



wwPDB EM Validation Summary Report ⓘ

Apr 18, 2024 – 10:06 PM JST

PDB ID : 8K8J
EMDB ID : EMD-36951
Title : Cannabinoid Receptor 1 bound to Fenofibrate coupling MiniGsq and Nb35 Complex
Authors : Tang, W.Q.; Wang, T.X.; Li, F.H.; Wang, J.Y.
Deposited on : 2023-07-30
Resolution : 2.88 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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

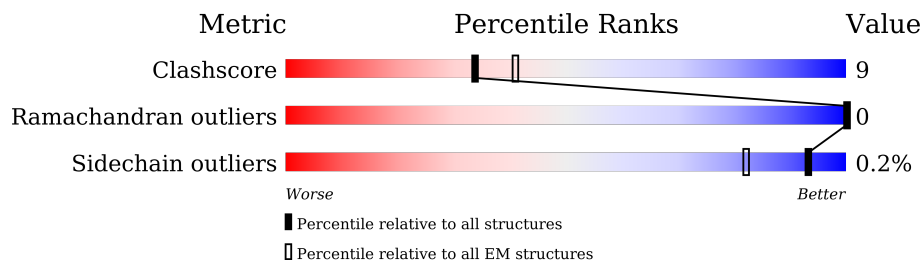
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	263	
2	B	340	
3	G	97	
4	N	139	
5	R	525	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8155 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	239	1970	1241	354	368	7	0	0

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP P63092
A	-8	GLY	-	expression tag	UNP P63092
A	-7	HIS	-	expression tag	UNP P63092
A	-6	HIS	-	expression tag	UNP P63092
A	-5	HIS	-	expression tag	UNP P63092
A	-4	HIS	-	expression tag	UNP P63092
A	-3	HIS	-	expression tag	UNP P63092
A	-2	HIS	-	expression tag	UNP P63092
A	-1	GLU	-	expression tag	UNP P63092
A	0	ASN	-	expression tag	UNP P63092
A	1	LEU	-	expression tag	UNP P63092
A	2	TYR	-	expression tag	UNP P63092
A	3	PHE	-	expression tag	UNP P63092
A	4	GLN	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	362	ALA	-	expression tag	UNP P63092
A	363	ARG	-	expression tag	UNP P63092
A	364	ARG	-	expression tag	UNP P63092
A	365	ILE	-	expression tag	UNP P63092
A	366	PHE	-	expression tag	UNP P63092
A	367	ASN	-	expression tag	UNP P63092
A	368	ASP	-	expression tag	UNP P63092
A	369	CYS	-	expression tag	UNP P63092
A	370	LYS	-	expression tag	UNP P63092
A	371	ASP	-	expression tag	UNP P63092
A	372	ILE	-	expression tag	UNP P63092
A	373	ILE	-	expression tag	UNP P63092
A	374	LEU	-	expression tag	UNP P63092
A	375	GLN	-	expression tag	UNP P63092
A	376	MET	-	expression tag	UNP P63092
A	377	ASN	-	expression tag	UNP P63092
A	378	LEU	-	expression tag	UNP P63092
A	379	ARG	-	expression tag	UNP P63092
A	380	GLU	-	expression tag	UNP P63092
A	381	TYR	-	expression tag	UNP P63092
A	382	ASN	-	expression tag	UNP P63092
A	383	LEU	-	expression tag	UNP P63092
A	384	VAL	-	expression tag	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
			Total	C	N	O	S		
2	B	338	2600	1604	467	508	21	0	0

- 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
			Total	C	N	O	S		
3	G	49	372	233	65	71	3	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-25	MET	-	initiating methionine	UNP P59768
G	-24	HIS	-	expression tag	UNP P59768
G	-23	HIS	-	expression tag	UNP P59768
G	-22	HIS	-	expression tag	UNP P59768
G	-21	HIS	-	expression tag	UNP P59768
G	-20	HIS	-	expression tag	UNP P59768
G	-19	HIS	-	expression tag	UNP P59768
G	-18	GLY	-	expression tag	UNP P59768
G	-17	GLY	-	expression tag	UNP P59768
G	-16	GLY	-	expression tag	UNP P59768
G	-15	SER	-	expression tag	UNP P59768
G	-14	ASP	-	expression tag	UNP P59768
G	-13	SER	-	expression tag	UNP P59768
G	-12	LEU	-	expression tag	UNP P59768
G	-11	GLU	-	expression tag	UNP P59768
G	-10	PHE	-	expression tag	UNP P59768
G	-9	ILE	-	expression tag	UNP P59768
G	-8	ALA	-	expression tag	UNP P59768
G	-7	SER	-	expression tag	UNP P59768
G	-6	LYS	-	expression tag	UNP P59768
G	-5	LEU	-	expression tag	UNP P59768
G	-4	ALA	-	expression tag	UNP P59768
G	-3	GLY	-	expression tag	UNP P59768
G	-2	GLY	-	expression tag	UNP P59768
G	-1	GLY	-	expression tag	UNP P59768
G	0	SER	-	expression tag	UNP P59768
G	68	SER	CYS	conflict	UNP P59768

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	126	961	599	168	188	6	0	0

- Molecule 5 is a protein called Soluble cytochrome b562,Cannabinoid receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	279	2227	1487	364	358	18	0	0

There are 71 discrepancies between the modelled and reference sequences:

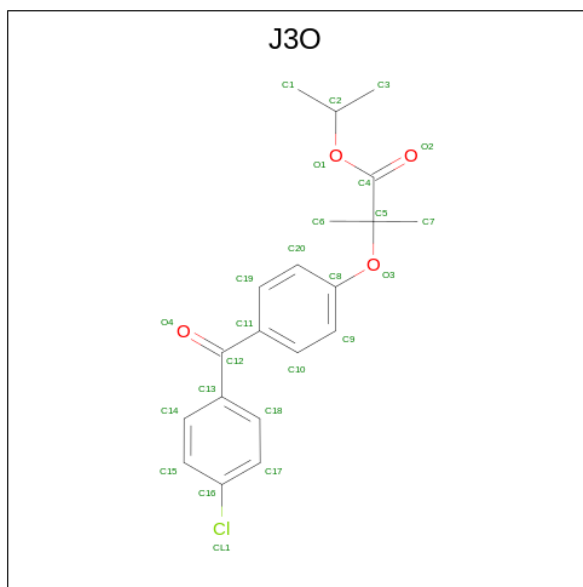
Chain	Residue	Modelled	Actual	Comment	Reference
R	-92	MET	-	initiating methionine	UNP P0ABE7
R	-91	LYS	-	expression tag	UNP P0ABE7
R	-90	THR	-	expression tag	UNP P0ABE7
R	-89	ILE	-	expression tag	UNP P0ABE7
R	-88	ILE	-	expression tag	UNP P0ABE7
R	-87	ALA	-	expression tag	UNP P0ABE7
R	-86	LEU	-	expression tag	UNP P0ABE7
R	-85	SER	-	expression tag	UNP P0ABE7
R	-84	TYR	-	expression tag	UNP P0ABE7
R	-83	ILE	-	expression tag	UNP P0ABE7
R	-82	PHE	-	expression tag	UNP P0ABE7
R	-81	CYS	-	expression tag	UNP P0ABE7
R	-80	LEU	-	expression tag	UNP P0ABE7
R	-79	VAL	-	expression tag	UNP P0ABE7
R	-78	PHE	-	expression tag	UNP P0ABE7
R	-77	ALA	-	expression tag	UNP P0ABE7
R	-76	ASP	-	expression tag	UNP P0ABE7
R	-75	TYR	-	expression tag	UNP P0ABE7
R	-74	LYS	-	expression tag	UNP P0ABE7
R	-73	ASP	-	expression tag	UNP P0ABE7
R	-72	ASP	-	expression tag	UNP P0ABE7
R	-71	ASP	-	expression tag	UNP P0ABE7
R	-70	ASP	-	expression tag	UNP P0ABE7
R	-69	ALA	-	expression tag	UNP P0ABE7
R	-68	LYS	-	expression tag	UNP P0ABE7
R	-67	LEU	-	expression tag	UNP P0ABE7
R	-66	GLN	-	expression tag	UNP P0ABE7
R	-65	THR	-	expression tag	UNP P0ABE7
R	-64	MET	-	expression tag	UNP P0ABE7
R	-63	HIS	-	expression tag	UNP P0ABE7
R	-62	HIS	-	expression tag	UNP P0ABE7
R	-61	HIS	-	expression tag	UNP P0ABE7
R	-60	HIS	-	expression tag	UNP P0ABE7
R	-59	HIS	-	expression tag	UNP P0ABE7
R	-58	HIS	-	expression tag	UNP P0ABE7
R	-57	HIS	-	expression tag	UNP P0ABE7
R	-56	HIS	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-55	HIS	-	expression tag	UNP P0ABE7
R	-54	HIS	-	expression tag	UNP P0ABE7
R	-53	GLU	-	expression tag	UNP P0ABE7
R	-52	ASN	-	expression tag	UNP P0ABE7
R	-51	LEU	-	expression tag	UNP P0ABE7
R	-50	TYR	-	expression tag	UNP P0ABE7
R	-49	PHE	-	expression tag	UNP P0ABE7
R	-48	GLN	-	expression tag	UNP P0ABE7
R	-47	GLY	-	expression tag	UNP P0ABE7
R	-46	GLY	-	expression tag	UNP P0ABE7
R	-45	GLY	-	expression tag	UNP P0ABE7
R	-44	ARG	-	expression tag	UNP P0ABE7
R	-37	TRP	MET	conflict	UNP P0ABE7
R	58	ILE	HIS	conflict	UNP P0ABE7
R	62	LEU	-	linker	UNP P0ABE7
R	63	LEU	-	linker	UNP P0ABE7
R	64	GLU	-	linker	UNP P0ABE7
R	65	VAL	-	linker	UNP P0ABE7
R	66	LEU	-	linker	UNP P0ABE7
R	67	PHE	-	linker	UNP P0ABE7
R	68	GLN	-	linker	UNP P0ABE7
R	69	GLY	-	linker	UNP P0ABE7
R	70	PRO	-	linker	UNP P0ABE7
R	210	ILE	THR	conflict	UNP P21554
R	273	LYS	GLU	conflict	UNP P21554
R	283	VAL	THR	conflict	UNP P21554
R	340	GLU	ARG	conflict	UNP P21554
R	426	HIS	-	expression tag	UNP P21554
R	427	HIS	-	expression tag	UNP P21554
R	428	HIS	-	expression tag	UNP P21554
R	429	HIS	-	expression tag	UNP P21554
R	430	HIS	-	expression tag	UNP P21554
R	431	HIS	-	expression tag	UNP P21554
R	432	HIS	-	expression tag	UNP P21554

- Molecule 6 is propan-2-yl 2-[4-(4-chlorophenyl)carbonylphenoxy]-2-methyl-propanoate (three-letter code: J3O) (formula: C₂₀H₂₁ClO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	Cl	O	
6	R	1	25	20	1	4	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	352452	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	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: J3O

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	0.27	0/2006	0.48	0/2699
2	B	0.28	0/2647	0.55	0/3589
3	G	0.24	0/375	0.49	0/505
4	N	0.30	0/981	0.53	0/1329
5	R	0.26	0/2281	0.45	0/3099
All	All	0.27	0/8290	0.50	0/11221

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	1970	0	1949	35	0
2	B	2600	0	2505	47	0
3	G	372	0	390	13	0
4	N	961	0	928	15	0
5	R	2227	0	2352	52	0
6	R	25	0	0	1	0
All	All	8155	0	8124	147	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 9.

The worst 5 of 147 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)
5:R:108:PHE:CE2	5:R:269:PRO:HG3	1.54	1.43
5:R:108:PHE:HE2	5:R:269:PRO:CG	1.57	1.17
5:R:108:PHE:CE2	5:R:269:PRO:CG	2.35	1.08
5:R:108:PHE:HE2	5:R:269:PRO:HG3	1.05	0.87
2:B:210:LEU:HD22	2:B:255:LEU:HD12	1.63	0.80

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	235/263 (89%)	223 (95%)	12 (5%)	0	100	100
2	B	336/340 (99%)	323 (96%)	13 (4%)	0	100	100
3	G	47/97 (48%)	42 (89%)	5 (11%)	0	100	100
4	N	124/139 (89%)	118 (95%)	6 (5%)	0	100	100
5	R	275/525 (52%)	257 (94%)	18 (6%)	0	100	100
All	All	1017/1364 (75%)	963 (95%)	54 (5%)	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	214/232 (92%)	213 (100%)	1 (0%)	88	96
2	B	281/283 (99%)	281 (100%)	0	100	100
3	G	39/76 (51%)	39 (100%)	0	100	100
4	N	104/116 (90%)	104 (100%)	0	100	100
5	R	249/461 (54%)	248 (100%)	1 (0%)	91	97
All	All	887/1168 (76%)	885 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	LYS
5	R	108	PHE

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 monosaccharides 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	J3O	R	501	-	26,26,26	0.29	0	37,37,37	0.92	2 (5%)

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	J3O	R	501	-	-	5/23/23/23	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	R	501	J3O	C10-C11-C12	2.85	126.83	120.57
6	R	501	J3O	C19-C11-C12	-2.70	114.64	120.57

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	501	J3O	C19-C11-C12-C13
6	R	501	J3O	O1-C4-C5-C6
6	R	501	J3O	O1-C4-C5-C7
6	R	501	J3O	O2-C4-C5-C6
6	R	501	J3O	O2-C4-C5-C7

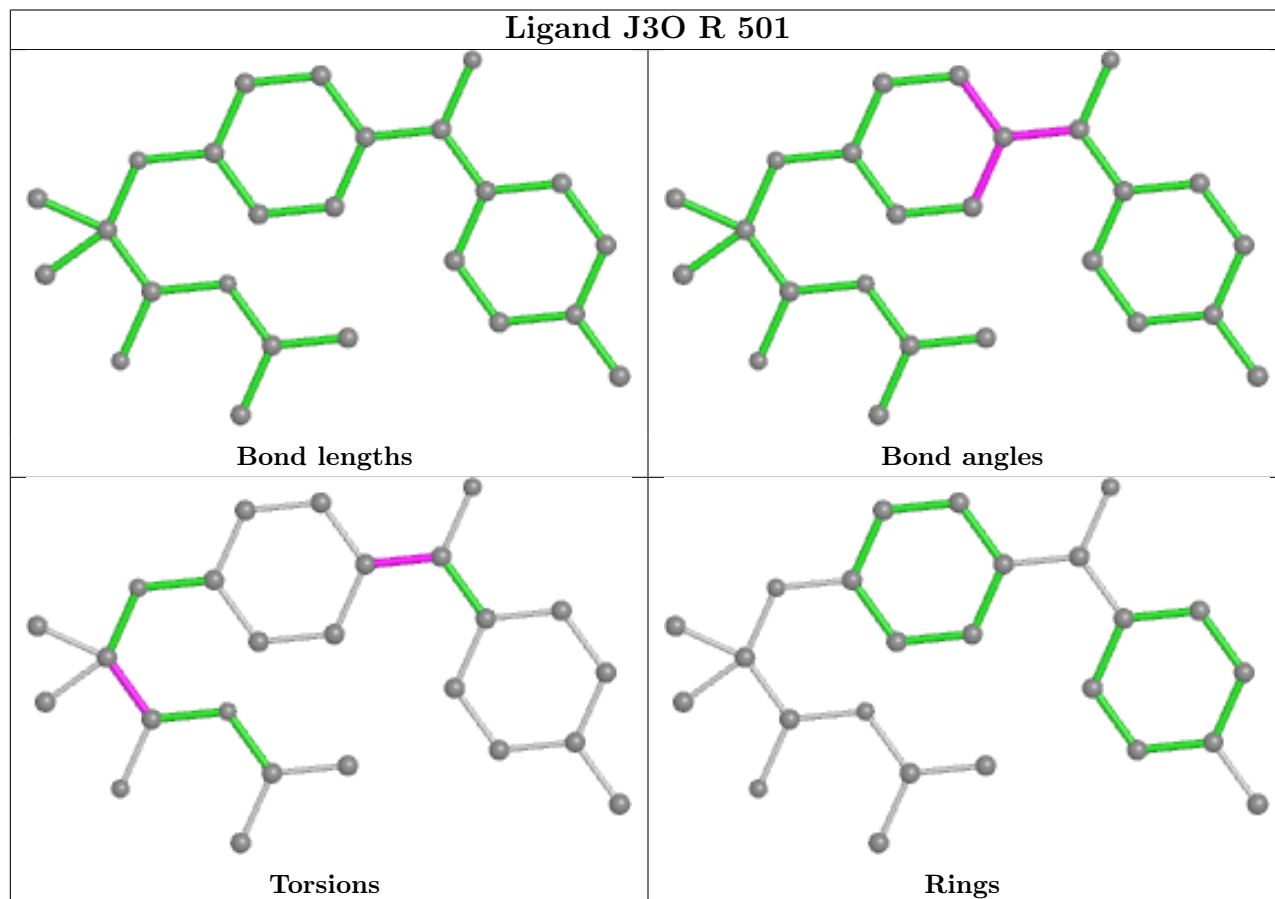
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	501	J3O	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 [i](#)

There are no chain breaks in this entry.