



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 12:52 PM JST

PDB ID : 8J6Q
EMDB ID : EMD-36011
Title : Cryo-EM structure of the 3-HB and compound 9n-bound human HCAR2-Gi1 complex
Authors : Mao, C.; Gao, M.; Zang, S.; Zhu, Y.; Ma, X.; Zhang, Y.
Deposited on : 2023-04-26
Resolution : 2.60 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

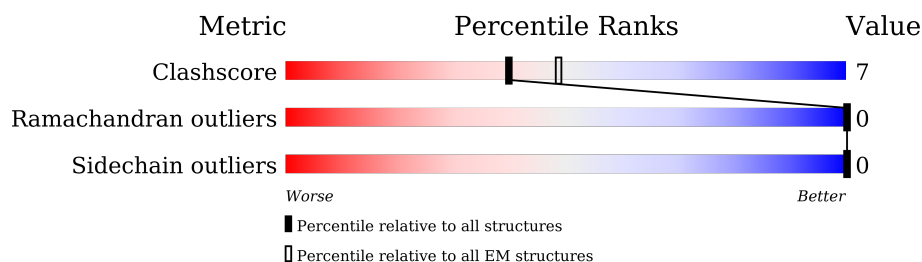
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	352	
2	B	339	
3	G	58	
4	S	250	
5	R	295	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9187 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
1	A	225	Total	C	N	O	S	0	0
			1811	1150	301	346	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- 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	339	Total	C	N	O	S	0	0
			2607	1607	468	511	21		

- 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	58	Total	C	N	O	S	0	0
			444	277	79	85	3		

- Molecule 4 is a protein called single Fab chain (scFv16).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	234	Total	C	N	O	S	0	0
			1795	1137	297	351	10		

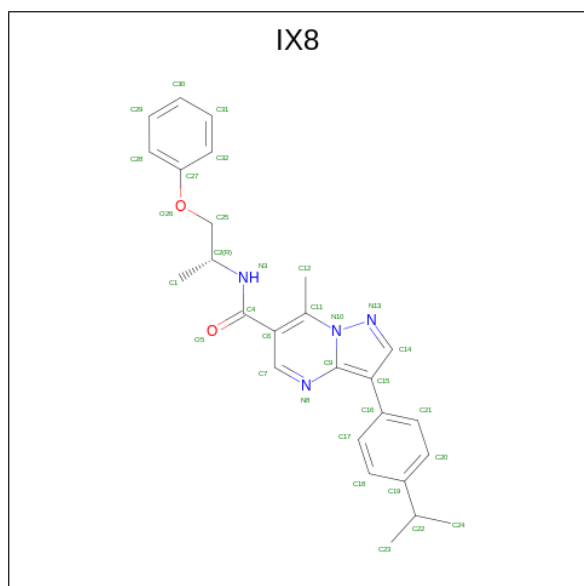
- Molecule 5 is a protein called Hydroxycarboxylic acid receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	295	Total	C	N	O	S	0	0
			2420	1613	404	382	21		

There is a discrepancy between the modelled and reference sequences:

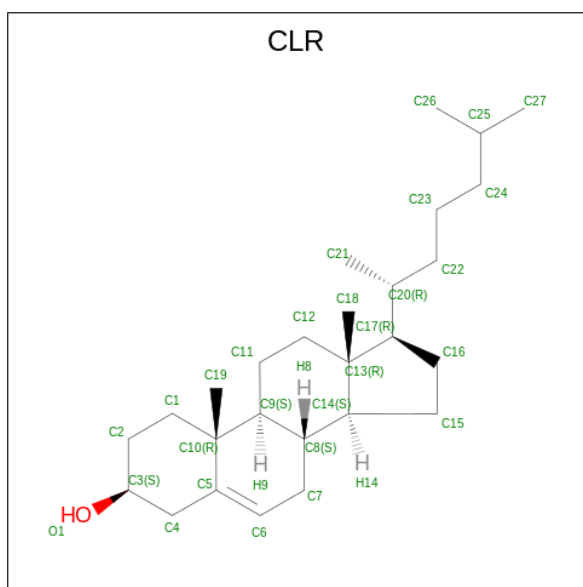
Chain	Residue	Modelled	Actual	Comment	Reference
R	302	ASN	-	expression tag	UNP Q8TDS4

- Molecule 6 is 7-methyl-N-[(2R)-1-phenoxypropan-2-yl]-3-(4-propan-2-ylphenyl)pyrazolo[1,5-a]pyrimidine-6-carboxamide (three-letter code: IX8) (formula: C₂₆H₂₈N₄O₂).



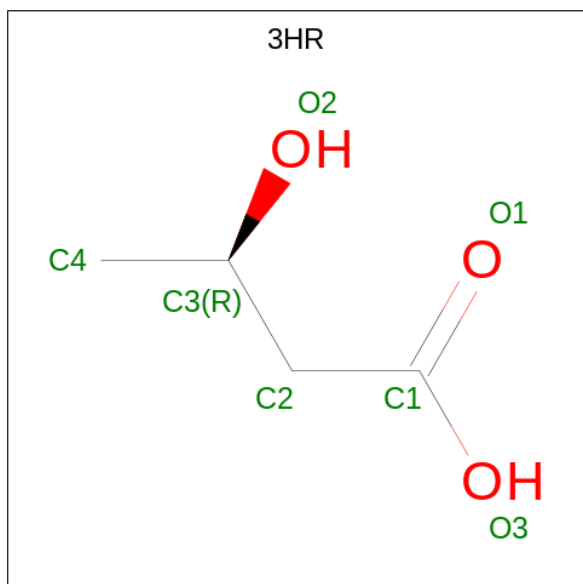
Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			32	26	4	2	

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			28	27	1	
7	R	1	Total	C	O	0
			28	27	1	

- Molecule 8 is (3R)-3-hydroxybutanoic acid (three-letter code: 3HR) (formula: $C_4H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
8	R	1	Total	C	O	0
			7	4	3	

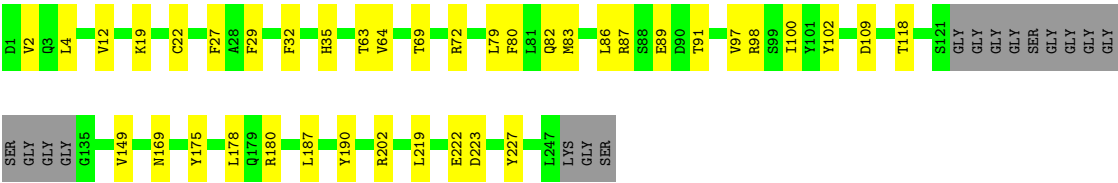
- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



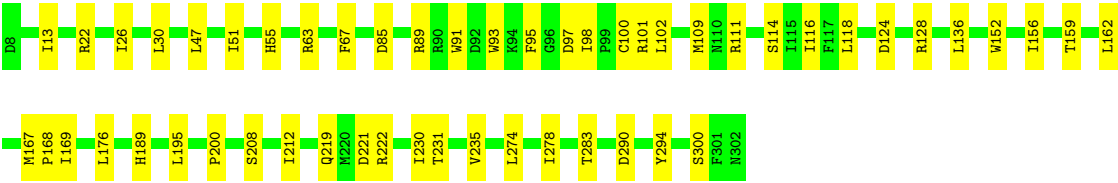
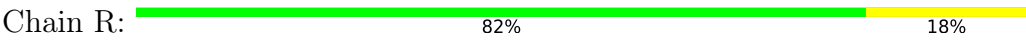
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	R	1	14	8	1	5	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		AltConf
10	R	1	Total	O	0
			1	1	



● Molecule 5: Hydroxycarboxylic acid receptor 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157251	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: NAG, 3HR, CLR, IX8

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	0.26	0/1841	0.46	0/2471
2	B	0.27	0/2654	0.55	0/3597
3	G	0.24	0/450	0.47	0/608
4	S	0.28	0/1839	0.52	0/2493
5	R	0.26	0/2491	0.50	0/3377
All	All	0.26	0/9275	0.51	0/12546

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	1811	0	1799	22	0
2	B	2607	0	2510	48	0
3	G	444	0	454	0	0
4	S	1795	0	1727	24	0
5	R	2420	0	2476	37	0
6	R	32	0	0	0	0
7	R	56	0	92	6	0
8	R	7	0	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	R	14	0	13	0	0
10	R	1	0	0	0	0
All	All	9187	0	9078	126	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 126 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)
4:S:187:LEU:HD21	4:S:190:TYR:HB3	1.76	0.67
2:B:158:VAL:HG12	2:B:190:LEU:HD21	1.76	0.67
5:R:111:ARG:HD3	5:R:283:THR:HG21	1.77	0.66
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.29	0.65
4:S:180:ARG:NH2	4:S:222:GLU:OE2	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	A	221/352 (63%)	218 (99%)	3 (1%)	0	100	100
2	B	337/339 (99%)	329 (98%)	8 (2%)	0	100	100
3	G	56/58 (97%)	56 (100%)	0	0	100	100
4	S	230/250 (92%)	225 (98%)	5 (2%)	0	100	100
5	R	293/295 (99%)	278 (95%)	15 (5%)	0	100	100
All	All	1137/1294 (88%)	1106 (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	200/304 (66%)	200 (100%)	0	100	100
2	B	282/282 (100%)	282 (100%)	0	100	100
3	G	47/47 (100%)	47 (100%)	0	100	100
4	S	198/202 (98%)	198 (100%)	0	100	100
5	R	268/268 (100%)	268 (100%)	0	100	100
All	All	995/1103 (90%)	995 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	331	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
7	CLR	R	404	-	31,31,31	0.65	0	48,48,48	1.06	3 (6%)
9	NAG	R	405	5	14,14,15	0.24	0	17,19,21	0.44	0
8	3HR	R	403	-	6,6,6	1.43	1 (16%)	6,7,7	1.54	2 (33%)
7	CLR	R	402	-	31,31,31	0.69	0	48,48,48	1.10	4 (8%)
6	IX8	R	401	-	28,35,35	1.79	7 (25%)	34,49,49	2.63	17 (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
7	CLR	R	404	-	-	6/10/68/68	0/4/4/4
9	NAG	R	405	5	-	0/6/23/26	0/1/1/1
8	3HR	R	403	-	-	1/4/4/4	-
7	CLR	R	402	-	-	5/10/68/68	0/4/4/4
6	IX8	R	401	-	-	6/21/21/21	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	401	IX8	C4-N3	4.81	1.44	1.34
6	R	401	IX8	C6-C4	3.56	1.57	1.50
6	R	401	IX8	C15-C16	3.13	1.55	1.49
6	R	401	IX8	C2-N3	2.84	1.54	1.46
8	R	403	3HR	O1-C1	2.57	1.30	1.22

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	401	IX8	C18-C19-C20	-6.31	110.42	118.29
6	R	401	IX8	C21-C16-C17	-4.37	108.87	117.59
6	R	401	IX8	C12-C11-C6	-4.22	119.26	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	401	IX8	C6-C4-N3	3.62	123.50	116.80
6	R	401	IX8	C21-C16-C15	3.49	126.73	120.86

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

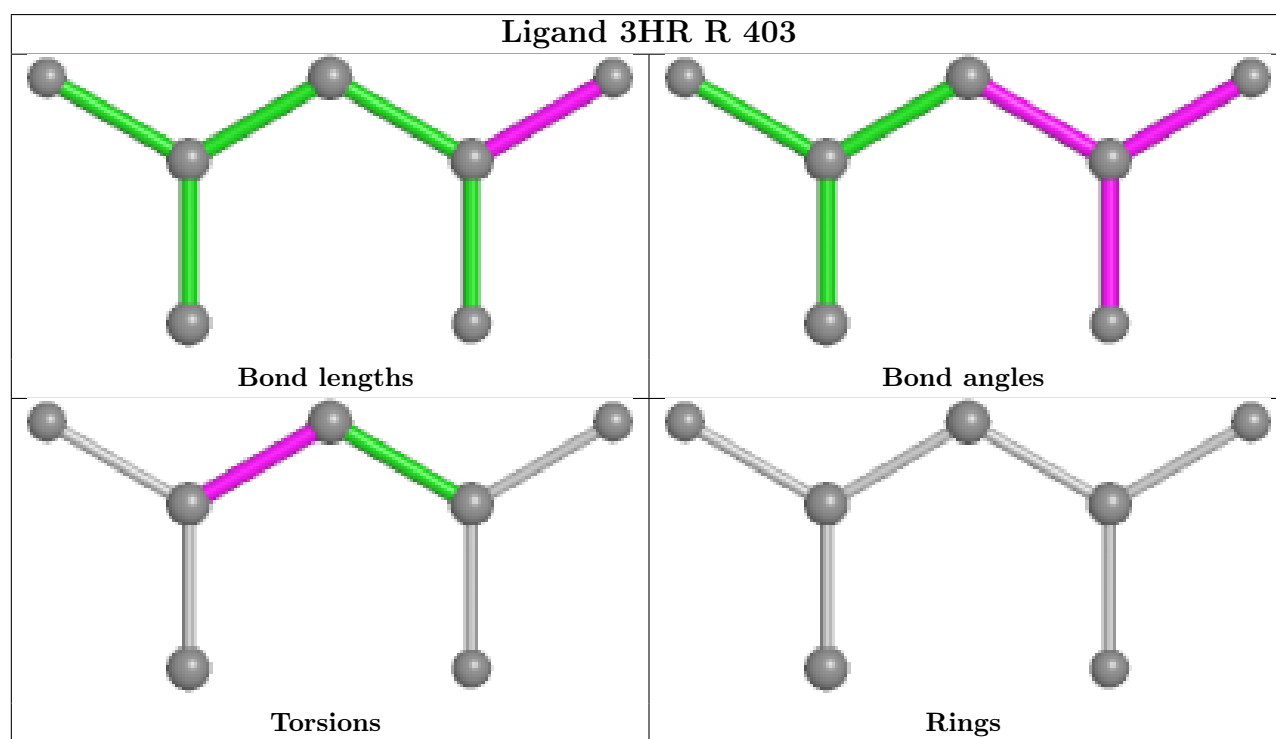
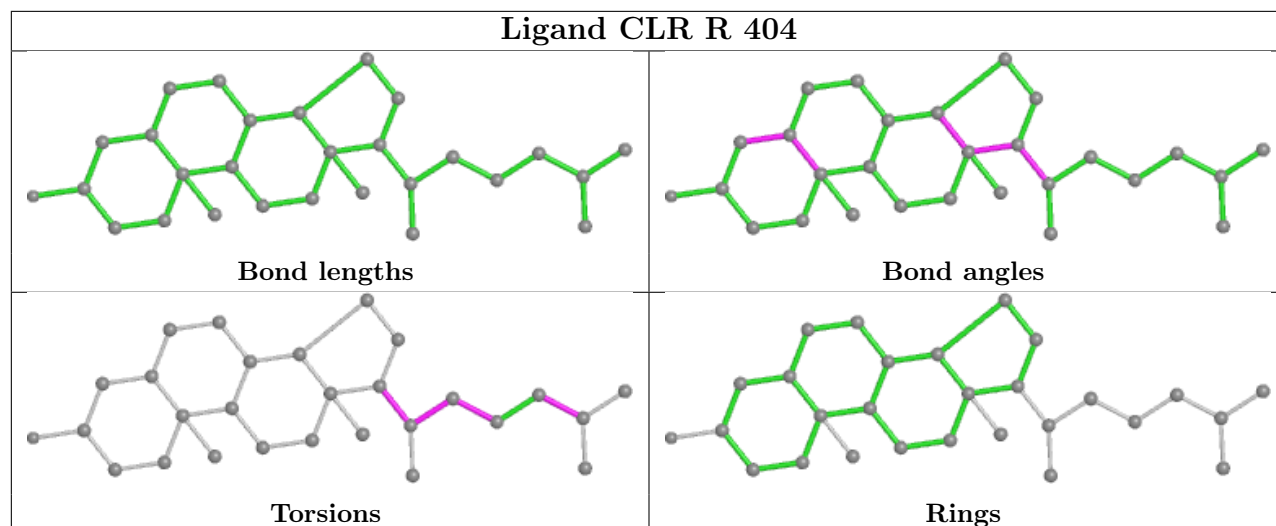
Mol	Chain	Res	Type	Atoms
6	R	401	IX8	C9-C15-C16-C17
6	R	401	IX8	C9-C15-C16-C21
6	R	401	IX8	C14-C15-C16-C17
6	R	401	IX8	C14-C15-C16-C21
7	R	402	CLR	C13-C17-C20-C21

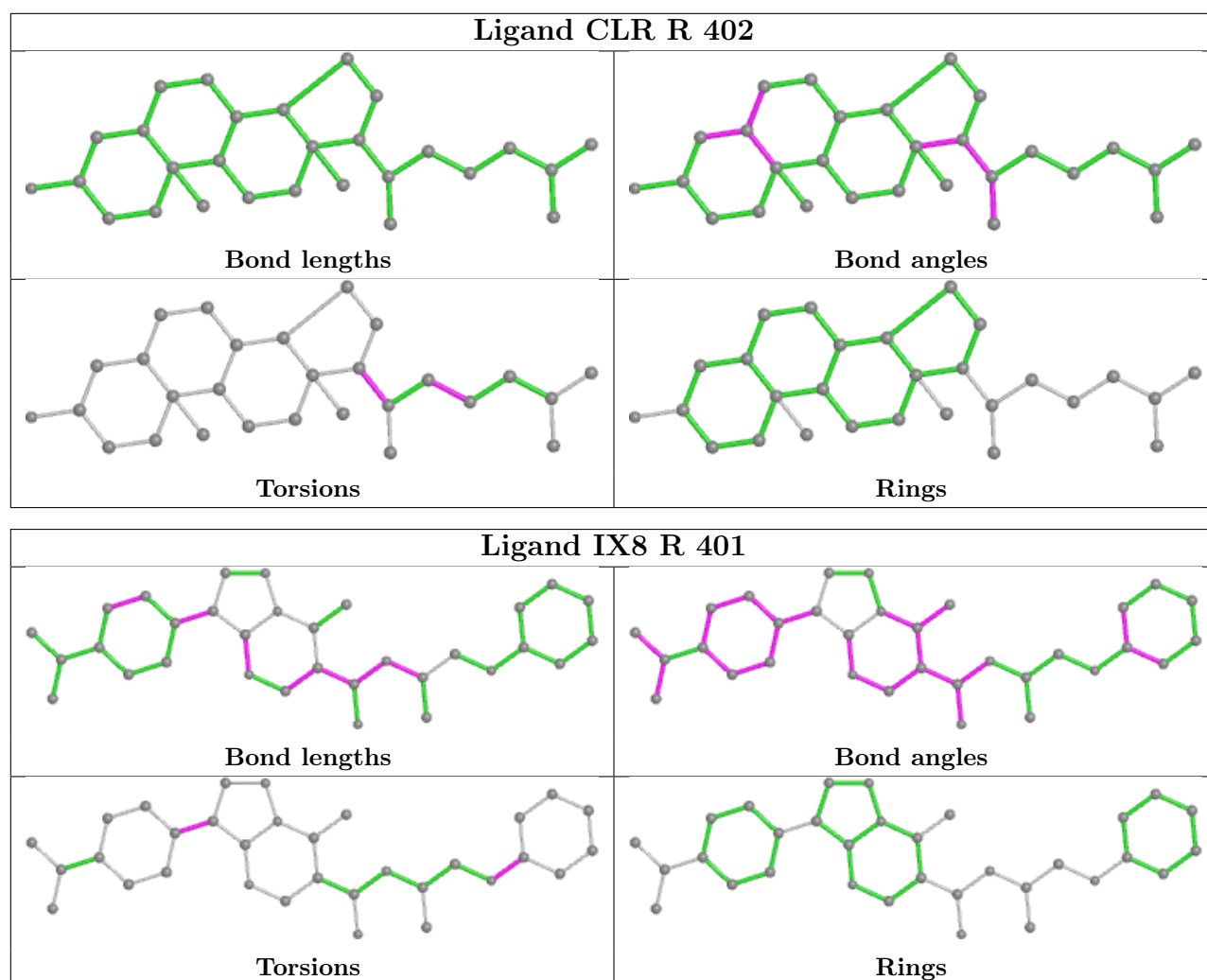
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	404	CLR	3	0
7	R	402	CLR	3	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.