



## Full wwPDB EM Validation Report ⓘ

Dec 24, 2023 – 12:07 AM JST

PDB ID : 8W88  
EMDB ID : EMD-37348  
Title : Cryo-EM structure of the SEP363856-bound TAAR1-Gs complex  
Authors : Liu, H.; Zheng, Y.; Wang, Y.; Wang, Y.; He, X.; Xu, P.; Huang, S.; Yuan, Q.;  
Zhang, X.; Wang, S.; Xu, H.E.; Xu, F.  
Deposited on : 2023-09-01  
Resolution : 2.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

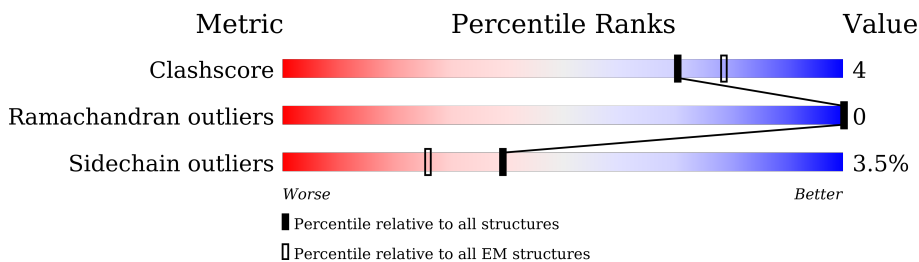
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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	54% (green), 6% (yellow), 40% (grey)
2	B	345	87% (green), 11% (yellow), 2% (grey)
3	G	71	75% (green), 6% (yellow), 20% (grey)
4	N	139	79% (green), 11% (yellow), 9% (grey)
5	R	339	76% (green), 6% (yellow), 17% (grey)

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8307 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	236	1957	1230	358	362	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ALA	GLY	conflict	UNP P63092
A	365	SER	ALA	variant	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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	initiating methionine	UNP P62873
B	10	GLY	-	expression tag	UNP P62873
B	11	SER	-	expression tag	UNP P62873
B	12	LEU	-	expression tag	UNP P62873
B	13	LEU	-	expression tag	UNP P62873
B	14	GLN	-	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	G	57	433	271	75	84	3	0	0

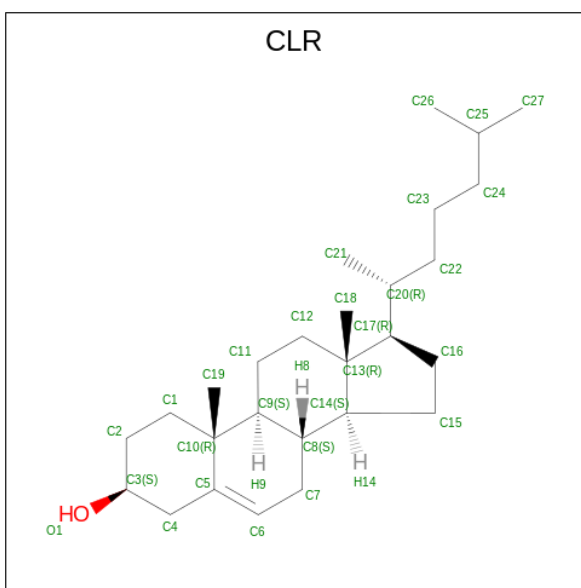
- Molecule 4 is a protein called Nanobody35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	127	967	602	169	190	6	0	0

- Molecule 5 is a protein called Trace amine-associated receptor 1.

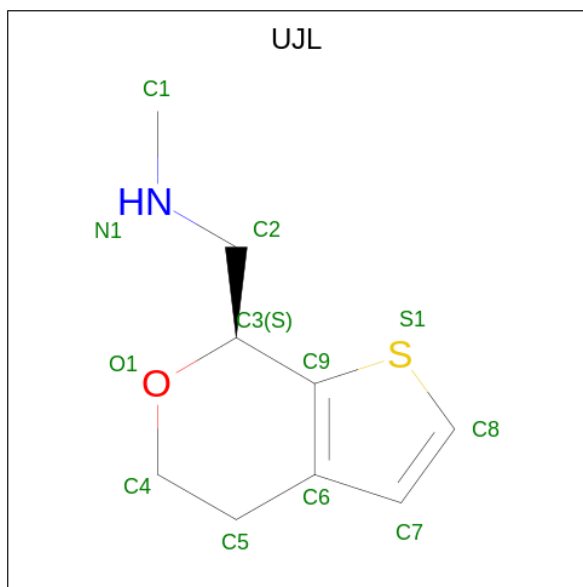
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	281	2254	1510	349	371	24	0	0

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ) (labeled as "Ligand of Interest" by depositor).



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


- Molecule 7 is 1-[(7 {S})-5,7-dihydro-4 {H}-thieno[2,3-c]pyran-7-yl]- {N}-methyl-methanamine (three-letter code: UJL) (formula:  $C_9H_{13}NOS$ ) (labeled as "Ligand of Interest" by depositor).

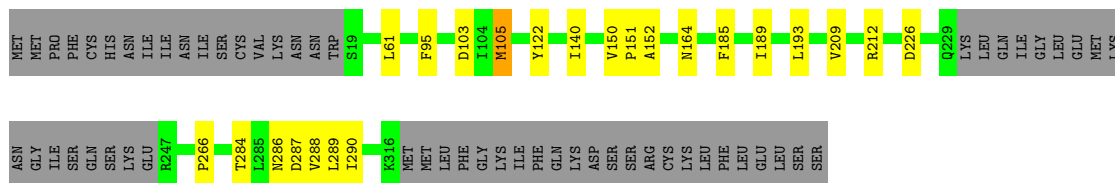


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
7	R	1	12	9	1	1	1	0



• Molecule 5: Trace amine-associated receptor 1

Chain R:  76% 6% 17%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	664918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	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: CLR, UJL

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	0.30	0/1992	0.54	0/2677
2	B	0.31	0/2647	0.54	0/3589
3	G	0.26	0/439	0.43	0/594
4	N	0.32	0/987	0.53	0/1337
5	R	0.31	0/2323	0.44	0/3160
All	All	0.31	0/8388	0.51	0/11357

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	1957	0	1941	15	0
2	B	2600	0	2505	22	0
3	G	433	0	441	5	0
4	N	967	0	934	8	0
5	R	2254	0	2265	14	0
6	R	84	0	138	1	0
7	R	12	0	0	2	0
All	All	8307	0	8224	58	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 4.

All (58) 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:326:GLU:N	1:A:326:GLU:OE2	2.14	0.81
5:R:103:ASP:OD2	7:R:404:UJL:C3	2.29	0.80
5:R:284:THR:O	5:R:288:VAL:HG23	1.98	0.64
4:N:54:GLN:N	4:N:54:GLN:OE1	2.32	0.63
1:A:19:ARG:NH1	2:B:101:ASN:OD1	2.33	0.62
4:N:53:SER:O	4:N:73:ARG:NH1	2.36	0.58
5:R:95:PHE:CZ	6:R:403:CLR:H191	2.38	0.57
5:R:105:MET:HG3	5:R:152:ALA:HA	1.88	0.56
2:B:176:ASP:O	2:B:177:THR:HB	2.05	0.56
2:B:86:ALA:HB2	2:B:116:CYS:SG	2.47	0.55
5:R:164:ASN:ND2	5:R:185:PHE:O	2.34	0.54
4:N:106:ARG:HB2	4:N:106:ARG:NH1	2.23	0.54
2:B:177:THR:CG2	2:B:177:THR:O	2.57	0.53
1:A:238:ASN:O	1:A:284:ILE:HD11	2.10	0.52
2:B:177:THR:O	2:B:177:THR:HG22	2.10	0.52
2:B:239:GLU:HB2	2:B:260:ASP:OD1	2.09	0.52
2:B:208:ASP:O	2:B:209:THR:OG1	2.27	0.52
5:R:122:TYR:OH	5:R:212:ARG:NH1	2.40	0.51
1:A:16:LYS:O	1:A:20:GLU:HG2	2.09	0.51
5:R:287:ASP:O	5:R:290:ILE:HG13	2.12	0.50
2:B:46:ILE:HG22	3:G:37:MET:HE1	1.93	0.49
2:B:43:LEU:HD23	2:B:275:MET:HE3	1.94	0.47
5:R:122:TYR:HB2	5:R:209:VAL:HG13	1.95	0.47
1:A:261:GLN:OE1	1:A:264:ARG:NH1	2.47	0.47
1:A:361:HIS:NE2	1:A:377:ASP:OD2	2.36	0.47
1:A:313:GLU:OE2	1:A:313:GLU:N	2.29	0.47
5:R:266:PRO:HB2	5:R:289:LEU:HD22	1.98	0.46
2:B:233:GLN:NE2	2:B:268:LEU:O	2.46	0.46
1:A:294:ASP:N	1:A:294:ASP:OD1	2.49	0.46
1:A:324:THR:O	1:A:324:THR:OG1	2.29	0.46
2:B:137:TYR:CE2	2:B:148:VAL:HG22	2.51	0.46
1:A:283:THR:O	1:A:283:THR:CG2	2.63	0.45
4:N:8:SER:N	4:N:22:SER:O	2.46	0.45
2:B:305:PHE:N	2:B:305:PHE:CD1	2.85	0.44
1:A:366:VAL:O	1:A:366:VAL:HG23	2.18	0.44
2:B:260:ASP:O	2:B:261:ALA:HB3	2.17	0.44
2:B:238:HIS:CD2	2:B:264:ARG:HE	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:61:LEU:HG	5:R:140:ILE:HG23	2.00	0.44
1:A:317:TYR:OH	1:A:342:ASP:OD2	2.23	0.44
5:R:189:ILE:O	5:R:193:LEU:HD23	2.18	0.44
5:R:103:ASP:OD2	7:R:404:UJL:O1	2.36	0.44
2:B:176:ASP:O	2:B:176:ASP:OD1	2.36	0.43
2:B:258:SER:OG	2:B:260:ASP:HB2	2.18	0.43
4:N:4:GLN:NE2	4:N:6:GLN:OE1	2.50	0.43
2:B:191:THR:HG22	2:B:192:THR:N	2.33	0.43
2:B:271:ASP:OD2	3:G:24:ILE:HD11	2.19	0.43
2:B:19:GLN:OE1	2:B:19:GLN:N	2.47	0.43
4:N:106:ARG:HB2	4:N:106:ARG:HH11	1.84	0.42
1:A:19:ARG:HH11	1:A:19:ARG:HG2	1.84	0.42
1:A:283:THR:O	1:A:283:THR:HG22	2.19	0.42
5:R:286:ASN:O	5:R:290:ILE:HG23	2.20	0.42
2:B:43:LEU:HD13	3:G:33:ALA:HB1	2.01	0.41
1:A:223:VAL:HG21	1:A:233:TRP:CZ3	2.56	0.41
4:N:92:THR:HG23	4:N:126:THR:HA	2.02	0.41
5:R:150:VAL:N	5:R:151:PRO:HD2	2.36	0.41
2:B:43:LEU:CD1	3:G:33:ALA:HB1	2.50	0.41
4:N:80:LEU:HD23	4:N:97:CYS:SG	2.61	0.40
2:B:46:ILE:HD12	3:G:33:ALA:HB3	2.03	0.40

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	230/394 (58%)	223 (97%)	7 (3%)	0	100	100
2	B	336/345 (97%)	322 (96%)	14 (4%)	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	N	125/139 (90%)	122 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	277/339 (82%)	273 (99%)	4 (1%)	0	100	100
All	All	1023/1288 (79%)	995 (97%)	28 (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	213/351 (61%)	207 (97%)	6 (3%)	43	69
2	B	281/287 (98%)	266 (95%)	15 (5%)	22	45
3	G	46/58 (79%)	45 (98%)	1 (2%)	52	76
4	N	105/116 (90%)	98 (93%)	7 (7%)	16	33
5	R	249/309 (81%)	247 (99%)	2 (1%)	81	92
All	All	894/1121 (80%)	863 (96%)	31 (4%)	39	62

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	18	GLN
1	A	26	GLU
1	A	27	LYS
1	A	316	ARG
1	A	356	HIS
2	B	21	ARG
2	B	72	TYR
2	B	91	LYS
2	B	114	MET
2	B	118	TYR
2	B	159	LEU
2	B	166	ASP
2	B	227	ARG

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Mol	Chain	Res	Type
2	B	230	MET
2	B	232	ARG
2	B	247	PHE
2	B	275	MET
2	B	287	THR
2	B	325	ASP
2	B	353	ASN
3	G	56	SER
4	N	6	GLN
4	N	22	SER
4	N	31	SER
4	N	68	ARG
4	N	77	LYS
4	N	81	TYR
4	N	109	PHE
5	R	105	MET
5	R	226	ASP

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	13	ASN
2	B	238	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
6	CLR	R	401	-	31,31,31	0.36	0	48,48,48	0.59	0
6	CLR	R	403	-	31,31,31	0.36	0	48,48,48	0.53	0
6	CLR	R	402	-	31,31,31	0.39	0	48,48,48	0.76	0
7	UJL	R	404	-	9,13,13	3.42	2 (22%)	4,17,17	2.87	2 (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
6	CLR	R	401	-	-	0/10/68/68	0/4/4/4
6	CLR	R	403	-	-	0/10/68/68	0/4/4/4
6	CLR	R	402	-	-	1/10/68/68	0/4/4/4
7	UJL	R	404	-	-	1/3/13/13	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	404	UJL	C9-S1	-9.29	1.56	1.74
7	R	404	UJL	C8-S1	-3.74	1.53	1.71

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	404	UJL	C4-C5-C6	5.07	118.13	110.87
7	R	404	UJL	O1-C4-C5	2.36	112.91	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	404	UJL	N1-C2-C3-O1

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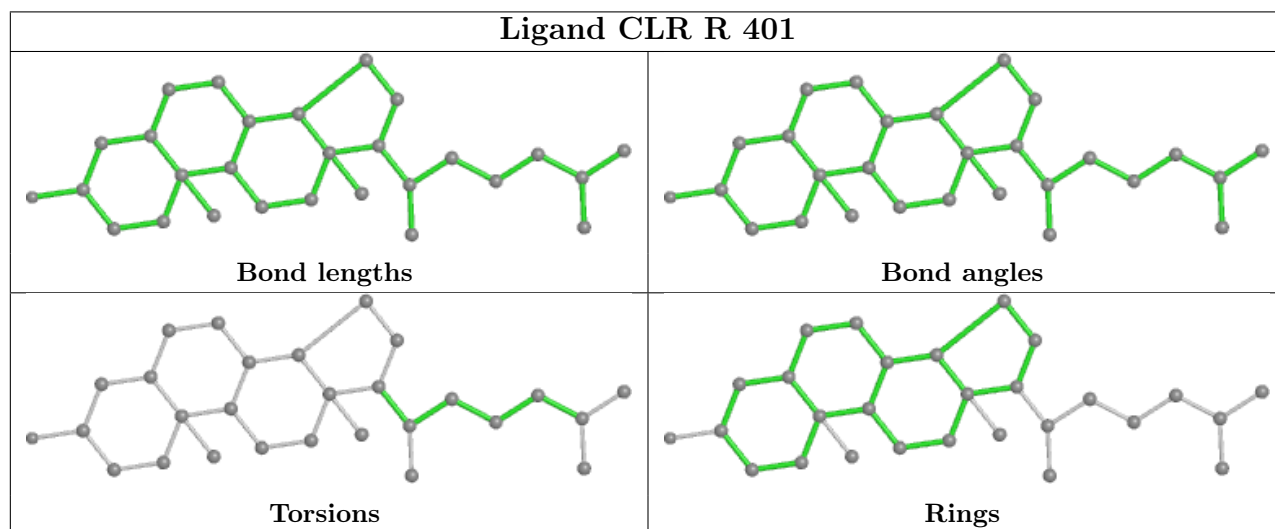
Mol	Chain	Res	Type	Atoms
6	R	402	CLR	C20-C22-C23-C24

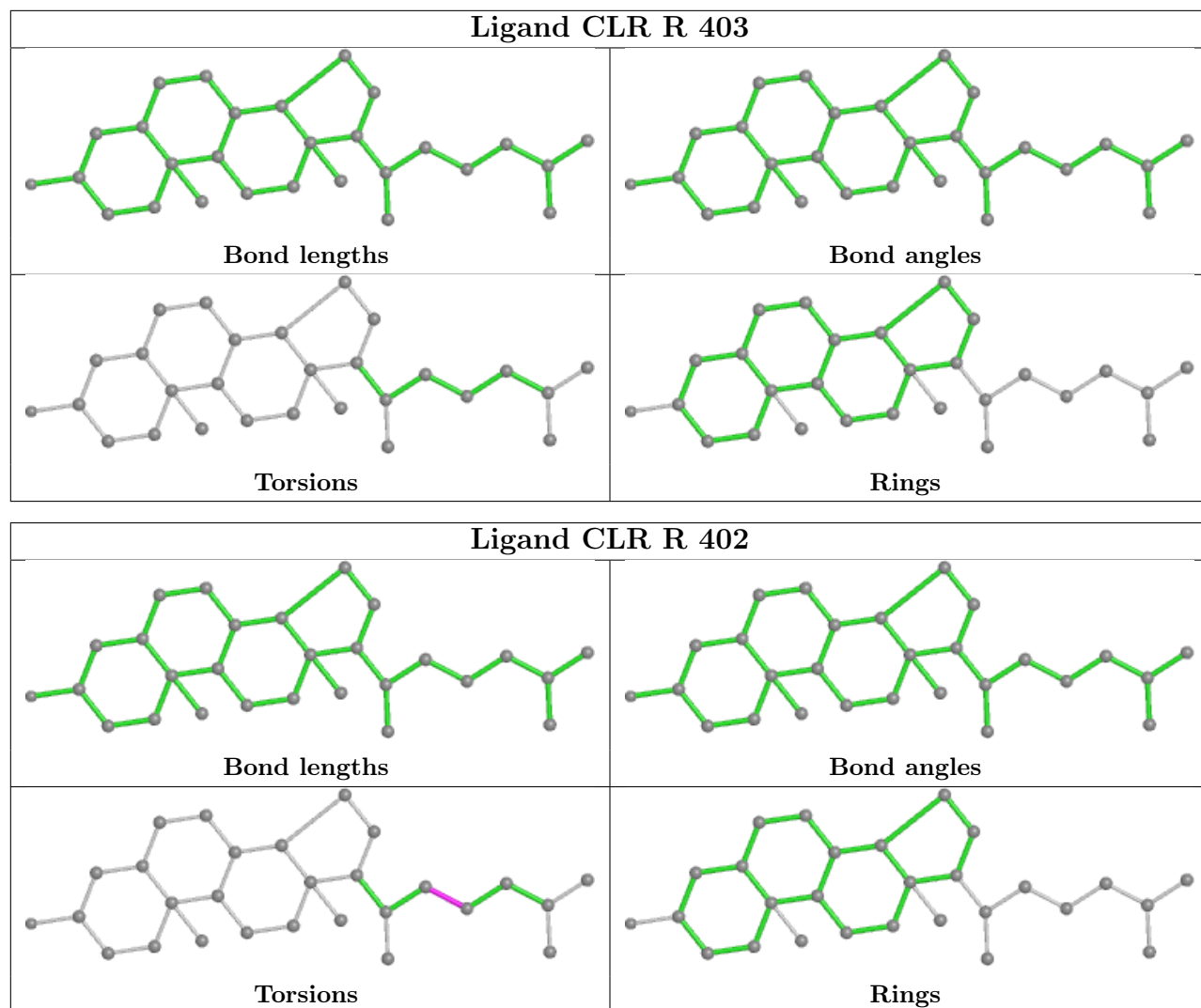
There are no ring outliers.

2 monomers are involved in 3 short contacts:

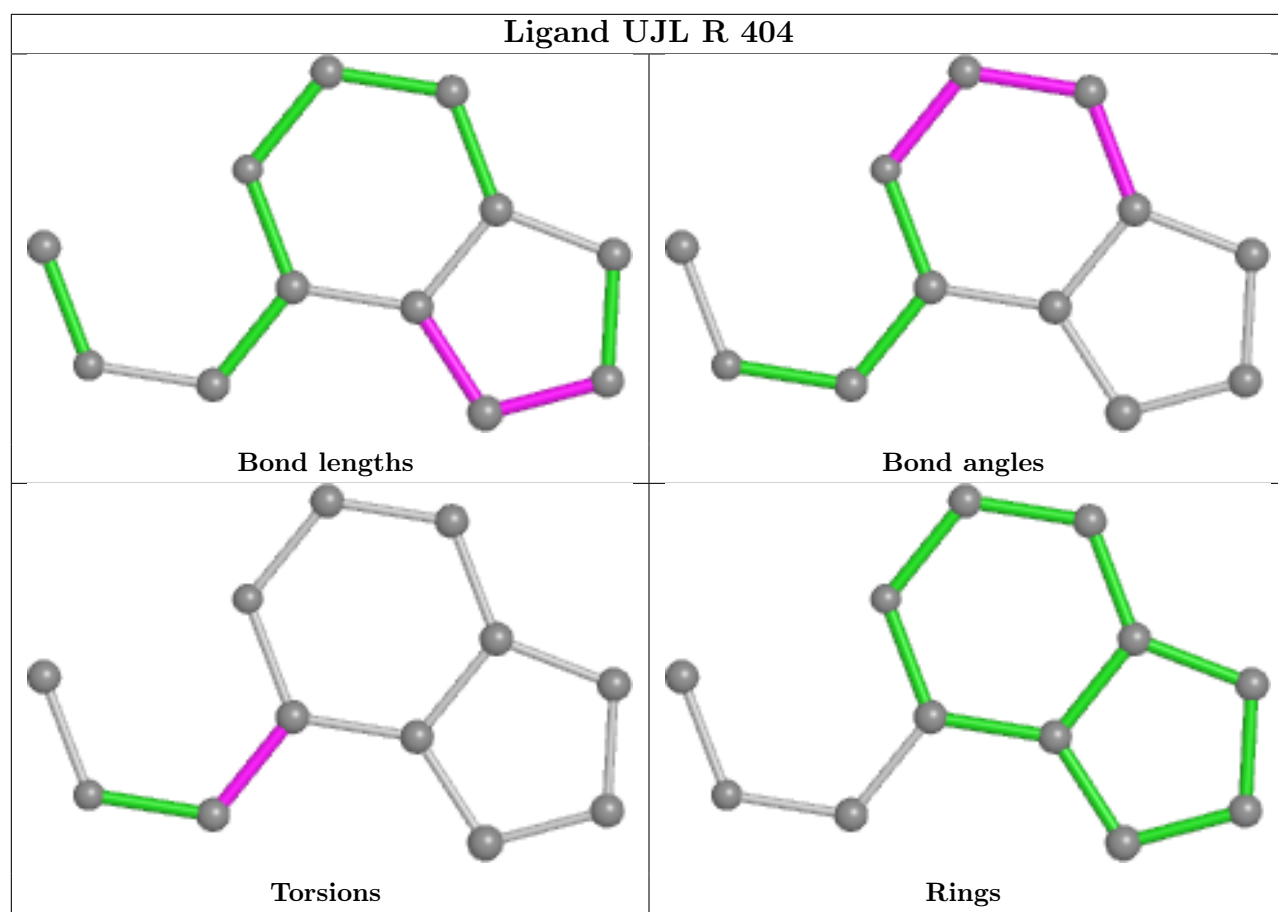
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	403	CLR	1	0
7	R	404	UJL	2	0

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.