



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 11:53 PM UTC

PDB ID : 7TYN / pdb_00007tyn
EMDB ID : EMD-26188
Title : Calcitonin Receptor in complex with Gs and salmon calcitonin peptide
Authors : Cao, J.; Belousoff, M.J.; Johnson, R.M.; Wootten, D.L.; Sexton, P.M.
Deposited on : 2022-02-13
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

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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

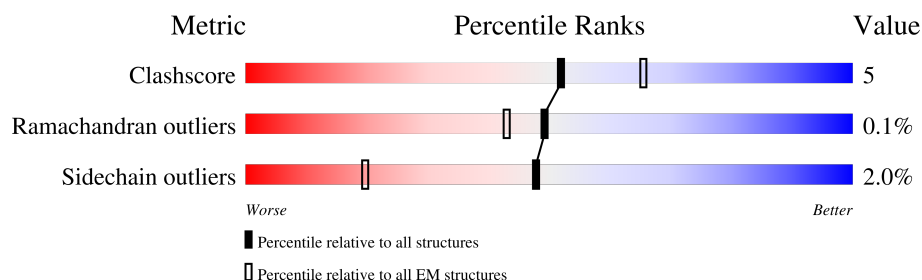
1 Overall quality at a glance

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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	P	33	82% 12% . .
2	R	501	64% 9% . 26%
3	A	394	49% 8% 42%
4	B	350	82% 15% .
5	G	71	65% 11% . 23%
6	N	138	75% 17% . 7%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9364 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 Calcitonin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	33	Total	C	N	O	S	0	1
			239	145	44	48	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	33	NH2	-	amidation	UNP B5XGR7

- Molecule 2 is a protein called Calcitonin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	373	Total	C	N	O	S	0	0
			2892	1917	479	471	25		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-7	MET	-	expression tag	UNP P30988
R	-6	LYS	-	expression tag	UNP P30988
R	-5	THR	-	expression tag	UNP P30988
R	-4	ILE	-	expression tag	UNP P30988
R	-3	ILE	-	expression tag	UNP P30988
R	-2	ALA	-	expression tag	UNP P30988
R	-1	LEU	-	expression tag	UNP P30988
R	0	SER	-	expression tag	UNP P30988
R	1	TYR	-	expression tag	UNP P30988
R	2	ILE	-	expression tag	UNP P30988
R	3	PHE	-	expression tag	UNP P30988
R	4	CYS	-	expression tag	UNP P30988
R	5	LEU	-	expression tag	UNP P30988
R	6	VAL	-	expression tag	UNP P30988
R	7	PHE	-	expression tag	UNP P30988
R	8	ALA	-	expression tag	UNP P30988

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Chain	Residue	Modelled	Actual	Comment	Reference
R	9	ASP	-	expression tag	UNP P30988
R	10	TYR	-	expression tag	UNP P30988
R	11	LYS	-	expression tag	UNP P30988
R	12	ASP	-	expression tag	UNP P30988
R	13	ASP	-	expression tag	UNP P30988
R	14	ASP	-	expression tag	UNP P30988
R	15	ASP	-	expression tag	UNP P30988
R	16	LEU	-	expression tag	UNP P30988
R	17	GLU	-	expression tag	UNP P30988
R	18	VAL	-	expression tag	UNP P30988
R	19	LEU	-	expression tag	UNP P30988
R	20	PHE	-	expression tag	UNP P30988
R	21	GLN	-	expression tag	UNP P30988
R	22	GLY	-	expression tag	UNP P30988
R	23	PRO	-	expression tag	UNP P30988
R	24	ALA	-	expression tag	UNP P30988
R	447	LEU	PRO	conflict	UNP P30988
R	475	PRO	-	expression tag	UNP P30988
R	476	ALA	-	expression tag	UNP P30988
R	477	GLY	-	expression tag	UNP P30988
R	478	LEU	-	expression tag	UNP P30988
R	479	GLU	-	expression tag	UNP P30988
R	480	VAL	-	expression tag	UNP P30988
R	481	LEU	-	expression tag	UNP P30988
R	482	PHE	-	expression tag	UNP P30988
R	483	GLN	-	expression tag	UNP P30988
R	484	GLY	-	expression tag	UNP P30988
R	485	PRO	-	expression tag	UNP P30988
R	486	HIS	-	expression tag	UNP P30988
R	487	HIS	-	expression tag	UNP P30988
R	488	HIS	-	expression tag	UNP P30988
R	489	HIS	-	expression tag	UNP P30988
R	490	HIS	-	expression tag	UNP P30988
R	491	HIS	-	expression tag	UNP P30988
R	492	HIS	-	expression tag	UNP P30988
R	493	HIS	-	expression tag	UNP P30988

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	227	Total	C	N	O	S	0	0
			1881	1188	342	345	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	conflict	UNP P63092
A	226	ALA	GLY	conflict	UNP P63092
A	268	ALA	GLU	conflict	UNP P63092
A	271	LYS	ASN	conflict	UNP P63092
A	274	ASP	LYS	conflict	UNP P63092
A	280	LYS	ARG	conflict	UNP P63092
A	284	ASP	THR	conflict	UNP P63092
A	285	THR	ILE	conflict	UNP P63092

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	339	Total	C	N	O	S	0	0
			2606	1607	468	510	21		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

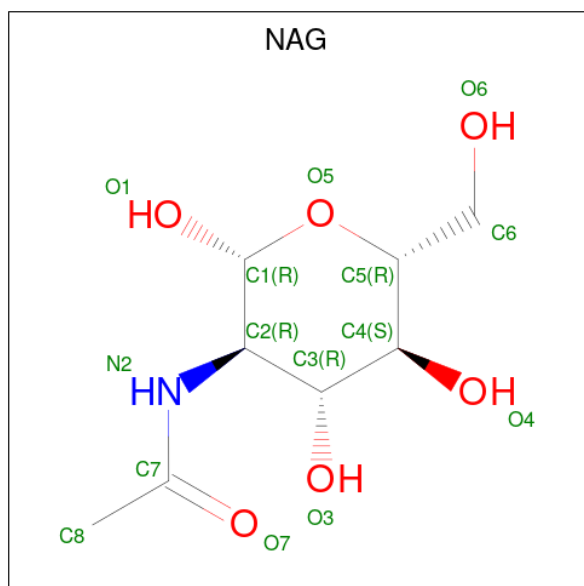
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	55	Total	C	N	O	S	0	0
			424	266	75	80	3		

- Molecule 6 is a protein called Nanobody 35.

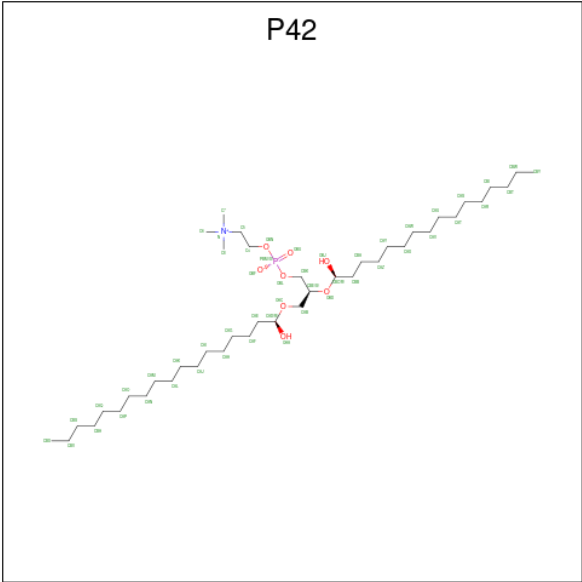
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	128	Total	C	N	O	S	0	0
			973	605	170	192	6		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



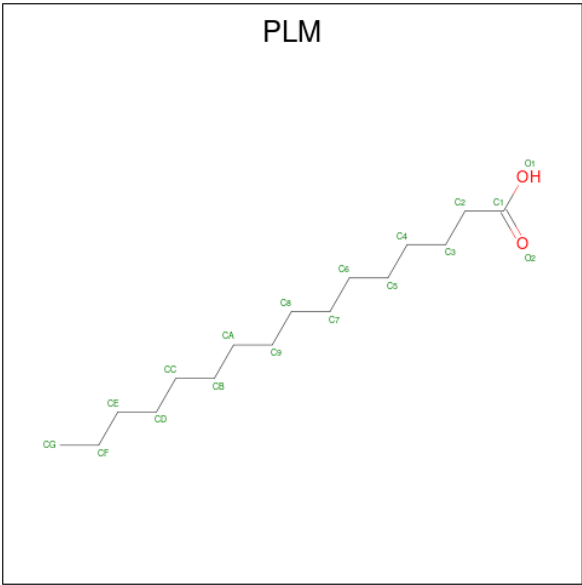
Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	N	O	0
			14	8	1	5	
7	R	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 8 is (2S)-2-([(1R)-1-hydroxyhexadecyl]oxy)-3-([(1R)-1-hydroxyoctadecyl]oxy)propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: P42) (formula: $C_{42}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
8	R	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 9 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



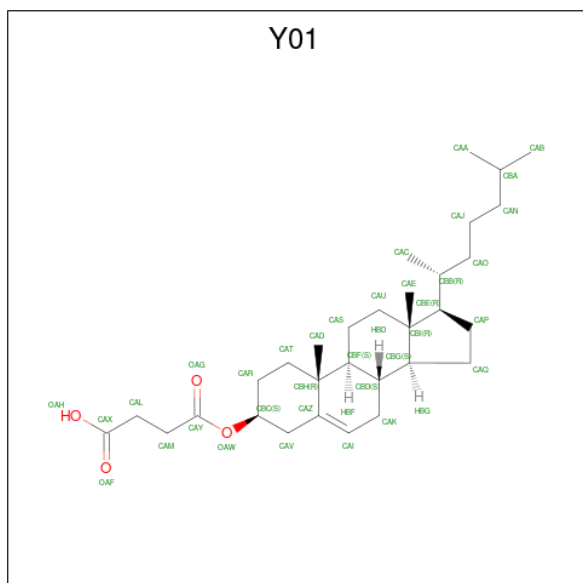
Mol	Chain	Residues	Atoms			AltConf
9	R	1	Total	C	O	0
			18	16	2	
9	R	1	Total	C	O	0
			18	16	2	
9	R	1	Total	C	O	0
			18	16	2	

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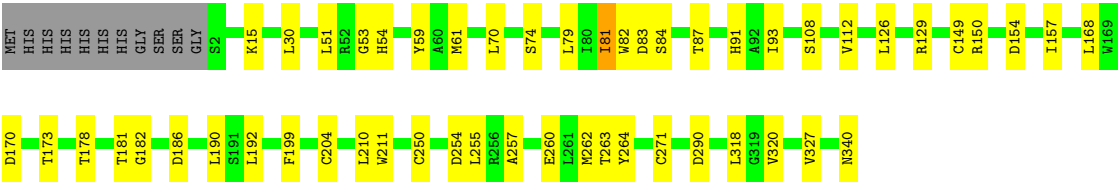
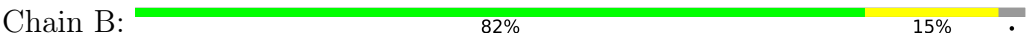
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- Molecule 10 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
10	R	1	Total	C	O	0
			35	31	4	



- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 6: Nanobody 35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	867000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: NH2, PLM, P42, NAG, Y01

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	P	0.52	0/241	1.22	3/326 (0.9%)
2	R	0.18	0/2987	0.35	0/4086
3	A	0.09	0/1916	0.27	0/2576
4	B	0.10	0/2653	0.29	0/3597
5	G	0.09	0/430	0.26	0/580
6	N	0.11	0/993	0.32	0/1345
All	All	0.16	0/9220	0.36	3/12510 (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
6	N	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	32	PRO	CA-N-CD	-15.69	90.04	112.00
1	P	31	THR	C-N-CD	5.51	147.58	125.00
1	P	27	THR	CB-CA-C	5.37	119.64	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	N	99	CYS	Peptide

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	P	239	0	241	4	0
2	R	2892	0	2700	34	0
3	A	1881	0	1866	22	0
4	B	2606	0	2510	30	0
5	G	424	0	436	5	0
6	N	973	0	938	14	0
7	R	28	0	26	0	0
8	R	52	0	88	2	0
9	R	234	0	403	9	0
10	R	35	0	49	0	0
All	All	9364	0	9257	101	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 5.

All (101) 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:B:87:THR:O	4:B:87:THR:HG22	1.90	0.70
2:R:38:PRO:HG2	2:R:41:TYR:HB2	1.79	0.63
4:B:129:ARG:HD3	4:B:129:ARG:H	1.65	0.62
2:R:220:LYS:HD3	9:R:515:PLM:H92	1.81	0.61
3:A:362:HIS:NE2	3:A:378:ASP:OD2	2.33	0.61
3:A:59:GLN:HG2	3:A:369:THR:HA	1.82	0.60
4:B:260:GLU:OE2	4:B:263:THR:OG1	2.22	0.58
4:B:81:ILE:HG13	4:B:91:HIS:HB2	1.86	0.58
3:A:289:LEU:HB3	3:A:361:PRO:HA	1.85	0.57
2:R:87:ALA:HB1	2:R:114:GLU:HA	1.86	0.57
2:R:302:HIS:HA	2:R:305:VAL:HB	1.86	0.56
4:B:271:CYS:HB2	4:B:290:ASP:HB2	1.86	0.56
3:A:250:SER:H	3:A:293:LYS:HB2	1.69	0.56
3:A:292:ASN:HA	3:A:364:THR:HB	1.88	0.55
2:R:221:ILE:HG13	9:R:515:PLM:HE2	1.88	0.55
2:R:203:VAL:HG23	2:R:204:GLU:HG2	1.89	0.55
4:B:340:ASN:OD1	5:G:59:ASN:ND2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:52:SER:O	6:N:72:ARG:NH1	2.39	0.54
5:G:16:VAL:HG12	5:G:20:LYS:HE3	1.89	0.54
2:R:360:PRO:HG3	9:R:513:PLM:HC2	1.91	0.53
4:B:320:VAL:HG22	4:B:327:VAL:HG22	1.89	0.53
6:N:29:PHE:O	6:N:72:ARG:NH2	2.41	0.53
4:B:182:GLY:H	4:B:211:TRP:HH2	1.55	0.53
3:A:232:ARG:HH21	4:B:204:CYS:HB3	1.73	0.52
4:B:170:ASP:OD2	4:B:173:THR:OG1	2.26	0.52
2:R:112:CYS:HA	2:R:118:TRP:HA	1.92	0.52
6:N:91:THR:HG23	6:N:125:THR:HA	1.92	0.51
4:B:254:ASP:HB3	4:B:257:ALA:HB3	1.93	0.51
6:N:99:CYS:HA	6:N:115:TYR:OH	2.10	0.51
2:R:256:LYS:NZ	2:R:258:ARG:HG2	2.26	0.51
4:B:108:SER:OG	4:B:154:ASP:OD1	2.28	0.50
3:A:364:THR:HG22	3:A:366:ALA:H	1.76	0.50
6:N:112:SER:HB2	6:N:115:TYR:HB2	1.94	0.50
4:B:168:LEU:HB3	4:B:178:THR:HB	1.94	0.49
4:B:87:THR:O	4:B:87:THR:CG2	2.59	0.49
2:R:264:LEU:O	2:R:269:PHE:N	2.42	0.49
2:R:345:THR:HG21	9:R:511:PLM:H92	1.94	0.49
6:N:83:MET:HB3	6:N:86:LEU:HD21	1.94	0.49
2:R:284:TYR:HB3	9:R:509:PLM:H21	1.94	0.49
4:B:149:CYS:HB2	4:B:157:ILE:HD11	1.94	0.49
2:R:220:LYS:HB3	9:R:515:PLM:HB2	1.94	0.49
6:N:83:MET:HE1	6:N:124:VAL:HG11	1.95	0.49
1:P:31:THR:O	1:P:32:PRO:C	2.57	0.48
5:G:8:SER:OG	5:G:9:ILE:N	2.45	0.48
3:A:368:ASP:OD1	3:A:368:ASP:N	2.45	0.48
1:P:18:LYS:HB2	2:R:100:PRO:HB2	1.96	0.47
1:P:16:LEU:HD11	2:R:149:TYR:HB2	1.96	0.47
2:R:248:ILE:O	3:A:384:GLN:NE2	2.34	0.47
9:R:514:PLM:HD2	9:R:515:PLM:HF2	1.97	0.47
3:A:344:GLU:OE1	3:A:347:ARG:NH2	2.48	0.47
2:R:296:HIS:HB2	9:R:508:PLM:H31	1.97	0.46
2:R:58:ARG:O	2:R:62:LEU:N	2.45	0.46
5:G:38:MET:O	5:G:42:GLU:HG2	2.16	0.46
4:B:149:CYS:O	4:B:150:ARG:NH1	2.49	0.46
2:R:347:ILE:HD11	3:A:393:LEU:HD23	1.97	0.46
2:R:183:LEU:HD21	2:R:259:LEU:HD22	1.98	0.46
2:R:154:VAL:HG13	8:R:503:P42:HBW	1.98	0.45
4:B:53:GLY:H	4:B:82:TRP:HH2	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:192:LEU:HD23	4:B:199:PHE:HB3	1.99	0.45
4:B:30:LEU:HD23	4:B:262:MET:HB2	1.98	0.45
2:R:374:TYR:O	2:R:378:SER:OG	2.26	0.45
3:A:24:LYS:HE3	3:A:24:LYS:HB3	1.67	0.45
2:R:199:ILE:O	2:R:203:VAL:HG22	2.17	0.45
1:P:1:CYS:HB3	2:R:293:VAL:HG22	1.98	0.44
3:A:301:VAL:HA	3:A:306:SER:HB2	2.00	0.44
2:R:154:VAL:HG11	8:R:503:P42:HAIA	2.00	0.44
6:N:37:VAL:HG23	6:N:95:TYR:HB2	2.00	0.44
3:A:232:ARG:CD	6:N:100:PRO:HG3	2.48	0.44
4:B:15:LYS:HB3	4:B:15:LYS:HE3	1.67	0.44
2:R:101:ASP:N	2:R:101:ASP:OD1	2.51	0.43
2:R:396:ASN:O	2:R:400:THR:HG23	2.18	0.43
4:B:79:LEU:HB3	4:B:93:ILE:HB	1.99	0.43
2:R:72:CYS:HB3	2:R:112:CYS:HB2	1.89	0.43
6:N:34:MET:HB3	6:N:79:LEU:HD22	2.00	0.43
6:N:67:ARG:CZ	6:N:87:LYS:HE2	2.48	0.43
4:B:51:LEU:HD13	4:B:82:TRP:CD2	2.54	0.43
3:A:207:ILE:HD11	3:A:222:PHE:HB3	2.00	0.43
2:R:272:VAL:HB	2:R:273:PRO:HD3	2.01	0.42
6:N:40:ALA:HB3	6:N:43:LYS:HD3	2.00	0.42
4:B:84:SER:HB2	5:G:61:PHE:HE1	1.83	0.42
2:R:256:LYS:HZ3	2:R:258:ARG:HG2	1.83	0.42
4:B:112:VAL:HG13	4:B:126:LEU:HD11	2.00	0.42
4:B:54:HIS:ND1	4:B:74:SER:HB3	2.34	0.42
6:N:33:LYS:HG3	6:N:51:ILE:O	2.19	0.42
4:B:186:ASP:N	4:B:186:ASP:OD1	2.53	0.42
4:B:51:LEU:HB3	4:B:82:TRP:CZ3	2.55	0.42
2:R:365:ASN:HB3	2:R:368:LEU:HB2	2.02	0.41
3:A:36:VAL:O	3:A:40:THR:HG22	2.20	0.41
9:R:510:PLM:H61	9:R:512:PLM:H31	2.01	0.41
3:A:372:ILE:H	3:A:372:ILE:HG13	1.65	0.41
3:A:229:ASP:OD1	3:A:229:ASP:N	2.53	0.41
3:A:233:LYS:HA	3:A:233:LYS:HD3	1.84	0.41
3:A:298:ALA:HA	3:A:334:VAL:HG21	2.03	0.41
6:N:37:VAL:HG12	6:N:47:TRP:HA	2.02	0.41
3:A:19:GLN:NE2	4:B:83:ASP:OD2	2.45	0.41
3:A:246:PHE:HB3	3:A:289:LEU:HD12	2.03	0.40
2:R:188:PHE:HE1	2:R:387:VAL:HG12	1.86	0.40
2:R:242:ILE:O	2:R:246:THR:HG23	2.21	0.40
2:R:82:TRP:CZ3	2:R:93:GLN:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:250:CYS:HB2	4:B:264:TYR:HB2	2.04	0.40
4:B:210:LEU:HD22	4:B:255:LEU:HD22	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	P	31/33 (94%)	30 (97%)	0	1 (3%)	3	5
2	R	371/501 (74%)	365 (98%)	6 (2%)	0	100	100
3	A	221/394 (56%)	220 (100%)	1 (0%)	0	100	100
4	B	337/350 (96%)	331 (98%)	6 (2%)	0	100	100
5	G	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
6	N	126/138 (91%)	126 (100%)	0	0	100	100
All	All	1139/1487 (77%)	1124 (99%)	14 (1%)	1 (0%)	49	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	32	PRO

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	P	29/29 (100%)	28 (97%)	1 (3%)	32	60
2	R	283/445 (64%)	277 (98%)	6 (2%)	47	73
3	A	202/349 (58%)	201 (100%)	1 (0%)	81	92
4	B	282/291 (97%)	275 (98%)	7 (2%)	42	69
5	G	45/58 (78%)	43 (96%)	2 (4%)	25	50
6	N	106/115 (92%)	104 (98%)	2 (2%)	50	75
All	All	947/1287 (74%)	928 (98%)	19 (2%)	48	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	32	PRO
2	R	112	CYS
2	R	293	VAL
2	R	305	VAL
2	R	334	GLU
2	R	339	LEU
2	R	367	MET
3	A	349	SER
4	B	59	TYR
4	B	61	MET
4	B	70	LEU
4	B	81	ILE
4	B	181	THR
4	B	190	LEU
4	B	318	LEU
5	G	9	ILE
5	G	15	LEU
6	N	12	VAL
6	N	120	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	3	ASN
1	P	20	GLN
2	R	208	ASN
2	R	288	ASN
2	R	396	ASN
3	A	278	ASN

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Mol	Chain	Res	Type
3	A	279	ASN
4	B	91	HIS
4	B	132	ASN
4	B	155	ASN
4	B	293	ASN
5	G	24	ASN
6	N	120	GLN

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](#)

17 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	$\# Z > 2$
9	PLM	R	508	-	17,17,17	0.54	0	17,17,17	0.50	0
9	PLM	R	509	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	515	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	506	-	17,17,17	0.53	0	17,17,17	0.50	0
7	NAG	R	502	2	14,14,15	0.89	1 (7%)	17,19,21	1.04	1 (5%)
9	PLM	R	510	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	513	-	17,17,17	0.54	0	17,17,17	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PLM	R	516	-	17,17,17	0.54	0	17,17,17	0.50	0
10	Y01	R	507	-	38,38,38	0.45	0	57,57,57	0.51	0
8	P42	R	503	-	51,51,51	0.35	0	53,59,59	0.43	0
9	PLM	R	505	-	17,17,17	0.53	0	17,17,17	0.49	0
9	PLM	R	511	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	517	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	512	-	17,17,17	0.53	0	17,17,17	0.50	0
7	NAG	R	501	2	14,14,15	0.26	0	17,19,21	0.38	0
9	PLM	R	514	-	17,17,17	0.54	0	17,17,17	0.50	0
9	PLM	R	504	-	17,17,17	0.54	0	17,17,17	0.50	0

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
9	PLM	R	508	-	-	2/15/15/15	-
9	PLM	R	509	-	-	2/15/15/15	-
9	PLM	R	515	-	-	0/15/15/15	-
9	PLM	R	506	-	-	2/15/15/15	-
7	NAG	R	502	2	-	2/6/23/26	0/1/1/1
9	PLM	R	510	-	-	2/15/15/15	-
9	PLM	R	513	-	-	0/15/15/15	-
9	PLM	R	516	-	-	2/15/15/15	-
10	Y01	R	507	-	-	3/19/77/77	0/4/4/4
8	P42	R	503	-	-	3/55/55/55	-
9	PLM	R	505	-	-	2/15/15/15	-
9	PLM	R	511	-	-	1/15/15/15	-
9	PLM	R	517	-	-	2/15/15/15	-
9	PLM	R	512	-	-	0/15/15/15	-
7	NAG	R	501	2	-	1/6/23/26	0/1/1/1
9	PLM	R	514	-	-	2/15/15/15	-
9	PLM	R	504	-	-	2/15/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	502	NAG	O5-C1	2.68	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	502	NAG	C1-O5-C5	3.97	117.50	112.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	503	P42	CBK-OBL-PBM-OB
10	R	507	Y01	OAG-CAY-OAW-CBC
10	R	507	Y01	CAM-CAY-OAW-CBC
7	R	502	NAG	O5-C5-C6-O6
7	R	502	NAG	C4-C5-C6-O6
10	R	507	Y01	CAO-CAJ-CAN-CBA
7	R	501	NAG	O5-C5-C6-O6
9	R	511	PLM	C4-C5-C6-C7
8	R	503	P42	OBN-C4-C5-N
8	R	503	P42	CBK-CBE-OB
9	R	510	PLM	O2-C1-C2-C3
9	R	517	PLM	O2-C1-C2-C3
9	R	504	PLM	O2-C1-C2-C3
9	R	516	PLM	O2-C1-C2-C3
9	R	510	PLM	O1-C1-C2-C3
9	R	516	PLM	O1-C1-C2-C3
9	R	508	PLM	O1-C1-C2-C3
9	R	517	PLM	O1-C1-C2-C3
9	R	504	PLM	O1-C1-C2-C3
9	R	506	PLM	O1-C1-C2-C3
9	R	505	PLM	O1-C1-C2-C3
9	R	509	PLM	O1-C1-C2-C3
9	R	514	PLM	O1-C1-C2-C3
9	R	508	PLM	O2-C1-C2-C3
9	R	506	PLM	O2-C1-C2-C3
9	R	509	PLM	O2-C1-C2-C3
9	R	514	PLM	O2-C1-C2-C3
9	R	505	PLM	O2-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 11 short contacts:

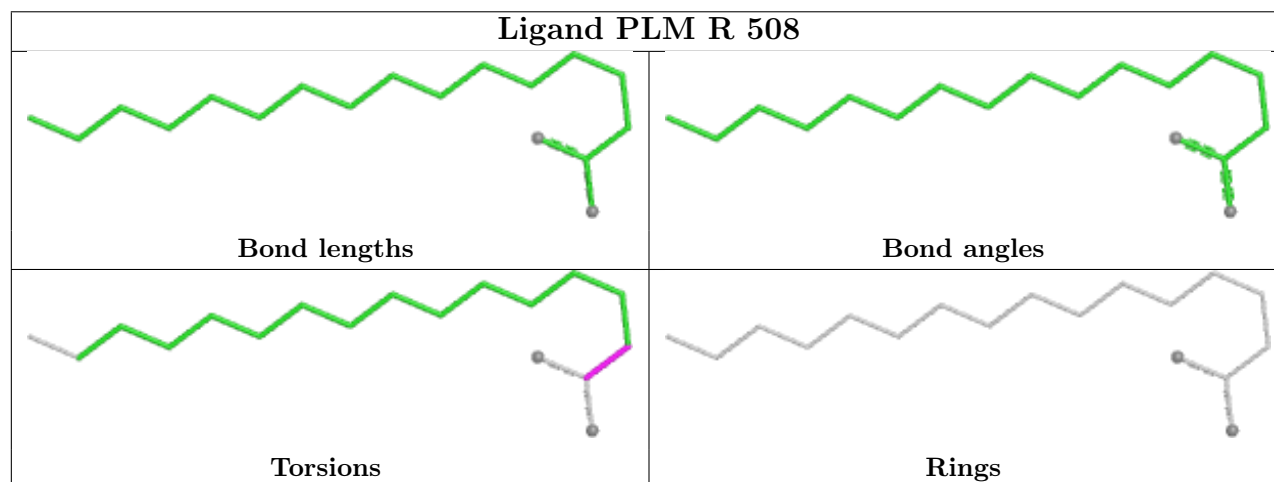
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	508	PLM	1	0

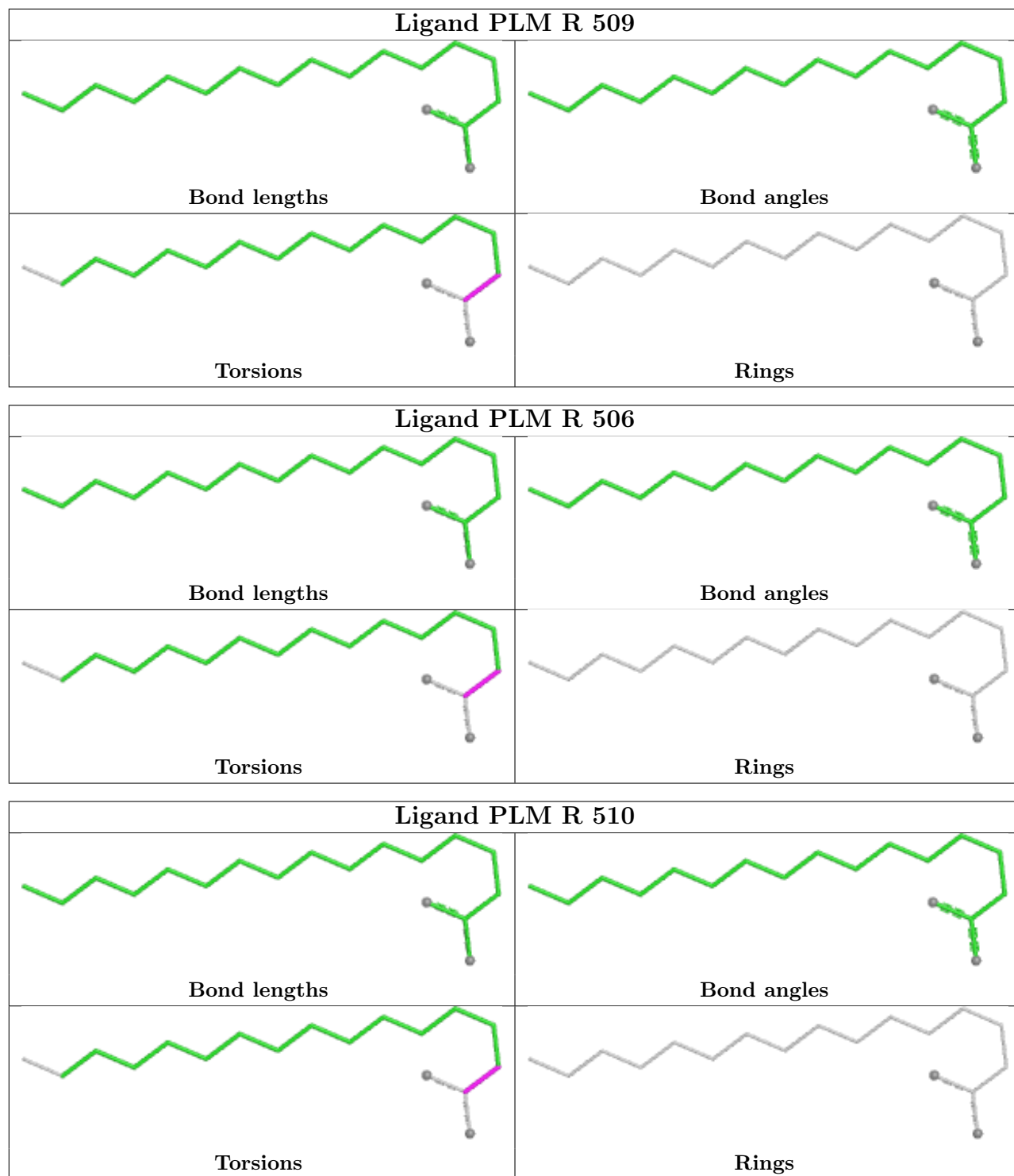
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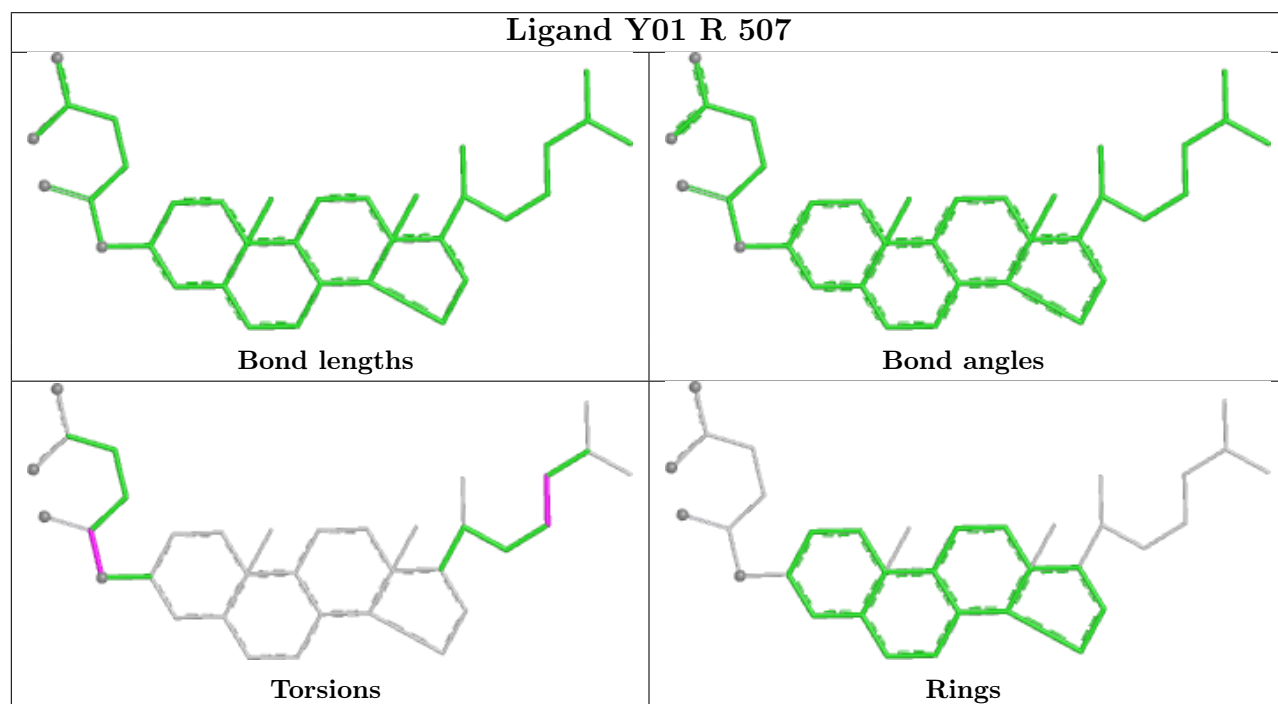
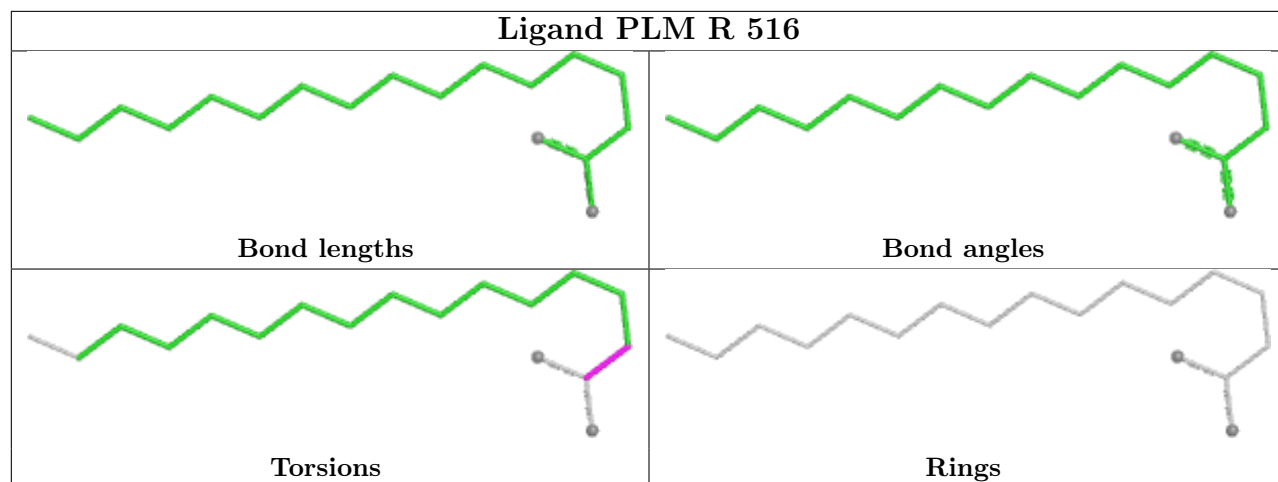
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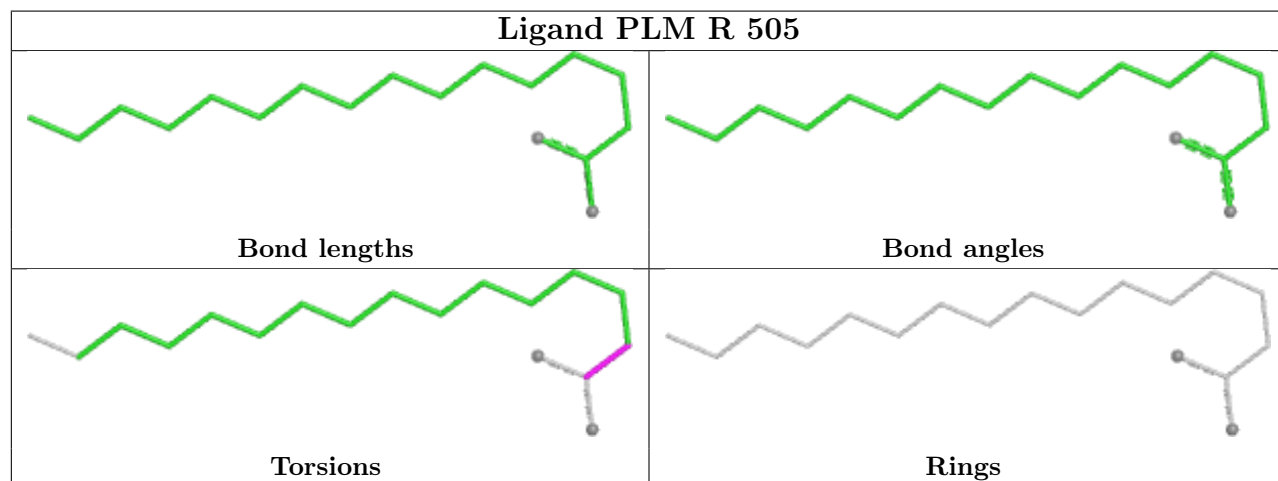
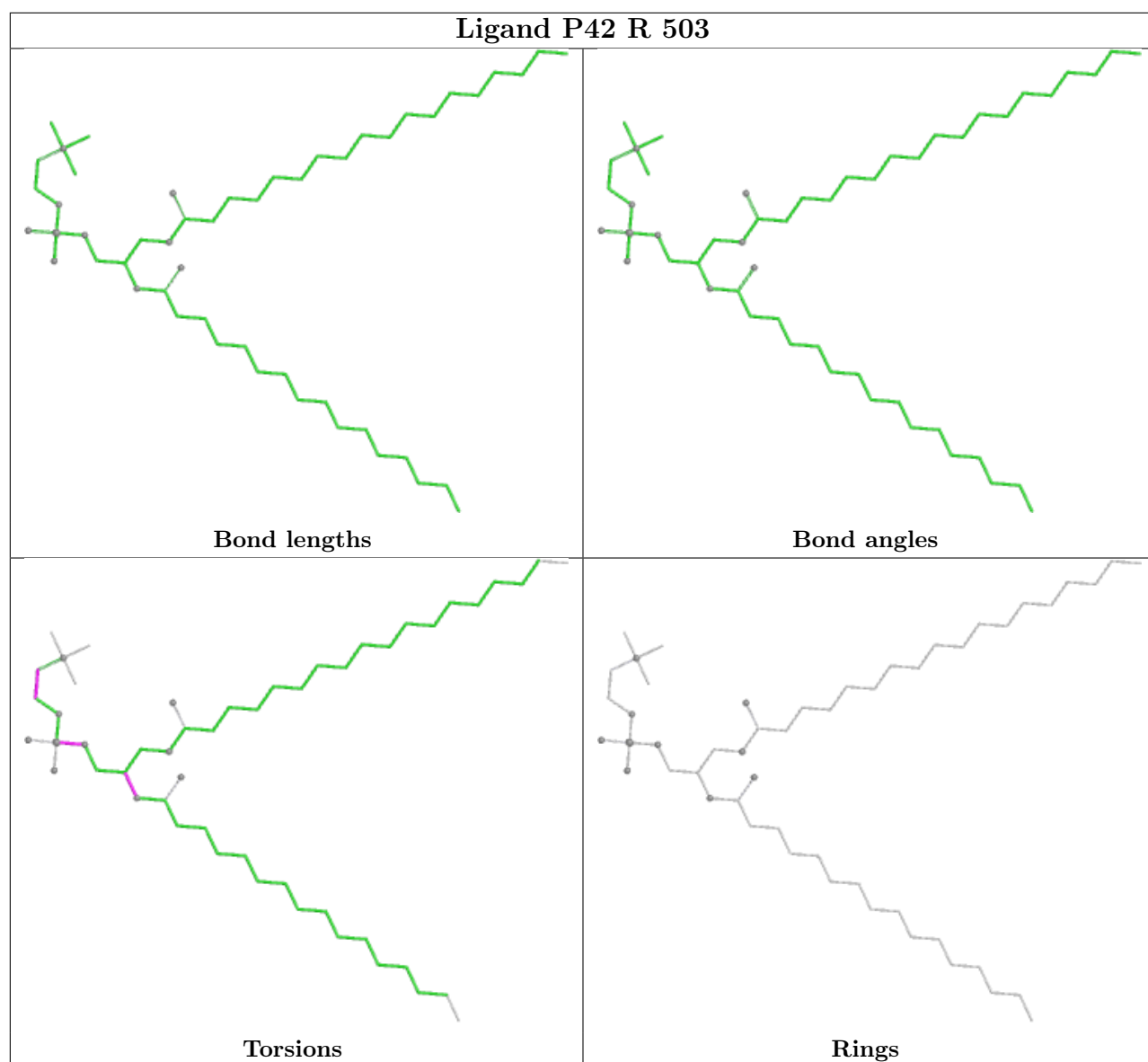
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	509	PLM	1	0
9	R	515	PLM	4	0
9	R	510	PLM	1	0
9	R	513	PLM	1	0
8	R	503	P42	2	0
9	R	511	PLM	1	0
9	R	512	PLM	1	0
9	R	514	PLM	1	0

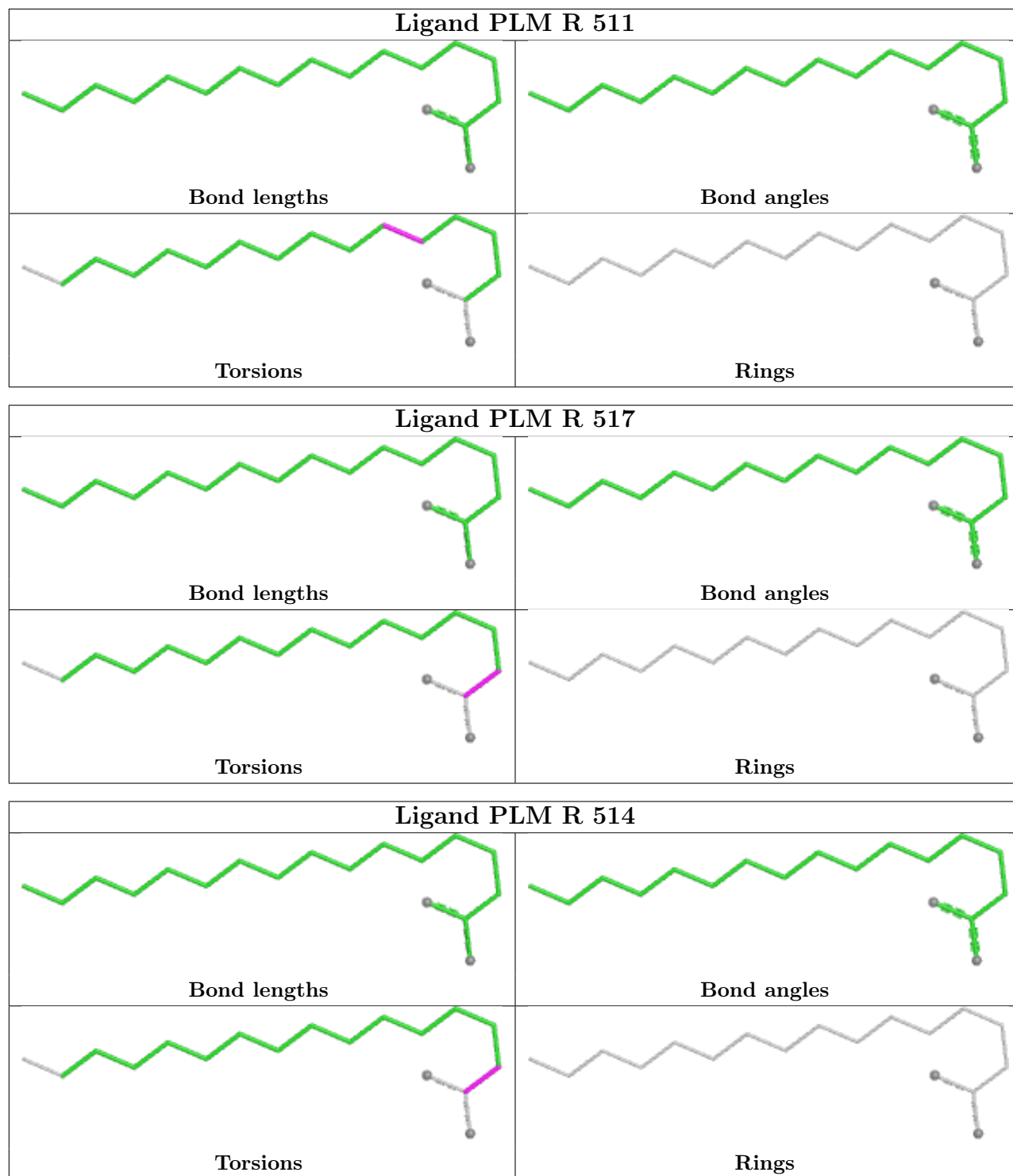
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

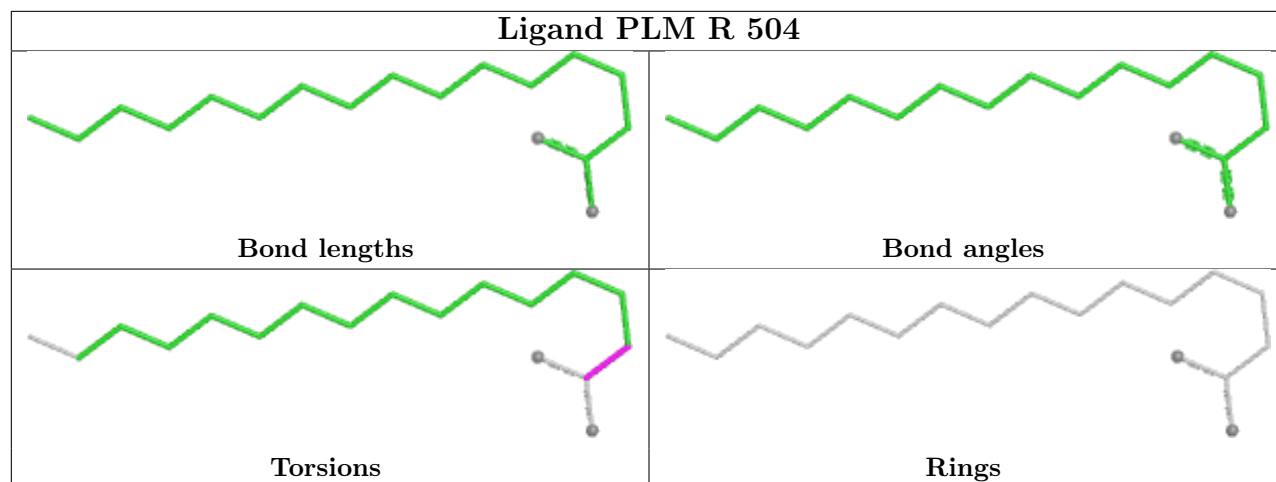












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26188. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.