	expression tag	UNP P63092
A	11	THR	-	expression tag	UNP P63092
A	12	LEU	-	expression tag	UNP P63092
A	13	SER	-	expression tag	UNP P63092
A	14	ALA	-	expression tag	UNP P63092
A	15	GLU	-	expression tag	UNP P63092
A	16	ASP	-	expression tag	UNP P63092
A	19	ALA	GLN	conflict	UNP P63092
A	20	VAL	ARG	conflict	UNP P63092
A	22	ARG	ALA	conflict	UNP P63092
A	23	SER	ASN	conflict	UNP P63092
A	25	MET	LYS	conflict	UNP P63092
A	49	ASP	GLY	conflict	UNP P63092
A	50	ASN	GLU	conflict	UNP P63092
A	196	GLY	-	linker	UNP P63092
A	197	GLY	-	linker	UNP P63092
A	198	SER	-	linker	UNP P63092
A	199	GLY	-	linker	UNP P63092
A	200	GLY	-	linker	UNP P63092
A	201	SER	-	linker	UNP P63092
A	202	GLY	-	linker	UNP P63092
A	203	GLY	-	linker	UNP P63092
A	249	ASP	ALA	conflict	UNP P63092
A	252	ASP	SER	conflict	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	MET	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	THR	deletion	UNP P63092
A	272	ASP	LEU	conflict	UNP P63092
A	372	ALA	ILE	conflict	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	375	ILE	VAL	conflict	UNP P63092
A	380	LYS	ARG	conflict	UNP P63092
A	384	LEU	GLN	conflict	UNP P63092
A	385	GLN	ARG	conflict	UNP P63092
A	387	ASN	HIS	conflict	UNP P63092
A	390	GLU	GLN	conflict	UNP P63092
A	392	ASN	GLU	conflict	UNP P63092
A	394	VAL	LEU	conflict	UNP P63092

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	329	Total	C	N	O	S	0	0
			2342	1472	412	440	18		

There are 19 discrepancies between the modelled and reference sequences:

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

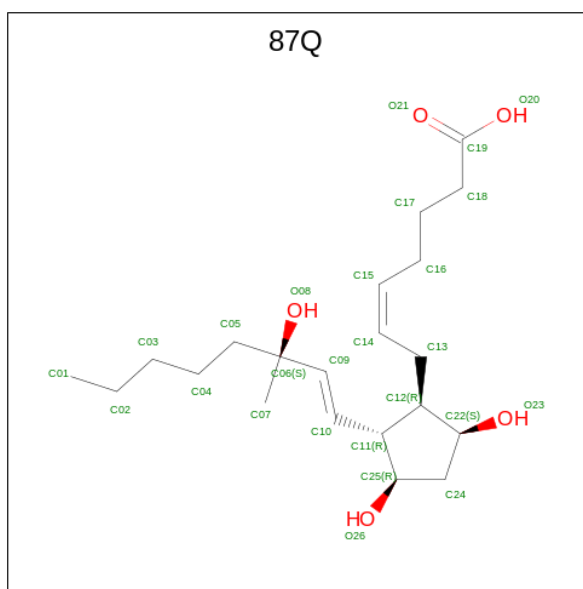
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	36	Total	C	N	O	S	0	0
			238	149	42	45	2		

- Molecule 5 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	114	Total	C	N	O	S	0	0
			845	533	145	161	6		

- Molecule 6 is Z-7-[(1R,2R,3R,5S)-2-[(E,3S)-3-methyl-3-oxidanyl-oct-1-enyl]-3,5-bis(oxidanyl)cyclopentyl]hept-5-enoic acid (three-letter code: 87Q) (formula: C₂₁H₃₆O₅).

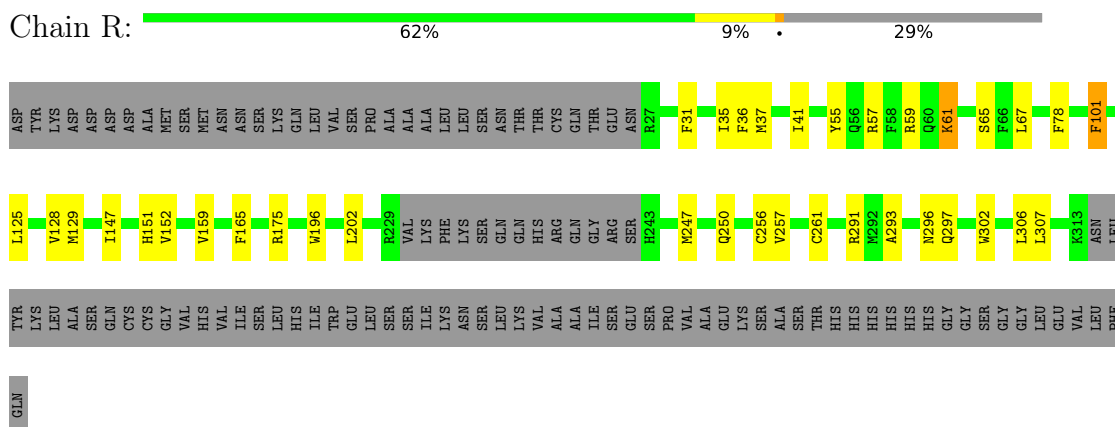


Mol	Chain	Residues	Atoms			AltConf
6	R	1	Total	C	O	0
			26	21	5	

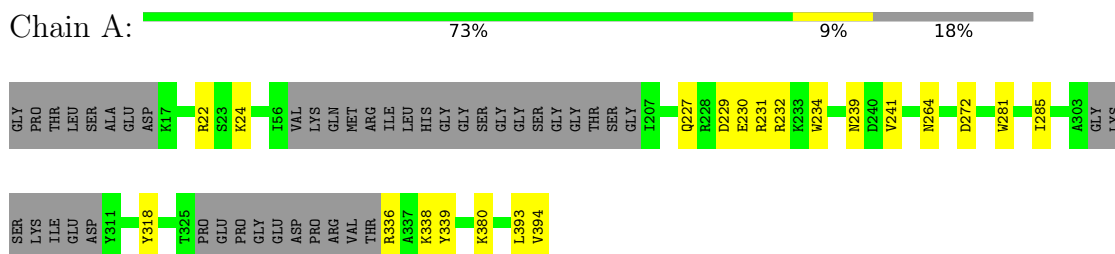
3 Residue-property plots [i](#)

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.

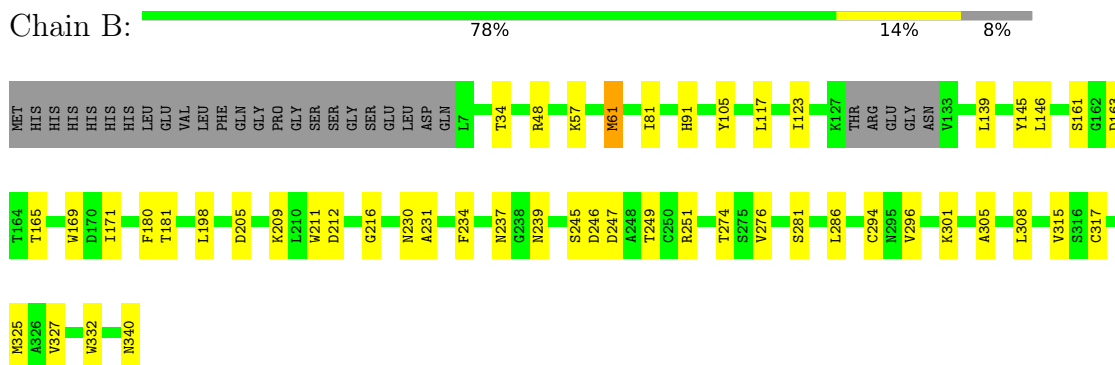
- Molecule 1: Prostaglandin F2-alpha receptor



- Molecule 2: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



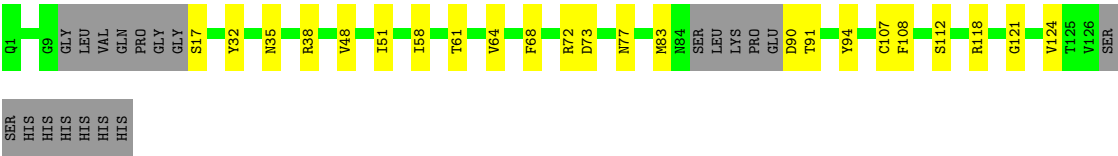
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



● Molecule 5: Nanobody 35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	327293	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: 87Q

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	R	0.25	0/2111	0.46	0/2870
2	A	0.25	0/1595	0.44	0/2163
3	B	0.25	0/2387	0.51	0/3258
4	G	0.23	0/240	0.40	0/329
5	N	0.27	0/863	0.51	0/1171
All	All	0.25	0/7196	0.48	0/9791

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	R	2065	0	2087	21	0
2	A	1564	0	1465	13	0
3	B	2342	0	2147	29	0
4	G	238	0	206	3	0
5	N	845	0	776	12	0
6	R	26	0	0	0	0
All	All	7080	0	6681	70	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 70 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:R:247:MET:SD	1:R:250:GLN:NE2	2.64	0.68
1:R:125:LEU:O	1:R:129:MET:HG3	1.94	0.67
2:A:239:ASN:ND2	2:A:281:TRP:O	2.29	0.66
5:N:94:TYR:O	5:N:121:GLY:HA2	1.96	0.65
2:A:231:ARG:NH2	2:A:272:ASP:OD1	2.31	0.63

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	R	270/384 (70%)	257 (95%)	13 (5%)	0	100	100
2	A	193/245 (79%)	193 (100%)	0	0	100	100
3	B	325/358 (91%)	312 (96%)	13 (4%)	0	100	100
4	G	34/71 (48%)	33 (97%)	1 (3%)	0	100	100
5	N	108/134 (81%)	98 (91%)	10 (9%)	0	100	100
All	All	930/1192 (78%)	893 (96%)	37 (4%)	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	R	211/335 (63%)	206 (98%)	5 (2%)	44	73
2	A	154/214 (72%)	151 (98%)	3 (2%)	52	79
3	B	221/298 (74%)	217 (98%)	4 (2%)	54	80
4	G	18/58 (31%)	18 (100%)	0	100	100
5	N	85/112 (76%)	84 (99%)	1 (1%)	67	86
All	All	689/1017 (68%)	676 (98%)	13 (2%)	52	79

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	380	LYS
3	B	61	MET
5	N	90	ASP
3	B	146	LEU
3	B	234	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	296	ASN
3	B	237	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	87Q	R	401	-	26,26,26	1.35	3 (11%)	27,34,34	2.41	3 (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	87Q	R	401	-	-	8/21/37/37	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	87Q	O08-C06	-3.72	1.39	1.44
6	R	401	87Q	C06-C09	2.60	1.54	1.51
6	R	401	87Q	C13-C14	2.13	1.56	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	401	87Q	C06-C09-C10	-8.06	114.94	127.11
6	R	401	87Q	C11-C10-C09	8.06	150.37	125.11
6	R	401	87Q	C13-C14-C15	-3.29	114.17	126.40

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	401	87Q	C09-C10-C11-C12
6	R	401	87Q	C09-C10-C11-C25

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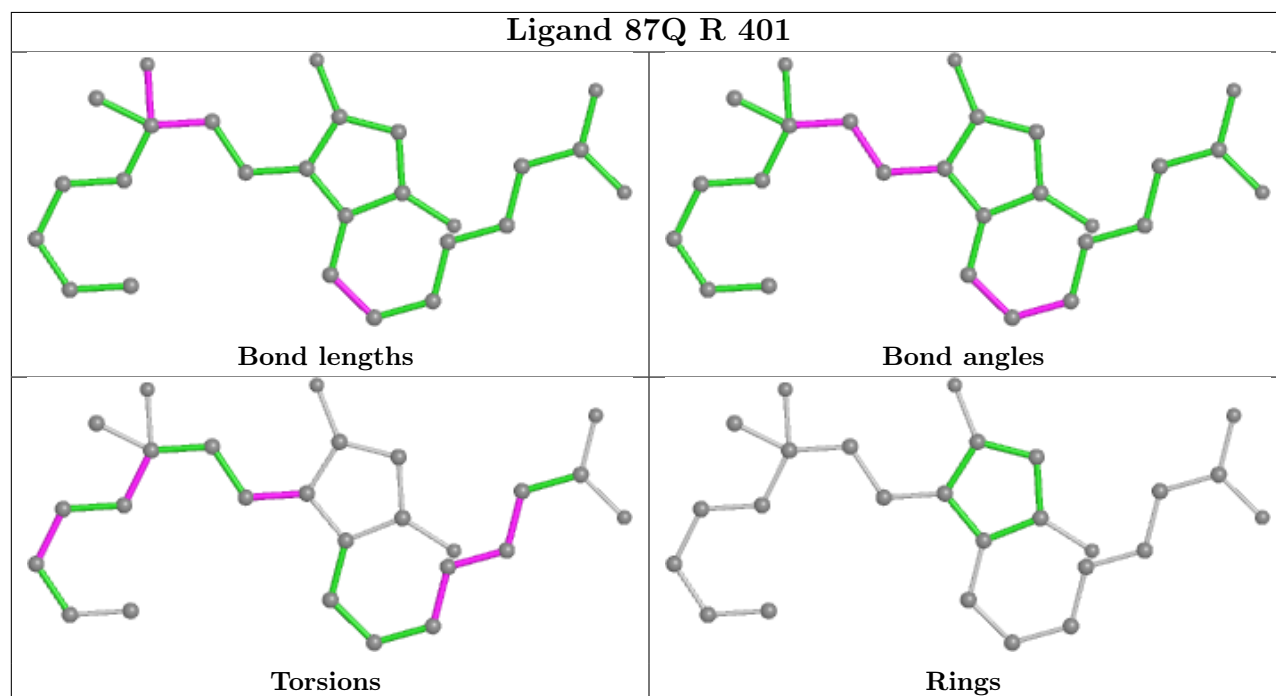
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Mol	Chain	Res	Type	Atoms
6	R	401	87Q	C04-C05-C06-C07
6	R	401	87Q	C16-C17-C18-C19
6	R	401	87Q	C02-C03-C04-C05

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 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.