Full wwPDB EM Validation Report ⓘ

Dec 24, 2023 – 12:08 AM JST

PDB ID	:	8W8B
EMDB ID	:	EMD-37351
Title	:	Cryo-EM structure of SEP-363856 bounded serotonin 1A (5-HT1A) receptor-Gi protein 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	:	3.00 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*
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:

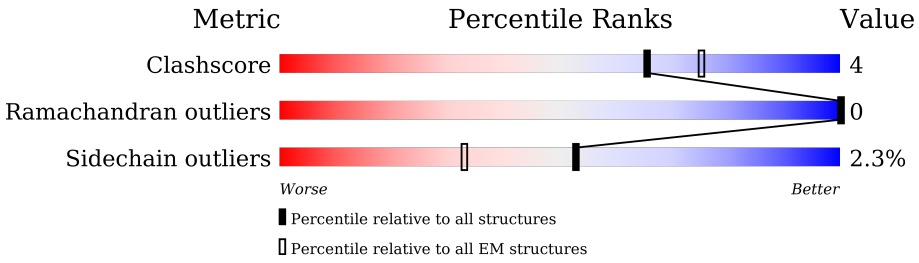
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	354	55% 6% 39%
2	B	345	81% 13% • 5%
3	E	267	76% 8% • 15%
4	G	71	55% 8% 37%
5	R	543	46% 5% 49%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8734 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	217	1751	1115	293	331	12	0	0

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
			Total	C	N	O	S		
2	B	328	2513	1553	452	487	21	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Antibody fragment scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	228	1756	1114	291	341	10	0	0

- 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	45	Total	C	N	O	S	0	0
			347	218	60	66	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	278	Total	C	N	O	S	0	0
			2197	1453	362	365	17		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-120	ASP	-	expression tag	UNP P0ABE7
R	-119	TYR	-	expression tag	UNP P0ABE7
R	-118	LYS	-	expression tag	UNP P0ABE7
R	-117	ASP	-	expression tag	UNP P0ABE7
R	-116	ASP	-	expression tag	UNP P0ABE7
R	-115	ASP	-	expression tag	UNP P0ABE7
R	-114	ASP	-	expression tag	UNP P0ABE7
R	-113	ALA	-	expression tag	UNP P0ABE7
R	-112	LYS	-	expression tag	UNP P0ABE7
R	-111	LEU	-	expression tag	UNP P0ABE7
R	-110	GLN	-	expression tag	UNP P0ABE7
R	-109	THR	-	expression tag	UNP P0ABE7
R	-108	MET	-	expression tag	UNP P0ABE7
R	-107	HIS	-	expression tag	UNP P0ABE7
R	-106	HIS	-	expression tag	UNP P0ABE7
R	-105	HIS	-	expression tag	UNP P0ABE7
R	-104	HIS	-	expression tag	UNP P0ABE7
R	-103	HIS	-	expression tag	UNP P0ABE7
R	-102	HIS	-	expression tag	UNP P0ABE7
R	-101	HIS	-	expression tag	UNP P0ABE7
R	-100	HIS	-	expression tag	UNP P0ABE7
R	-99	HIS	-	expression tag	UNP P0ABE7
R	-98	HIS	-	expression tag	UNP P0ABE7
R	-97	HIS	-	expression tag	UNP P0ABE7
R	-96	HIS	-	expression tag	UNP P0ABE7
R	-95	HIS	-	expression tag	UNP P0ABE7
R	-94	HIS	-	expression tag	UNP P0ABE7
R	-93	HIS	-	expression tag	UNP P0ABE7

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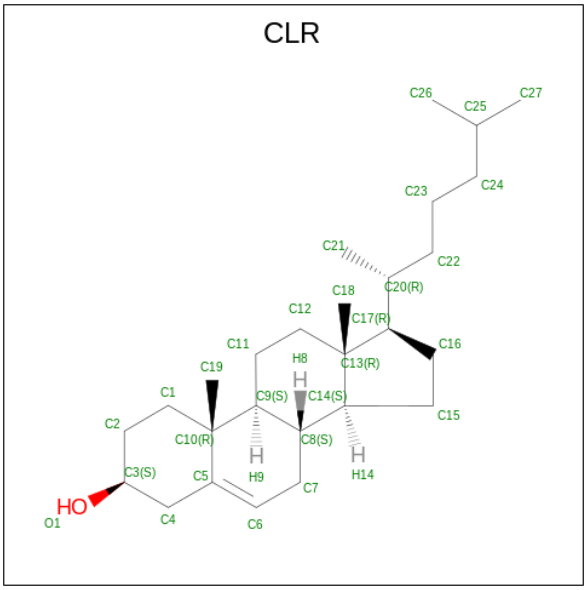
Chain	Residue	Modelled	Actual	Comment	Reference
R	-86	TRP	MET	conflict	UNP P0ABE7
R	9	ILE	HIS	conflict	UNP P0ABE7
R	13	LEU	-	linker	UNP P0ABE7
R	14	ALA	-	linker	UNP P0ABE7
R	15	SER	-	linker	UNP P0ABE7
R	16	GLU	-	linker	UNP P0ABE7
R	17	ASN	-	linker	UNP P0ABE7
R	18	LEU	-	linker	UNP P0ABE7
R	19	TYR	-	linker	UNP P0ABE7
R	20	PHE	-	linker	UNP P0ABE7
R	21	GLN	-	linker	UNP P0ABE7
R	24	THR	ASN	conflict	UNP P08908
R	125	TRP	LEU	conflict	UNP P08908

- 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
6	R	1	Total C O 28 27 1	0
6	R	1	Total C O 28 27 1	0
6	R	1	Total C O 28 27 1	0
6	R	1	Total C O 28 27 1	0

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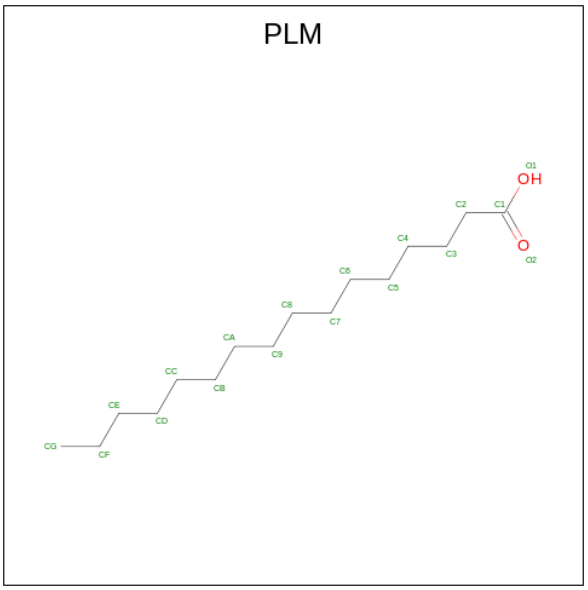
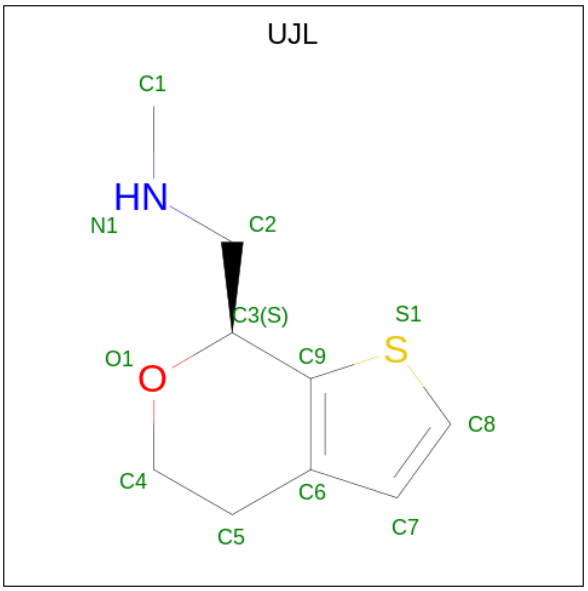
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	R	1	28	27	1	0

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	R	1	18	16	2	0

- Molecule 8 is 1-[(7 {S})-5,7-dihydro-4 {H}-thieno[2,3-c]pyran-7-yl]- {N}-methyl-metha namine (three-letter code: UJL) (formula: $C_9H_{13}NOS$) (labeled as "Ligand of Interest" by depositor).



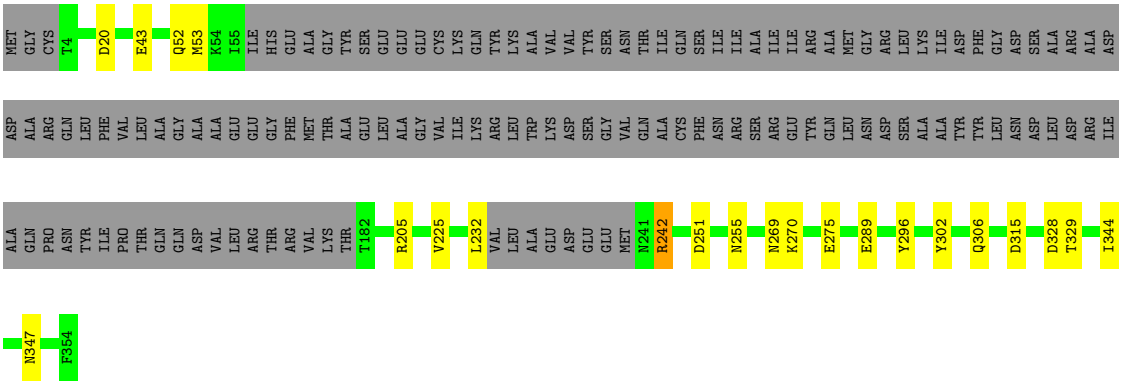
Mol	Chain	Residues	Atoms					AltConf
8	R	1	Total	C	N	O	S	0
			12	9	1	1	1	

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.

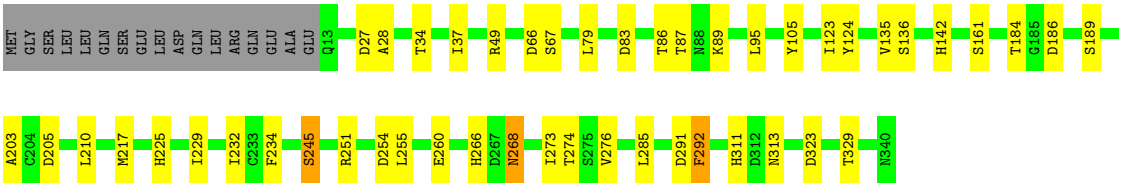
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



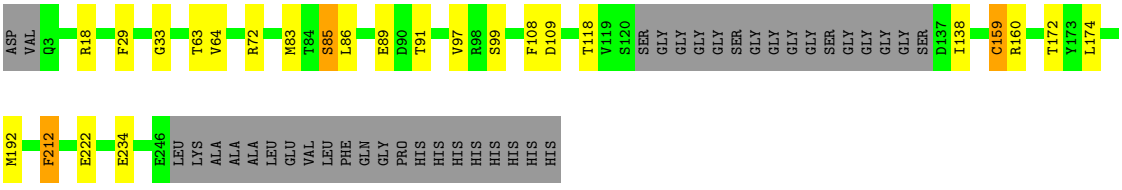
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



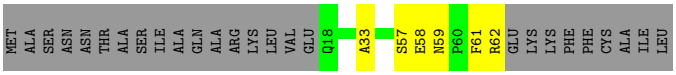
• Molecule 3: Antibody fragment scFv16

Chain E:



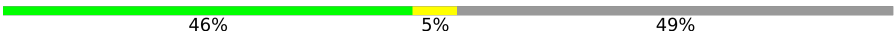
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

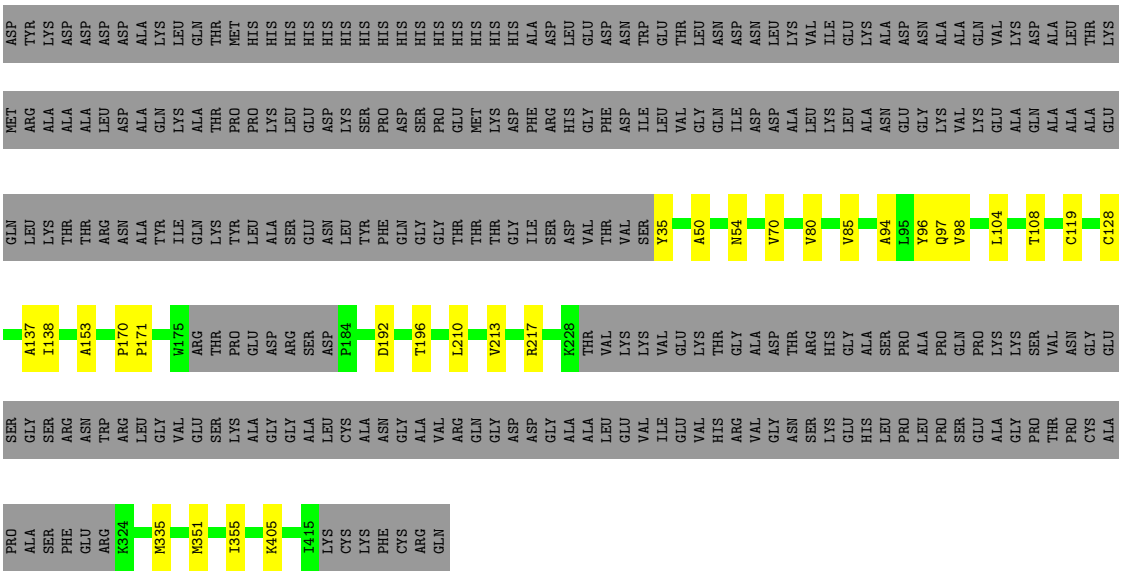
Chain G:



• Molecule 5: Soluble cytochrome b562,5-hydroxytryptamine receptor 1A

Chain R:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	396934	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 ($e^-/Å^2$)	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UJL, CLR, PLM

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	0.25	0/1780	0.44	0/2386
2	B	0.26	0/2560	0.53	0/3471
3	E	0.28	0/1800	0.50	0/2440
4	G	0.26	0/353	0.49	0/477
5	R	0.26	0/2248	0.46	0/3058
All	All	0.26	0/8741	0.49	0/11832

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

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	1751	0	1748	12	0
2	B	2513	0	2425	30	0
3	E	1756	0	1691	13	0
4	G	347	0	350	5	0
5	R	2197	0	2300	16	0
6	R	140	0	230	4	0
7	R	18	0	31	0	0
8	R	12	0	0	0	0
All	All	8734	0	8775	71	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 (71) 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:52:GLN:NE2	1:A:53:MET:SD	2.56	0.79
4:G:57:SER:OG	4:G:58:GLU:OE2	2.06	0.73
5:R:35:TYR:HH	6:R:501:CLR:H1	1.39	0.71
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.24	0.70
1:A:289:GLU:N	1:A:289:GLU:OE1	2.30	0.64
5:R:97:GLN:NE2	6:R:501:CLR:H192	2.12	0.64
5:R:50:ALA:O	5:R:54:ASN:ND2	2.33	0.61
3:E:85:SER:O	3:E:85:SER:OG	2.21	0.58
5:R:80:VAL:HG11	6:R:504:CLR:H6	1.87	0.56
2:B:311:HIS:HE2	2:B:329:THR:HG1	1.57	0.53
1:A:328:ASP:OD1	1:A:329:THR:N	2.42	0.52
3:E:174:LEU:HD22	3:E:212:PHE:CG	2.45	0.52
2:B:276:VAL:HG13	2:B:285:LEU:HD11	1.91	0.51
2:B:27:ASP:OD1	2:B:28:ALA:N	2.44	0.51
3:E:29:PHE:O	3:E:72:ARG:NH2	2.44	0.50
2:B:225:HIS:ND1	2:B:245:SER:HB3	2.26	0.50
2:B:273:ILE:N	2:B:273:ILE:HD12	2.26	0.50
3:E:109:ASP:N	3:E:109:ASP:OD1	2.42	0.50
2:B:229:ILE:HA	2:B:245:SER:HB2	1.93	0.49
1:A:232:LEU:HB2	1:A:242:ARG:HE	1.77	0.48
5:R:85:VAL:HG22	5:R:119:CYS:HB3	1.95	0.48
3:E:138:ILE:HD11	3:E:234:GLU:OE2	2.13	0.48
1:A:302:TYR:O	1:A:306:GLN:HG2	2.12	0.48
5:R:104:LEU:HD23	5:R:108:THR:HG21	1.96	0.48
5:R:94:ALA:O	5:R:98:VAL:HG22	2.14	0.48
3:E:159:CYS:SG	3:E:160:ARG:N	2.87	0.48
5:R:213:VAL:O	5:R:217:ARG:HG3	2.14	0.47
1:A:347:ASN:ND2	5:R:137:ALA:O	2.44	0.47
2:B:124:TYR:CE2	2:B:135:VAL:HG22	2.50	0.47
2:B:66:ASP:O	2:B:67:SER:OG	2.27	0.47
5:R:192:ASP:O	5:R:196:THR:HG22	2.15	0.46
4:G:59:ASN:C	4:G:59:ASN:OD1	2.53	0.46
2:B:266:HIS:NE2	2:B:268:ASN:OD1	2.49	0.46
2:B:79:LEU:HD22	2:B:95:LEU:HD21	1.98	0.46
1:A:344:ILE:HD12	5:R:138:ILE:O	2.14	0.46
2:B:203:ALA:HB3	2:B:205:ASP:OD1	2.15	0.45
1:A:225:VAL:O	1:A:269:ASN:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:HIS:CD2	2:B:329:THR:HG1	2.34	0.45
5:R:97:GLN:HE21	6:R:501:CLR:H192	1.81	0.45
5:R:128:CYS:SG	5:R:210:LEU:HD23	2.55	0.45
2:B:210:LEU:HD11	2:B:255:LEU:HD13	1.98	0.45
4:G:62:ARG:HG2	4:G:62:ARG:HH11	1.82	0.45
2:B:210:LEU:CD1	2:B:255:LEU:HD13	2.47	0.44
2:B:311:HIS:NE2	2:B:329:THR:OG1	2.48	0.44
2:B:225:HIS:CE1	2:B:245:SER:HB3	2.52	0.44
1:A:20:ASP:OD1	2:B:89:LYS:NZ	2.46	0.44
2:B:184:THR:HG22	2:B:184:THR:O	2.17	0.44
2:B:254:ASP:OD2	4:G:33:ALA:HB1	2.18	0.44
5:R:70:VAL:HG13	5:R:153:ALA:HB2	2.00	0.43
2:B:142:HIS:CG	2:B:161:SER:HG	2.37	0.43
2:B:49:ARG:NH1	4:G:61:PHE:O	2.51	0.43
3:E:63:THR:HG23	3:E:64:VAL:HG13	1.99	0.43
3:E:97:VAL:HG11	3:E:108:PHE:CD2	2.53	0.42
2:B:329:THR:OG1	2:B:329:THR:O	2.38	0.42
3:E:192:MET:O	3:E:192:MET:HG2	2.19	0.42
3:E:83:MET:HE3	3:E:86:LEU:HD21	2.01	0.42
5:R:170:PRO:N	5:R:171:PRO:HD2	2.33	0.42
5:R:351:MET:O	5:R:355:ILE:HG12	2.19	0.42
2:B:83:ASP:O	2:B:87:THR:N	2.52	0.42
1:A:43:GLU:O	1:A:270:LYS:NZ	2.42	0.42
2:B:291:ASP:O	2:B:292:PHE:CD1	2.73	0.42
3:E:91:THR:HG23	3:E:118:THR:HA	2.01	0.41
3:E:172:THR:HG21	3:E:192:MET:SD	2.60	0.41
3:E:33:GLY:N	3:E:99:SER:O	2.54	0.41
2:B:189:SER:OG	2:B:232:ILE:HG22	2.20	0.41
2:B:86:THR:O	2:B:87:THR:OG1	2.23	0.41
2:B:123:ILE:O	2:B:136:SER:N	2.52	0.41
2:B:292:PHE:HD2	2:B:313:ASN:O	2.03	0.41
2:B:34:THR:O	2:B:37:ILE:HG22	2.21	0.40
2:B:251:ARG:HD3	2:B:260:GLU:OE1	2.22	0.40
1:A:275:GLU:OE2	1:A:296:TYR:HB2	2.22	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	211/354 (60%)	210 (100%)	1 (0%)	0	100	100
2	B	326/345 (94%)	311 (95%)	15 (5%)	0	100	100
3	E	224/267 (84%)	216 (96%)	8 (4%)	0	100	100
4	G	43/71 (61%)	43 (100%)	0	0	100	100
5	R	272/543 (50%)	271 (100%)	1 (0%)	0	100	100
All	All	1076/1580 (68%)	1051 (98%)	25 (2%)	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	193/305 (63%)	190 (98%)	3 (2%)	62	86
2	B	271/287 (94%)	262 (97%)	9 (3%)	38	73
3	E	193/216 (89%)	187 (97%)	6 (3%)	40	75
4	G	37/58 (64%)	37 (100%)	0	100	100
5	R	237/453 (52%)	234 (99%)	3 (1%)	69	89
All	All	931/1319 (71%)	910 (98%)	21 (2%)	53	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ARG
1	A	242	ARG
1	A	315	ASP
2	B	105	TYR
2	B	186	ASP
2	B	217	MET
2	B	234	PHE
2	B	245	SER
2	B	268	ASN
2	B	274	THR
2	B	292	PHE
2	B	323	ASP
3	E	18	ARG
3	E	85	SER
3	E	89	GLU
3	E	159	CYS
3	E	212	PHE
3	E	222	GLU
5	R	96	TYR
5	R	335	MET
5	R	405	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

7 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	504	-	31,31,31	0.36	0	48,48,48	0.81	2 (4%)
6	CLR	R	501	-	31,31,31	0.36	0	48,48,48	0.65	0
6	CLR	R	503	-	31,31,31	0.35	0	48,48,48	0.48	0
6	CLR	R	505	-	31,31,31	0.36	0	48,48,48	0.53	0
6	CLR	R	502	-	31,31,31	0.40	0	48,48,48	0.66	0
8	UJL	R	507	-	9,13,13	3.92	3 (33%)	4,17,17	2.26	2 (50%)
7	PLM	R	506	-	17,17,17	0.94	1 (5%)	17,17,17	0.74	1 (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	CLR	R	504	-	-	6/10/68/68	0/4/4/4
6	CLR	R	501	-	-	2/10/68/68	0/4/4/4
6	CLR	R	503	-	-	0/10/68/68	0/4/4/4
6	CLR	R	505	-	-	0/10/68/68	0/4/4/4
6	CLR	R	502	-	-	2/10/68/68	0/4/4/4
8	UJL	R	507	-	-	1/3/13/13	0/2/2/2
7	PLM	R	506	-	-	2/15/15/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	R	507	UJL	C9-S1	-10.80	1.54	1.74
8	R	507	UJL	C8-S1	-3.82	1.52	1.71
7	R	506	PLM	C2-C1	3.06	1.57	1.50
8	R	507	UJL	C5-C6	-2.10	1.47	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	507	UJL	C4-C5-C6	3.83	116.37	110.87
6	R	504	CLR	C16-C17-C20	2.81	116.49	112.15
6	R	504	CLR	C15-C14-C13	2.22	106.51	103.84
7	R	506	PLM	O1-C1-O2	2.19	128.76	123.30
8	R	507	UJL	C3-C2-N1	-2.18	107.41	110.88

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	507	UJL	C3-C2-N1-C1
6	R	504	CLR	C16-C17-C20-C21
6	R	504	CLR	C13-C17-C20-C21
6	R	504	CLR	C13-C17-C20-C22
6	R	504	CLR	C16-C17-C20-C22
6	R	502	CLR	C21-C20-C22-C23
6	R	504	CLR	C23-C24-C25-C26
6	R	501	CLR	C21-C20-C22-C23
6	R	504	CLR	C23-C24-C25-C27
7	R	506	PLM	O1-C1-C2-C3
7	R	506	PLM	O2-C1-C2-C3
6	R	501	CLR	C22-C23-C24-C25
6	R	502	CLR	C23-C24-C25-C26

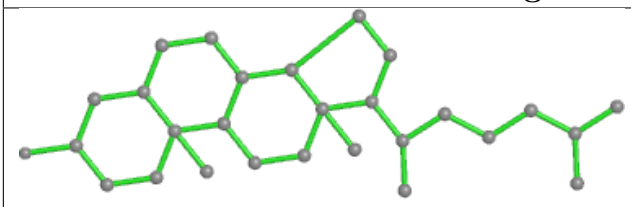
There are no ring outliers.

2 monomers are involved in 4 short contacts:

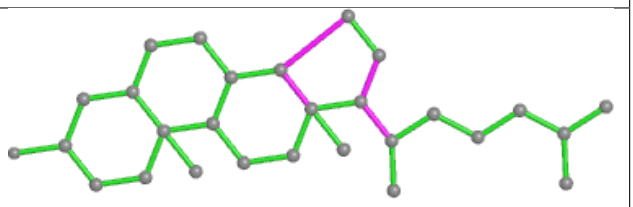
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	504	CLR	1	0
6	R	501	CLR	3	0

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 then 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.

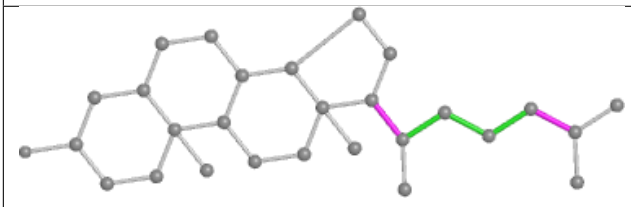
Ligand CLR R 504



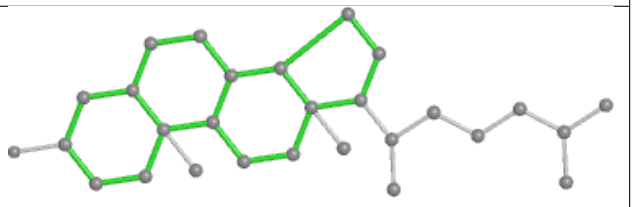
Bond lengths



Bond angles

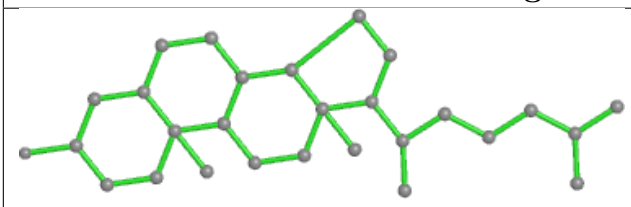


Torsions

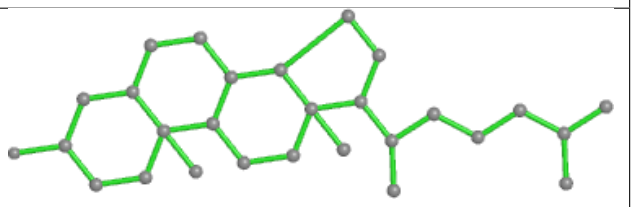


Rings

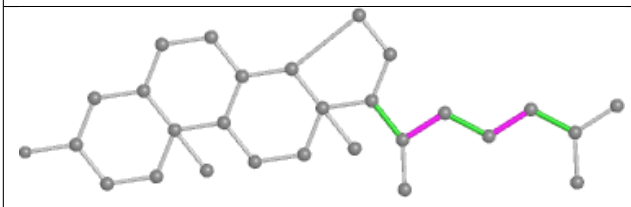
Ligand CLR R 501



Bond lengths



Bond angles



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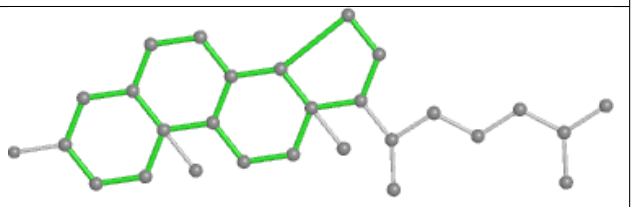
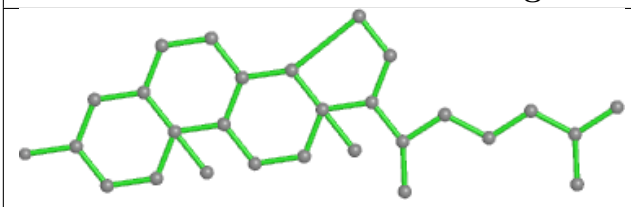
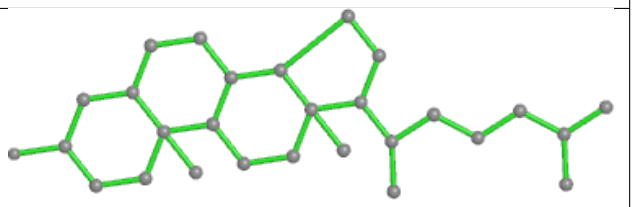


Rings

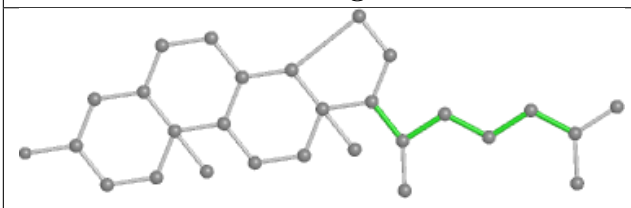
Ligand CLR R 503



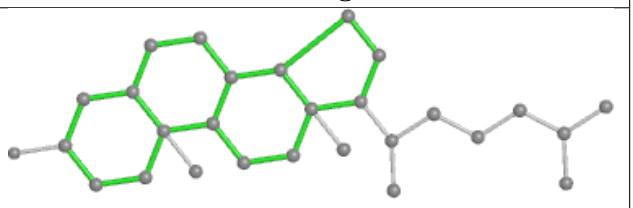
Bond lengths



Bond angles

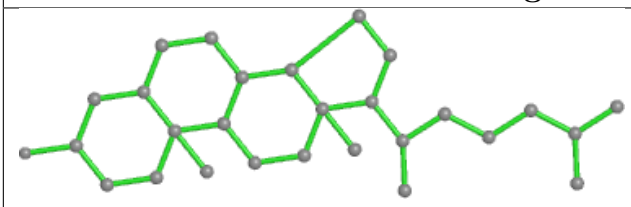


Torsions

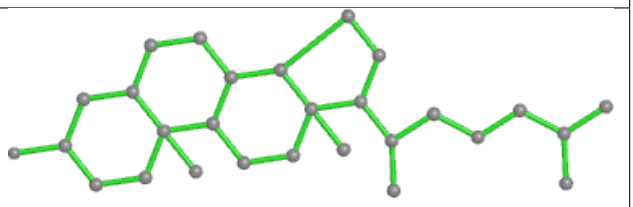


Rings

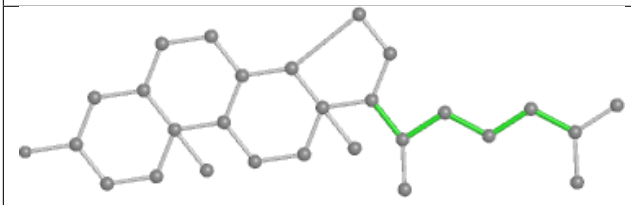
Ligand CLR R 505



Bond lengths



Bond angles



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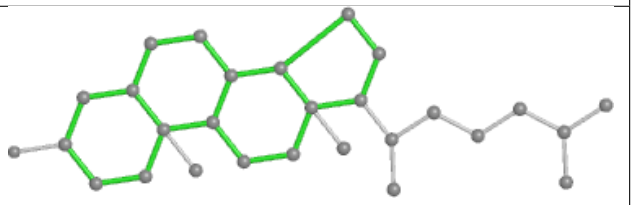
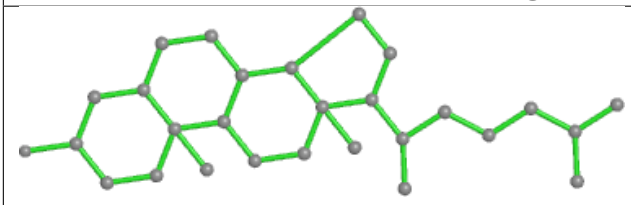
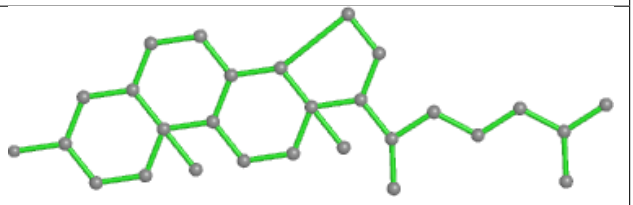


Rings

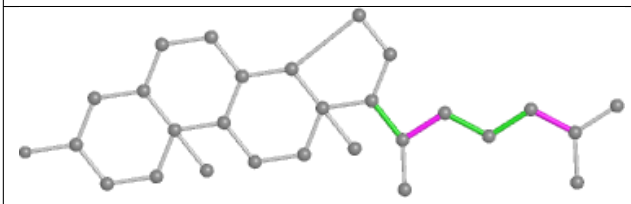
Ligand CLR R 502



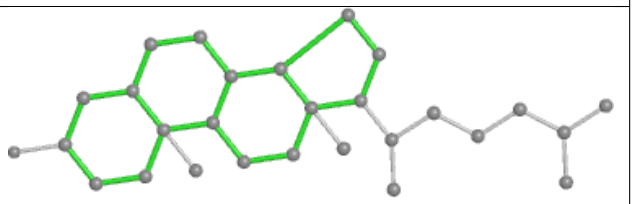
Bond lengths



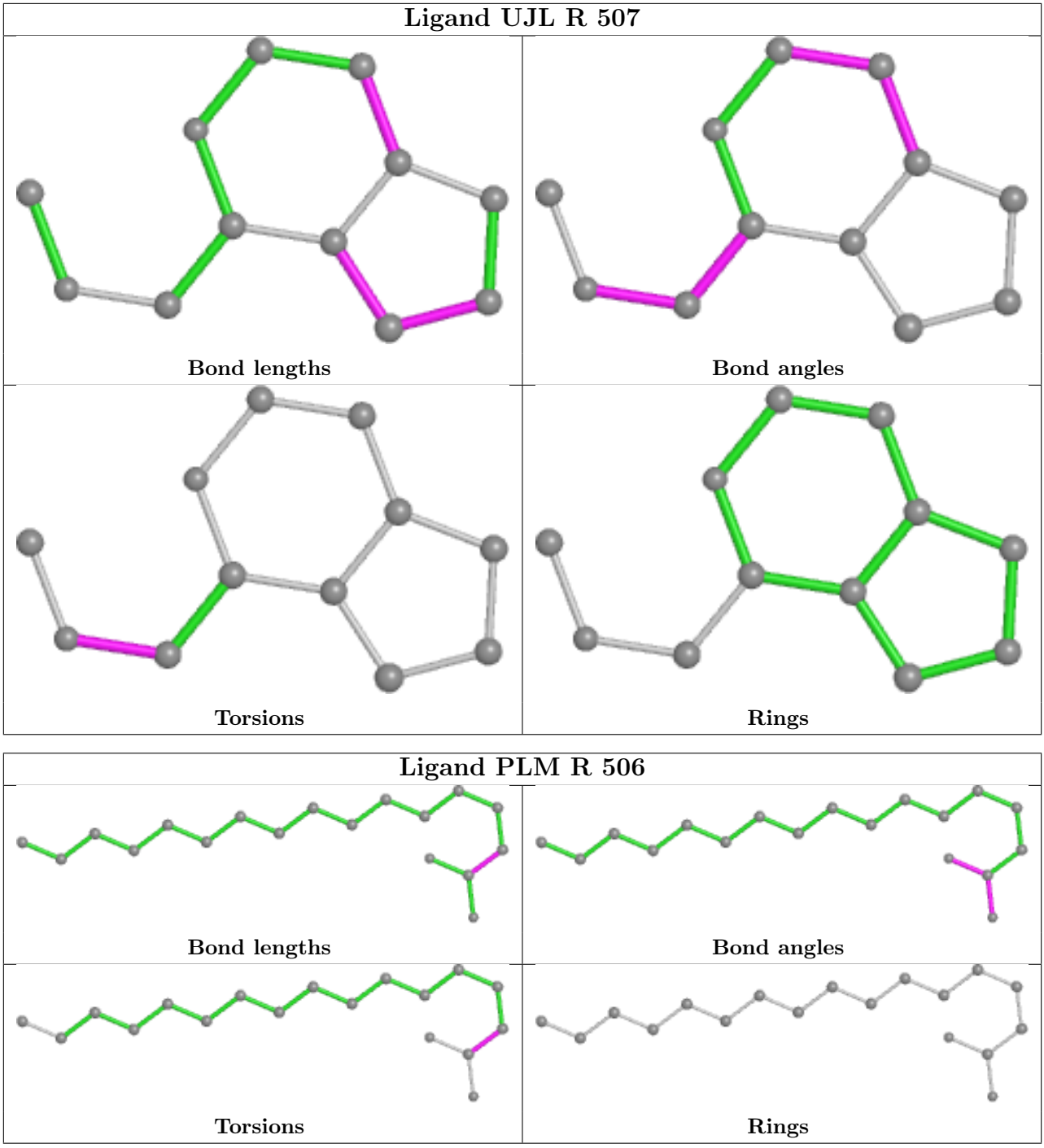
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.