

wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Feb 4, 2020 – 10:41 AM EST

PDB ID : 6KPG
EMDB ID: : EMD-0745
Title : Cryo-EM structure of CB1-G protein complex
Authors : Hua, T.; Li, X.T.; Wu, L.J.; Makriyannis, A.; Wang, Y.X.; Shen, L.; Liu, Z.J.
Deposited on : 2019-08-15
Resolution : 3.00 Å(reported)
Based on PDB ID : 6N4B

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

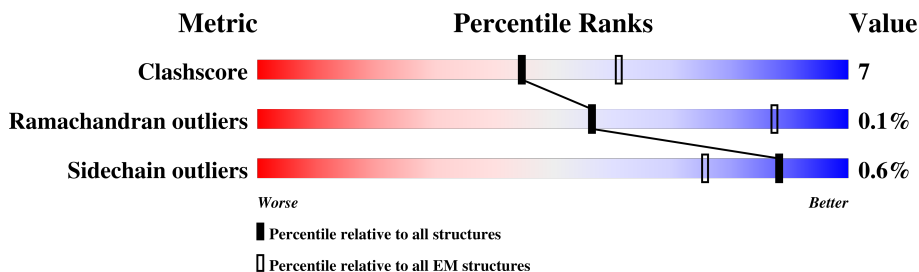
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	353	
2	B	346	
3	C	71	
4	R	469	
5	S	259	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8805 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(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	225	1771	1131	295	332	13	0	0

- 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	2592	1601	466	504	21	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	ILE	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	ARG	-	expression tag	UNP P62873
B	-2	ALA	-	expression tag	UNP P62873
B	-1	ARG	-	expression tag	UNP P62873
B	0	GLY	-	expression tag	UNP P62873
B	1	PHE	-	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
			Total	C	N	O	S		
3	C	56	433	271	76	83	3	0	0

- Molecule 4 is a protein called Cannabinoid receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	285	2223	1477	368	359	19	0	0

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-43	ALA	-	expression tag	UNP P21554
R	-42	ASP	-	expression tag	UNP P21554
R	-41	LEU	-	expression tag	UNP P21554
R	-40	GLU	-	expression tag	UNP P21554
R	-39	ASP	-	expression tag	UNP P21554
R	-38	ASN	-	expression tag	UNP P21554
R	-37	TRP	-	expression tag	UNP P21554
R	-36	GLU	-	expression tag	UNP P21554
R	-35	THR	-	expression tag	UNP P21554
R	-34	LEU	-	expression tag	UNP P21554
R	-33	ASN	-	expression tag	UNP P21554
R	-32	ASP	-	expression tag	UNP P21554
R	-31	ASN	-	expression tag	UNP P21554
R	-30	LEU	-	expression tag	UNP P21554
R	-29	LYS	-	expression tag	UNP P21554
R	-28	VAL	-	expression tag	UNP P21554
R	-27	ILE	-	expression tag	UNP P21554
R	-26	GLU	-	expression tag	UNP P21554
R	-25	LYS	-	expression tag	UNP P21554
R	-24	ALA	-	expression tag	UNP P21554
R	-23	ASP	-	expression tag	UNP P21554
R	-22	ASN	-	expression tag	UNP P21554
R	-21	ALA	-	expression tag	UNP P21554
R	-20	ALA	-	expression tag	UNP P21554
R	-19	GLN	-	expression tag	UNP P21554
R	-18	VAL	-	expression tag	UNP P21554
R	-17	LYS	-	expression tag	UNP P21554
R	-16	ASP	-	expression tag	UNP P21554
R	-15	ALA	-	expression tag	UNP P21554
R	-14	LEU	-	expression tag	UNP P21554
R	-13	THR	-	expression tag	UNP P21554
R	-12	LYS	-	expression tag	UNP P21554
R	-11	MET	-	expression tag	UNP P21554
R	-10	ARG	-	expression tag	UNP P21554
R	-9	ALA	-	expression tag	UNP P21554
R	-8	ALA	-	expression tag	UNP P21554
R	-7	ALA	-	expression tag	UNP P21554
R	-6	LEU	-	expression tag	UNP P21554
R	-5	ASP	-	expression tag	UNP P21554
R	-4	ALA	-	expression tag	UNP P21554
R	-3	GLN	-	expression tag	UNP P21554
R	-2	LYS	-	expression tag	UNP P21554

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ALA	-	expression tag	UNP P21554
R	0	THR	-	expression tag	UNP P21554
R	1	PRO	-	expression tag	UNP P21554
R	2	PRO	-	expression tag	UNP P21554
R	3	LYS	-	expression tag	UNP P21554
R	4	LEU	-	expression tag	UNP P21554
R	5	GLU	-	expression tag	UNP P21554
R	6	ASP	-	expression tag	UNP P21554
R	7	LYS	-	expression tag	UNP P21554
R	8	SER	-	expression tag	UNP P21554
R	9	PRO	-	expression tag	UNP P21554
R	10	ASP	-	expression tag	UNP P21554
R	11	SER	-	expression tag	UNP P21554
R	12	PRO	-	expression tag	UNP P21554
R	13	GLU	-	expression tag	UNP P21554
R	14	MET	-	expression tag	UNP P21554
R	15	LYS	-	expression tag	UNP P21554
R	16	ASP	-	expression tag	UNP P21554
R	17	PHE	-	expression tag	UNP P21554
R	18	ARG	-	expression tag	UNP P21554
R	19	HIS	-	expression tag	UNP P21554
R	20	GLY	-	expression tag	UNP P21554
R	21	PHE	-	expression tag	UNP P21554
R	22	ASP	-	expression tag	UNP P21554
R	23	ILE	-	expression tag	UNP P21554
R	24	LEU	-	expression tag	UNP P21554
R	25	VAL	-	expression tag	UNP P21554
R	26	GLY	-	expression tag	UNP P21554
R	27	GLN	-	expression tag	UNP P21554
R	28	ILE	-	expression tag	UNP P21554
R	29	ASP	-	expression tag	UNP P21554
R	30	ASP	-	expression tag	UNP P21554
R	31	ALA	-	expression tag	UNP P21554
R	32	LEU	-	expression tag	UNP P21554
R	33	LYS	-	expression tag	UNP P21554
R	34	LEU	-	expression tag	UNP P21554
R	35	ALA	-	expression tag	UNP P21554
R	36	ASN	-	expression tag	UNP P21554
R	37	GLU	-	expression tag	UNP P21554
R	38	GLY	-	expression tag	UNP P21554
R	39	LYS	-	expression tag	UNP P21554
R	40	VAL	-	expression tag	UNP P21554

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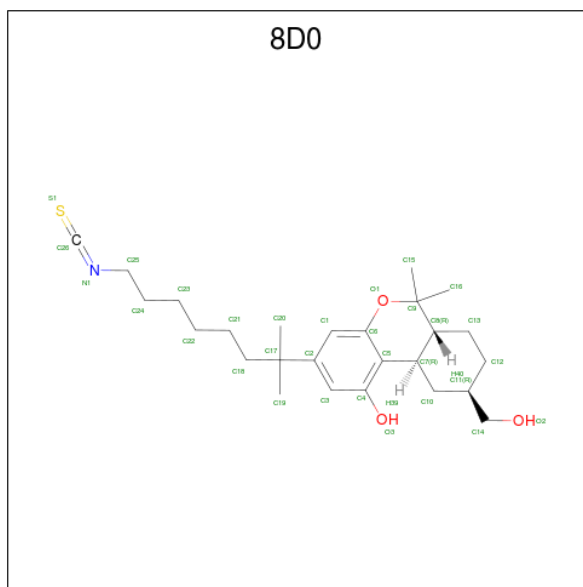
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Chain	Residue	Modelled	Actual	Comment	Reference
R	41	LYS	-	expression tag	UNP P21554
R	42	GLU	-	expression tag	UNP P21554
R	43	ALA	-	expression tag	UNP P21554
R	44	GLN	-	expression tag	UNP P21554
R	45	ALA	-	expression tag	UNP P21554
R	46	ALA	-	expression tag	UNP P21554
R	47	ALA	-	expression tag	UNP P21554
R	48	GLU	-	expression tag	UNP P21554
R	49	GLN	-	expression tag	UNP P21554
R	50	LEU	-	expression tag	UNP P21554
R	51	LYS	-	expression tag	UNP P21554
R	52	THR	-	expression tag	UNP P21554
R	53	THR	-	expression tag	UNP P21554
R	54	ARG	-	expression tag	UNP P21554
R	55	ASN	-	expression tag	UNP P21554
R	56	ALA	-	expression tag	UNP P21554
R	57	TYR	-	expression tag	UNP P21554
R	58	ILE	-	expression tag	UNP P21554
R	59	GLN	-	expression tag	UNP P21554
R	60	LYS	-	expression tag	UNP P21554
R	61	TYR	-	expression tag	UNP P21554
R	62	LEU	-	expression tag	UNP P21554
R	63	LEU	-	expression tag	UNP P21554
R	64	GLU	-	expression tag	UNP P21554
R	65	VAL	-	expression tag	UNP P21554
R	66	LEU	-	expression tag	UNP P21554
R	67	PHE	-	expression tag	UNP P21554
R	68	GLN	-	expression tag	UNP P21554
R	69	GLY	-	expression tag	UNP P21554
R	70	PRO	-	expression tag	UNP P21554
R	273	LYS	GLU	engineered mutation	UNP P21554
R	283	VAL	THR	engineered mutation	UNP P21554
R	340	GLU	ARG	engineered mutation	UNP P21554

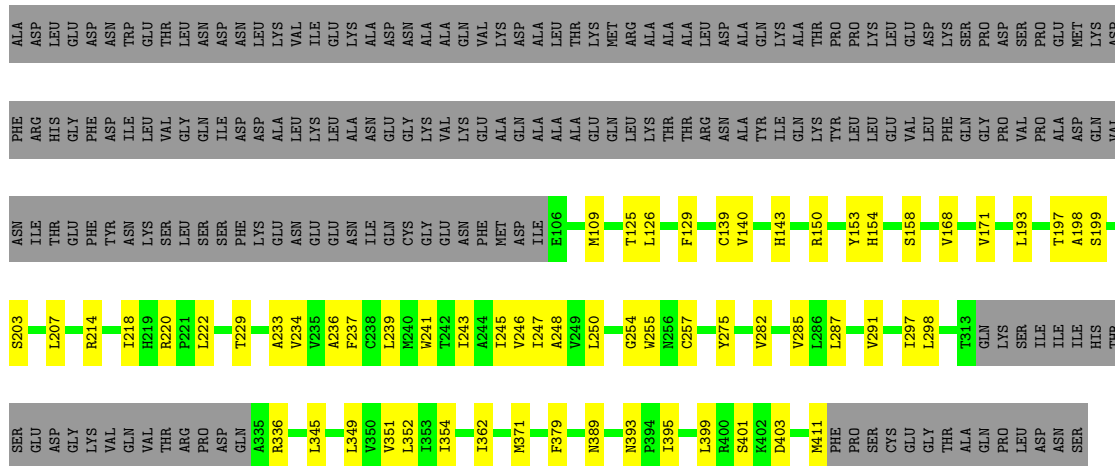
- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	231	1755	1117	294	334	10	0	0

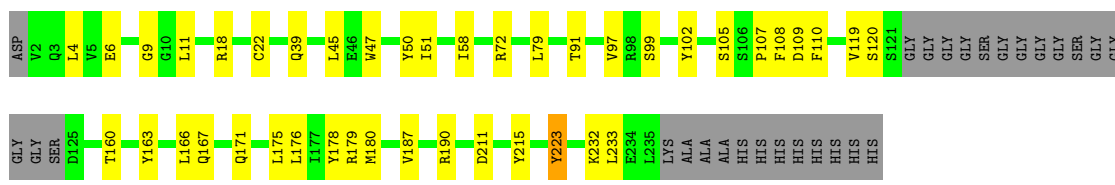
- Molecule 6 is (6 {a} {R},9 {R},10 {a} {R})-9-(hydroxymethyl)-3-(8-isothiocyanato-2-methyl-octan-2-yl)-6,6-dimethyl-6 {a},7,8,9,10,10 {a}-hexahydrobenzo[c]chromen-1-ol (three-letter code: 8D0) (formula: C₂₆H₃₉NO₃S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
6	R	1	31	26	1	3	1	0



• Molecule 5: scFv16



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	505644	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 ($e^-/\text{\AA}^2$)	1.333	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: 8D0

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 >2	RMSZ	# Z >2
1	A	0.55	0/1801	0.56	0/2421
2	B	0.74	1/2639 (0.0%)	0.67	1/3577 (0.0%)
3	C	0.39	0/439	0.50	0/592
4	R	0.36	0/2275	0.59	1/3092 (0.0%)
5	S	0.62	0/1799	0.65	0/2441
All	All	0.58	1/8953 (0.0%)	0.62	2/12123 (0.0%)

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
2	B	0	1
5	S	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	103	CYS	CB-SG	-6.84	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	R	193	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	79	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	86	THR	Peptide
5	S	223	TYR	Peptide

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	1771	0	1744	28	0
2	B	2592	0	2497	48	0
3	C	433	0	442	3	0
4	R	2223	0	2301	36	0
5	S	1755	0	1695	23	0
6	R	31	0	0	0	0
All	All	8805	0	8679	130	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 7.

The worst 5 of 130 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:271:LYS:HG2	1:A:325:CYS:HB3	1.73	0.70
4:R:255:TRP:HE1	4:R:275:TYR:HB2	1.57	0.69
5:S:160:THR:HB	5:S:180:MET:HB2	1.78	0.66
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.81	0.62
2:B:253:PHE:HA	2:B:260:GLU:HA	1.80	0.62

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	221/353 (63%)	206 (93%)	15 (7%)	0	100	100
2	B	336/346 (97%)	305 (91%)	31 (9%)	0	100	100
3	C	54/71 (76%)	49 (91%)	5 (9%)	0	100	100
4	R	281/469 (60%)	264 (94%)	17 (6%)	0	100	100
5	S	227/259 (88%)	211 (93%)	15 (7%)	1 (0%)	36	76
All	All	1119/1498 (75%)	1035 (92%)	83 (7%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	S	223	TYR

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	189/304 (62%)	189 (100%)	0	100	100
2	B	278/286 (97%)	277 (100%)	1 (0%)	92	97
3	C	46/58 (79%)	45 (98%)	1 (2%)	55	84
4	R	238/411 (58%)	234 (98%)	4 (2%)	63	88
5	S	191/209 (91%)	191 (100%)	0	100	100
All	All	942/1268 (74%)	936 (99%)	6 (1%)	88	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	222	LEU
4	R	371	MET
4	R	257	CYS
3	C	62	ARG

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Mol	Chain	Res	Type
4	R	336	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	ASN
2	B	156	GLN
3	C	44	HIS
2	B	88	ASN
2	B	91	HIS

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 carbohydrates 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	8D0	R	501	-	32,33,33	1.69	7 (21%)	46,48,48	1.64	10 (21%)

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	8D0	R	501	-	-	5/17/46/46	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	8D0	C10-C7	4.51	1.60	1.53
6	R	501	8D0	C13-C8	3.76	1.60	1.53
6	R	501	8D0	C4-C5	3.02	1.44	1.40
6	R	501	8D0	O1-C9	-2.99	1.41	1.46
6	R	501	8D0	C5-C7	2.85	1.56	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	8D0	C25-N1-C26	-5.28	120.25	159.28
6	R	501	8D0	O3-C4-C5	3.20	127.13	118.84
6	R	501	8D0	C13-C12-C11	-2.82	107.67	112.42
6	R	501	8D0	C13-C8-C9	-2.76	109.61	114.67
6	R	501	8D0	C10-C7-C5	2.75	117.08	113.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

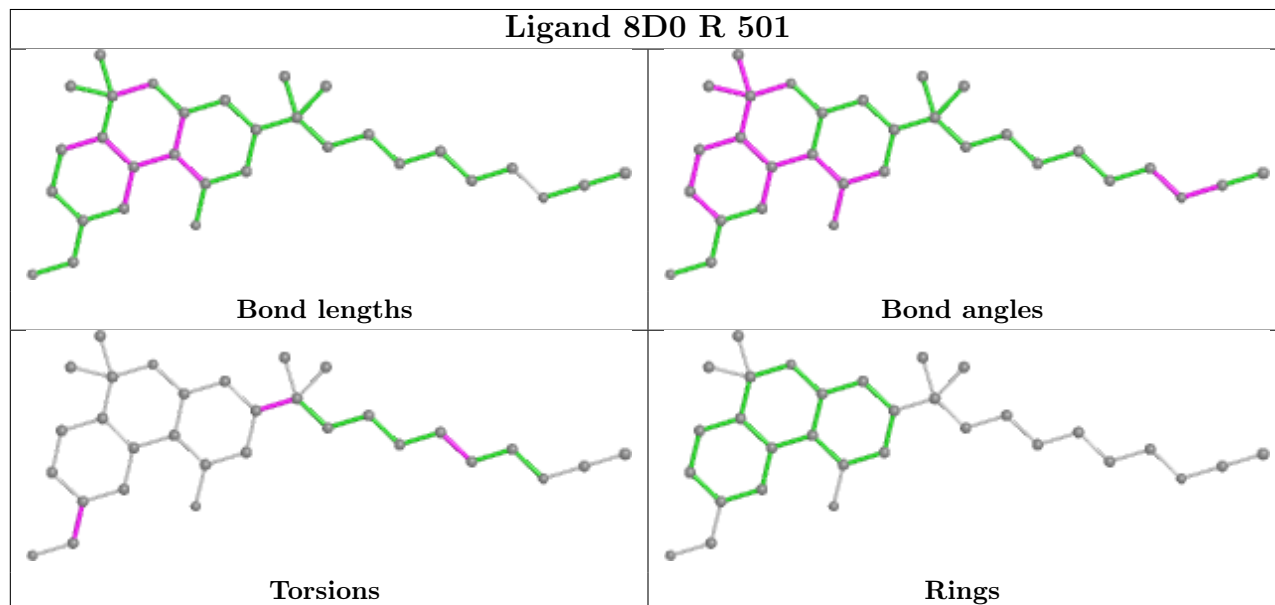
Mol	Chain	Res	Type	Atoms
6	R	501	8D0	C10-C11-C14-O2
6	R	501	8D0	C12-C11-C14-O2
6	R	501	8D0	C22-C23-C24-C25
6	R	501	8D0	C20-C17-C2-C1
6	R	501	8D0	C20-C17-C2-C3

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 [i](#)

There are no chain breaks in this entry.