wwPDB EM Validation Summary Report

Oct 6, 2024 – 11:21 AM EDT

PDB ID	:	8SI6
EMDB ID	:	EMD-40500
Title	:	Cryo-EM structure of TRPM7 in MSP2N2 nanodisc in complex with agonist naltriben in closed state
Authors	:	Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on	:	2023-04-14
Resolution	:	2.44 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:

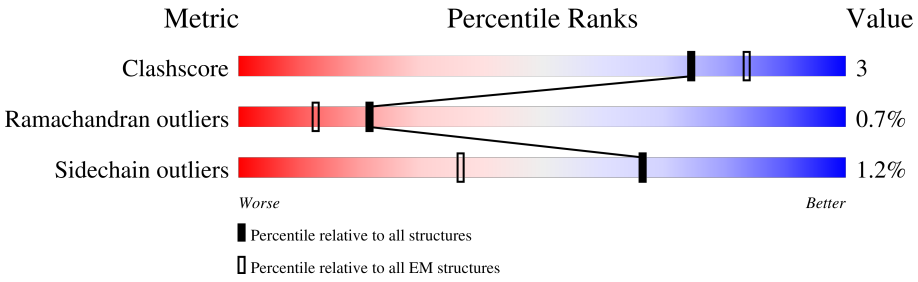
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.44 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1279	48% 79% 7% 13%
1	B	1279	48% 79% 7% 13%
1	C	1279	48% 79% 7% 13%
1	D	1279	48% 79% 7% 13%

2 Entry composition (i)

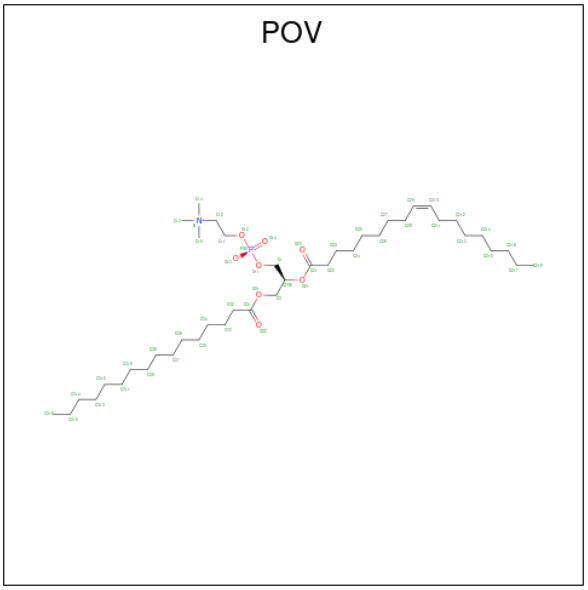
There are 6 unique types of molecules in this entry. The entry contains 79305 atoms, of which 40656 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1107	Total	C	H	N	O	S	0	0
			18006	5813	9060	1493	1580	60		
1	B	1107	Total	C	H	N	O	S	0	0
			18006	5813	9060	1493	1580	60		
1	C	1107	Total	C	H	N	O	S	0	0
			18006	5813	9060	1493	1580	60		
1	D	1107	Total	C	H	N	O	S	0	0
			18006	5813	9060	1493	1580	60		

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
2	A	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 82 25 49 1 6 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	A	1	Total C H 44 15 29	0
2	A	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 82 25 49 1 6 1	0

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Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H N O P 134 42 82 1 8 1	0
2	B	1	Total C H 44 15 29	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 82 25 49 1 6 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H N O P 134 42 82 1 8 1	0
2	C	1	Total C H 44 15 29	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H 44 15 29	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0

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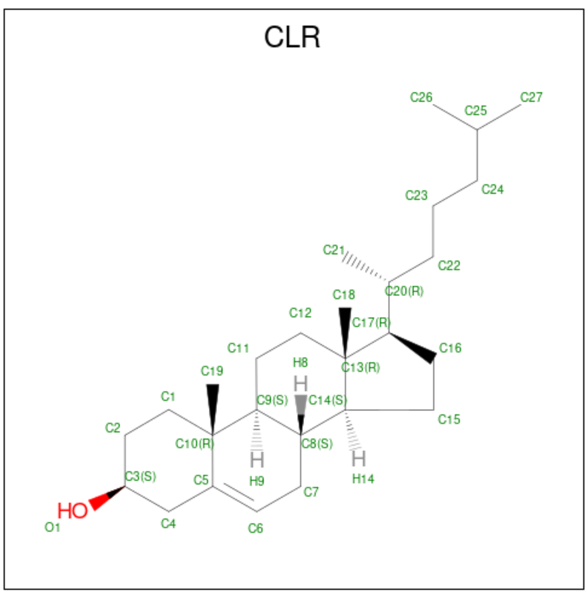
Mol	Chain	Residues	Atoms	AltConf
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0
2	D	1	Total C H N O P 82 25 49 1 6 1	0
2	D	1	Total C H N O P 134 42 82 1 8 1	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C H O 74 27 46 1	0
3	B	1	Total C H O 74 27 46 1	0
3	C	1	Total C H O 74 27 46 1	0

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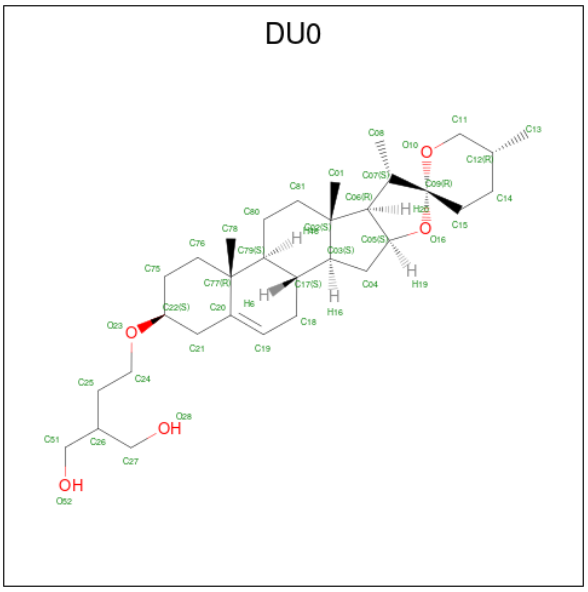
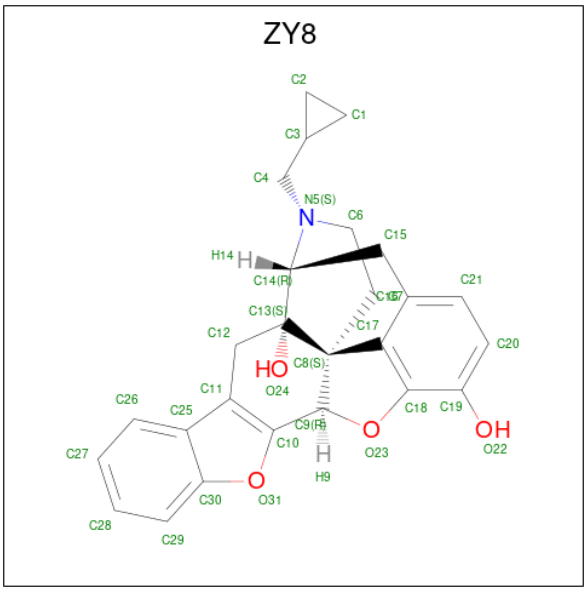
Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	H	O	0
			74	27	46	1	

- Molecule 4 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (three-letter code: DU0) (formula: $C_{32}H_{52}O_5$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			89	32	52	5	
4	B	1	Total	C	H	O	0
			89	32	52	5	
4	C	1	Total	C	H	O	0
			89	32	52	5	
4	D	1	Total	C	H	O	0
			89	32	52	5	

- Molecule 5 is (4bS,8R,8aS,14bR)-7-(cyclopropylmethyl)-5,6,7,8,9,14b-hexahydro-8aH-4,8-methanobis[1]benzofuro[3,2-e:2',3'-g]isoquinoline-1,8a-diol (three-letter code: ZY8) (formula: $C_{26}H_{25}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	0
			57	26	26	1	4	
5	B	1	Total	C	H	N	O	0
			57	26	26	1	4	
5	C	1	Total	C	H	N	O	0
			57	26	26	1	4	
5	D	1	Total	C	H	N	O	0
			57	26	26	1	4	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

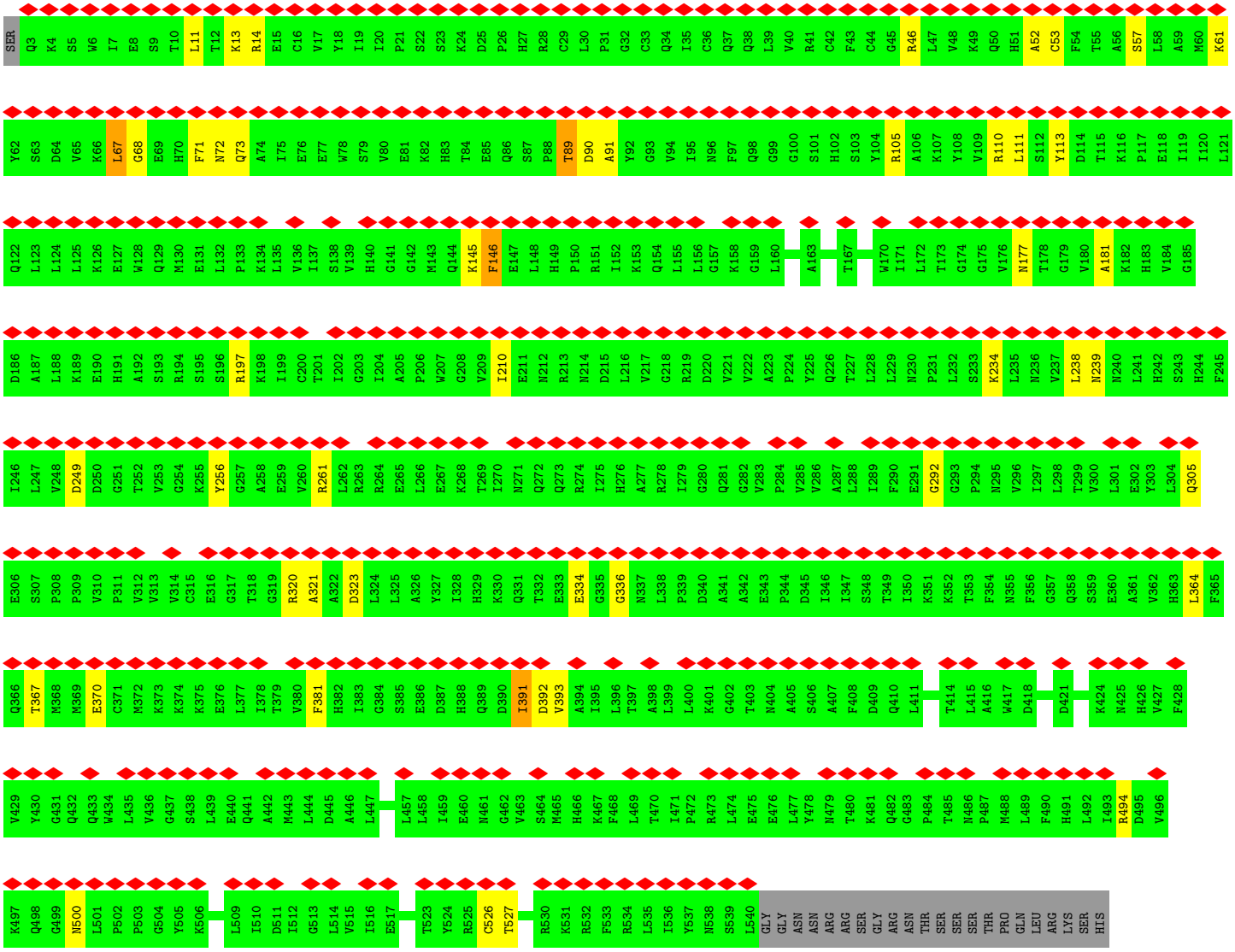
Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Ca	0
			1	1	

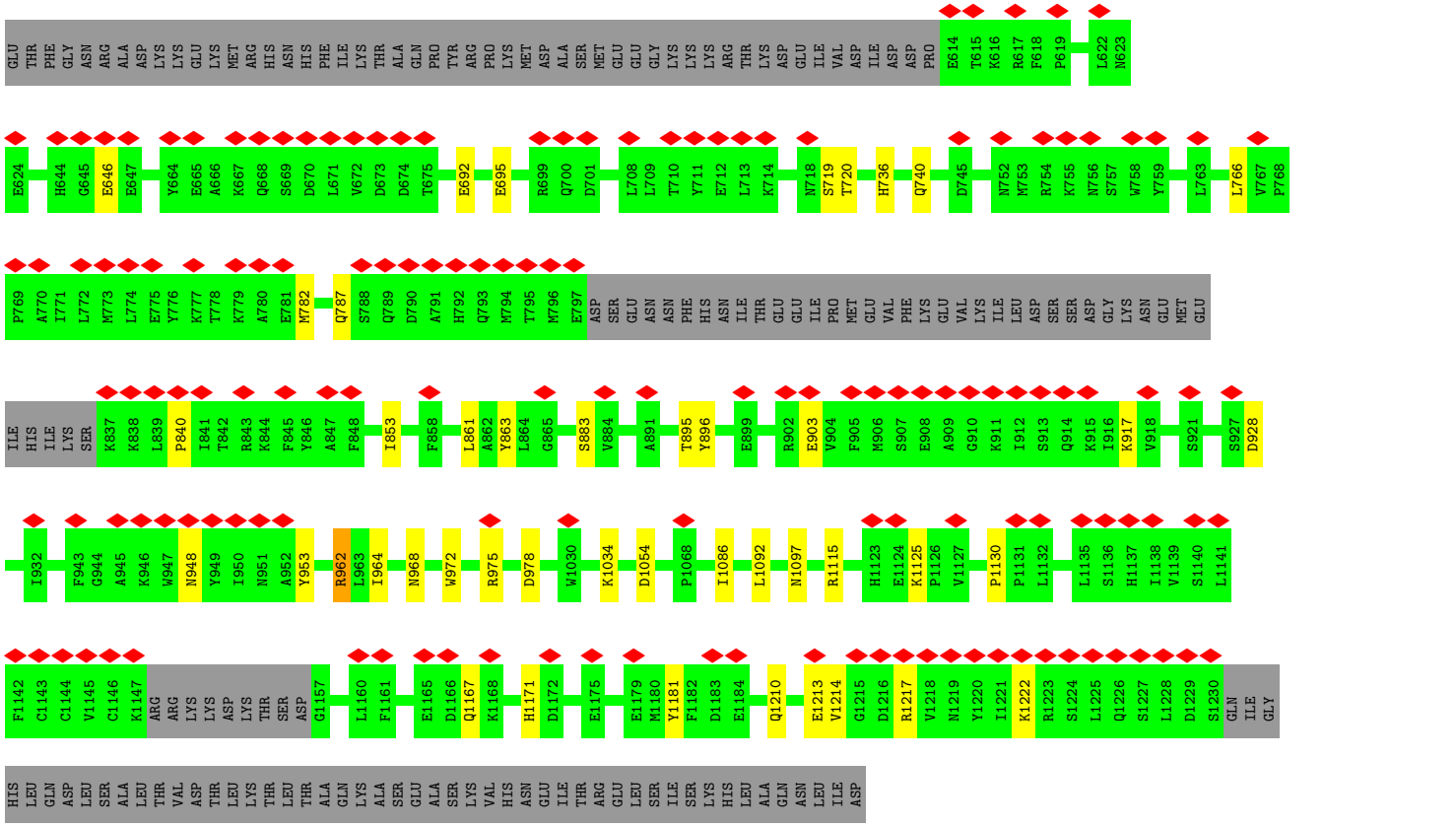
3 Residue-property plots (i)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Transient receptor potential cation channel subfamily M member 7

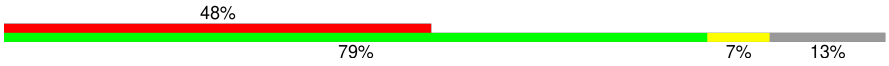
Chain A:

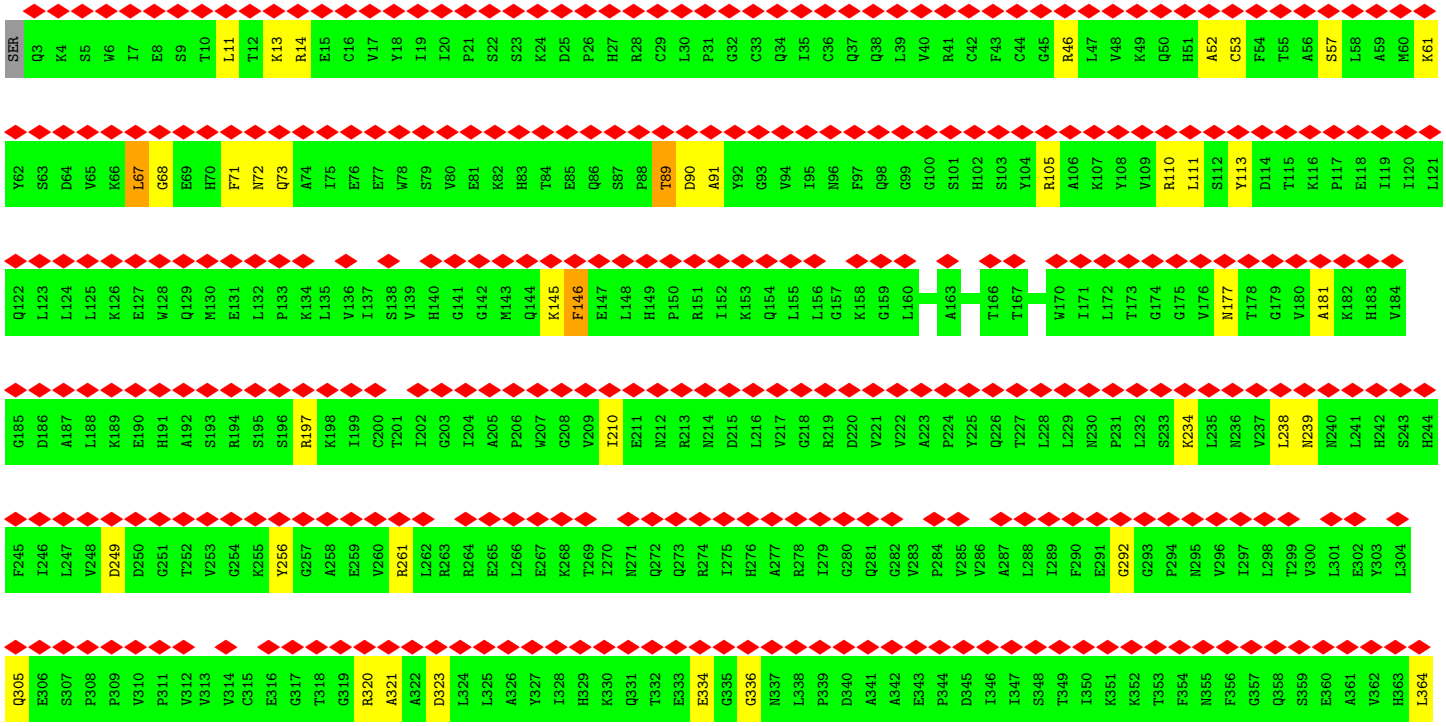


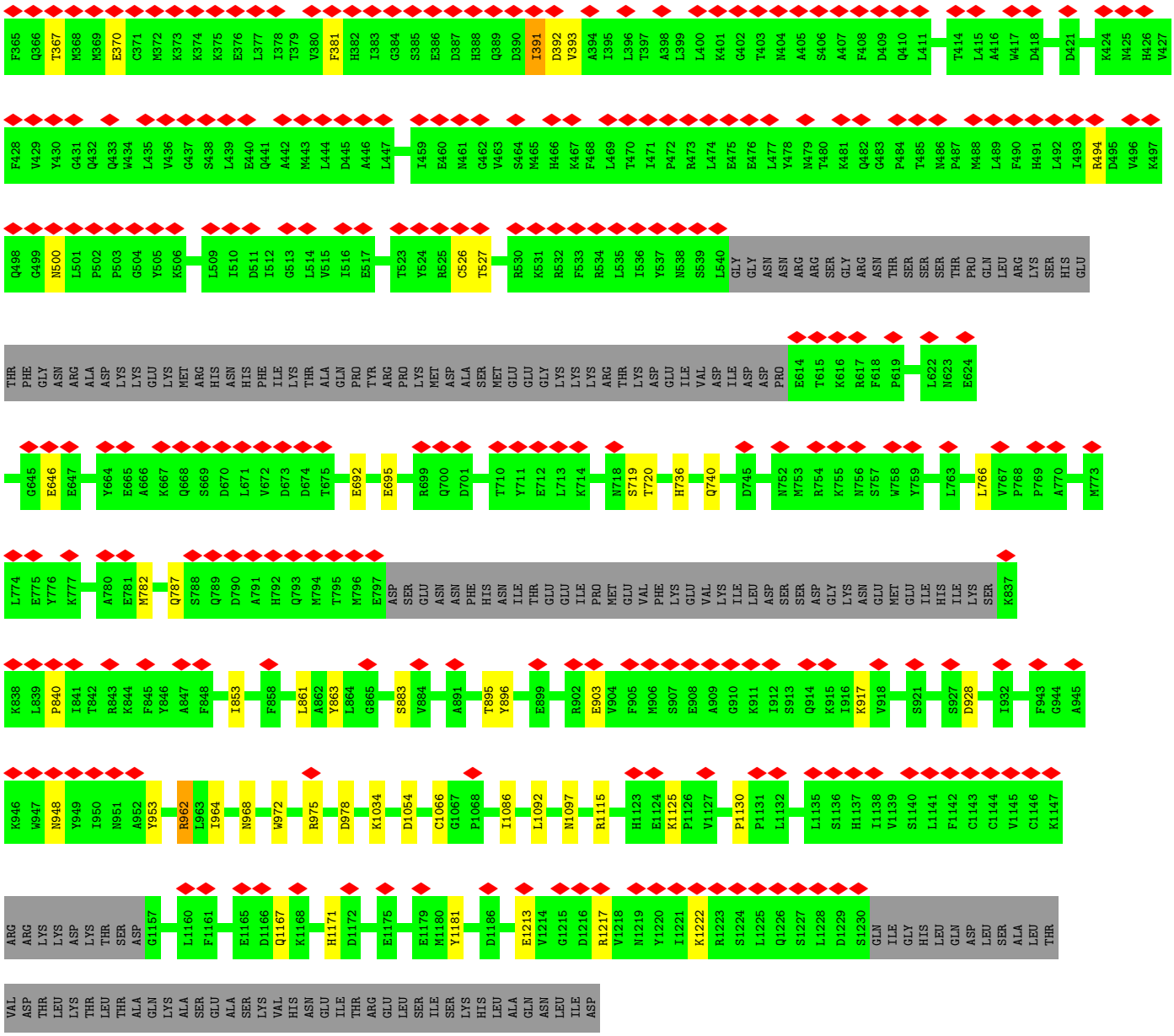


• Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain B:

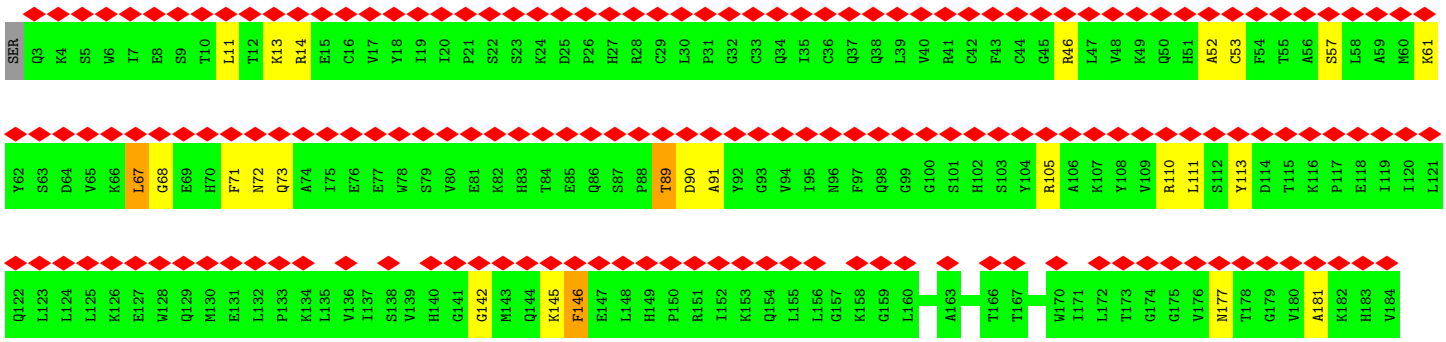


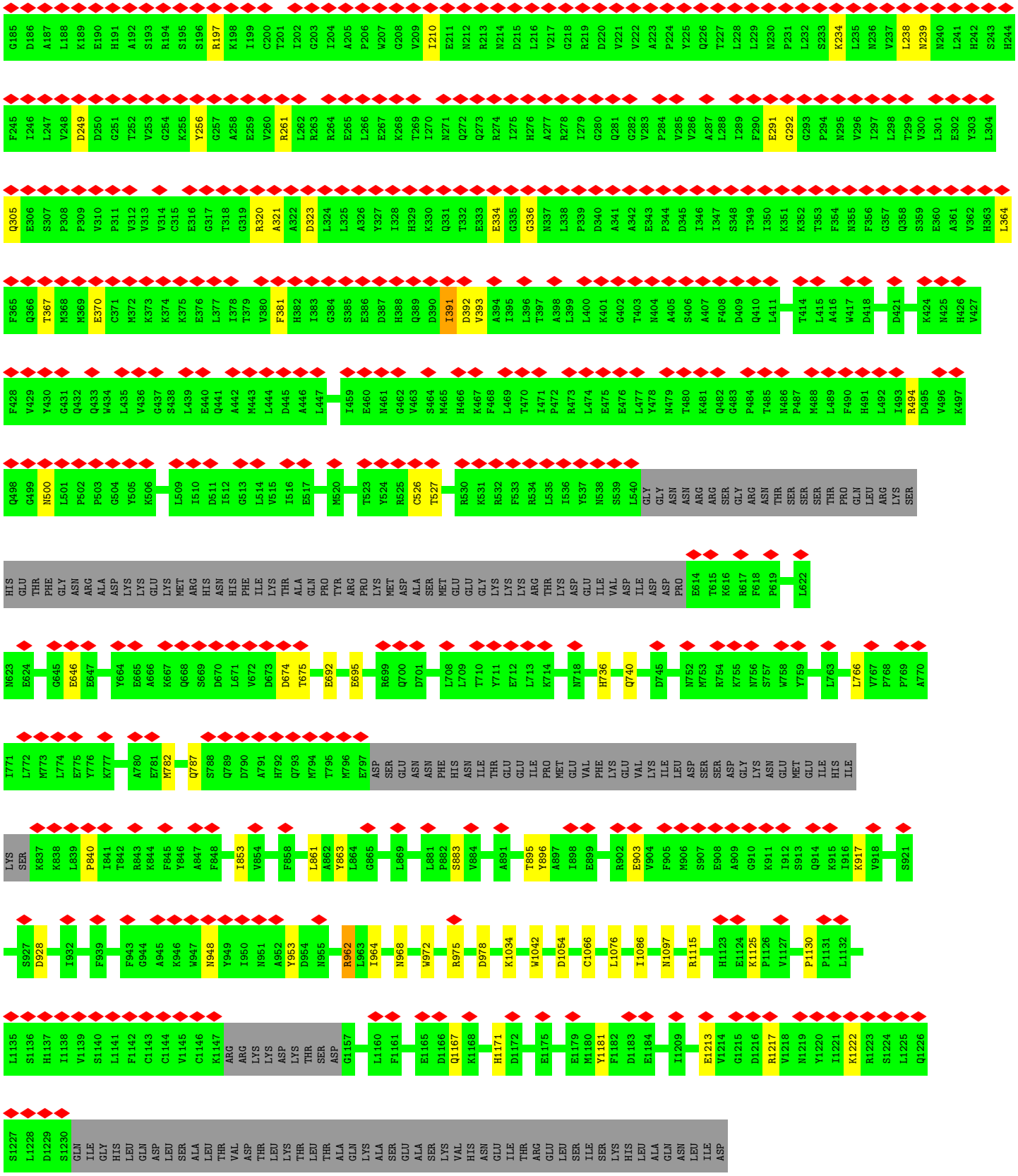




• Molecule 1: Transient receptor potential cation channel subfamily M member 7

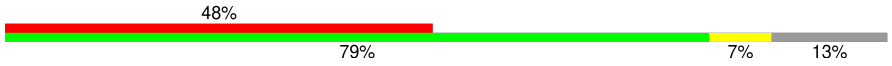
Chain C:

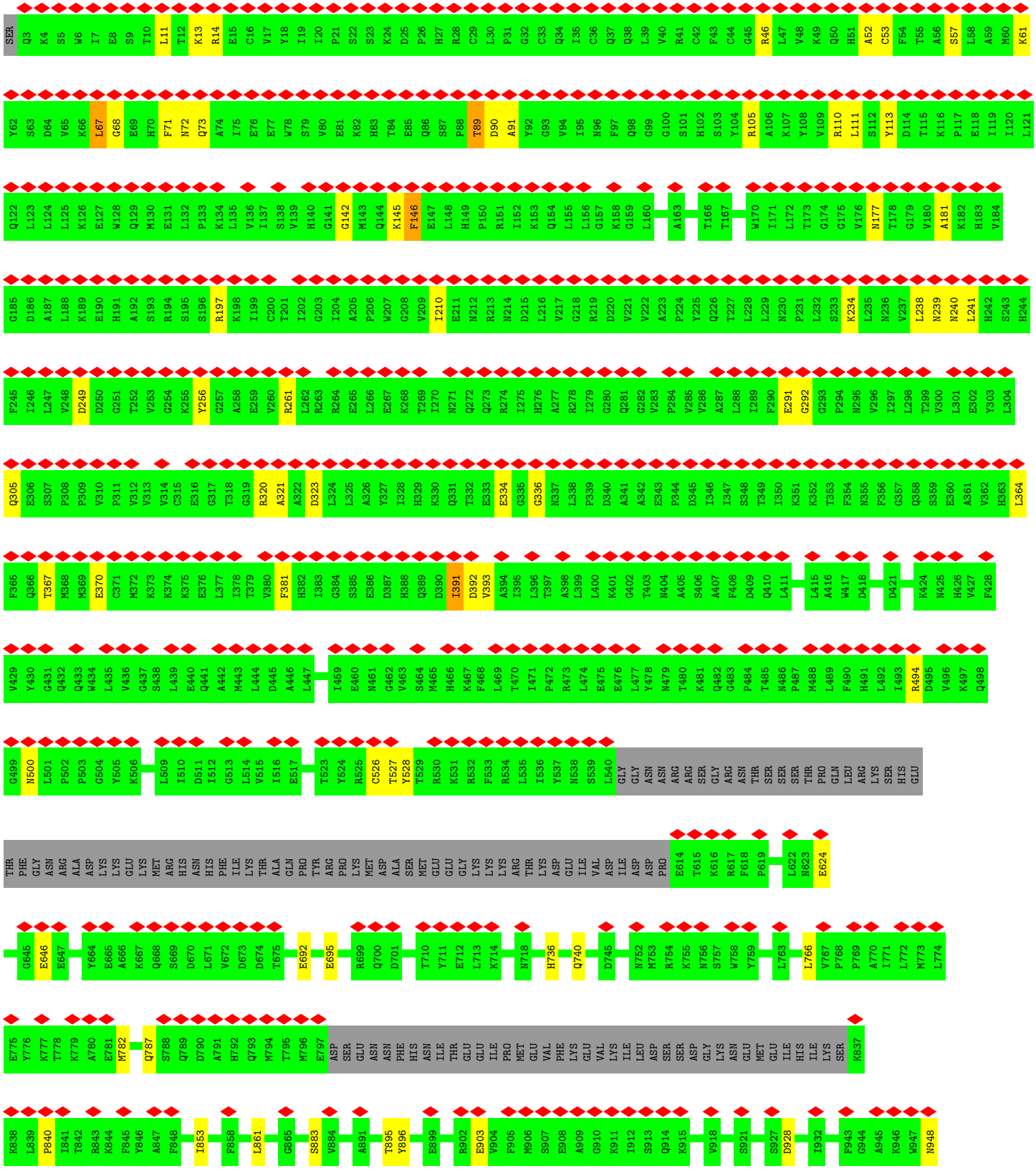


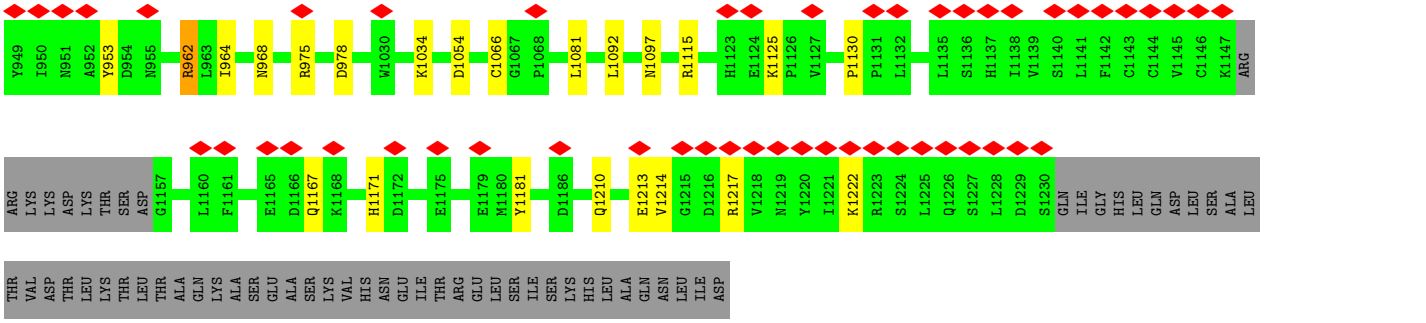


• Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain D:


48%
79%
7%
13%


SER Q3 K4 S5 W6 I7 E8 S9 T10 L11 T12 K13 R14 E15 C16 V17 Y18 I19 I20 P21 S22 S23 K24 D25 P26 H27 R28 C29 L30 P31 G32 C33 Q34 I35 C36 Q37 Q38 L39 V40 R41 C42 F43 C44 G45 R46 L47 V48 K49 Q50 H51 A52 C53 F54 T55 A56 S57 L58 A59 M60 K61
Y62 S63 D64 V65 K66 L67 G68 E69 H70 F71 N72 Q73 A74 I75 E76 E77 W78 S79 V80 E81 K82 H83 T84 E85 Q86 S87 P88 T89 D90 A91 Y92 G93 V94 I95 N96 F97 Q98 G99 G100 S101 H102 S103 Y104 R105 A106 K107 Y108 V109 R110 L111 S112 Y113 D114 T115 K116 P117 E118 I119 I120 L121
Q122 L123 L124 L125 K126 E127 W128 Q129 M130 E131 L132 P133 K134 L135 V136 I137 S138 V139 H140 G141 G142 M143 Q144 K145 F146 E147 L148 H149 P150 R151 I152 K153 Q154 L155 L156 G157 K158 G159 L160 A163 T166 T167 W170 I171 L172 T173 G174 G175 V176 N177 T178 G179 V180 A181 K182 H183 V184
G185 D186 A187 L188 K189 E190 H191 A192 S193 R194 S195 S196 R197 K198 I199 C200 T201 I202 G203 I204 A205 P206 W207 G208 V209 I210 E211 N212 R213 N214 D215 L216 V217 G218 R219 D220 V221 V222 A223 P224 Y225 Q226 T227 L228 L229 N230 P231 L232 S233 K234 L235 N236 V237 L238 N239 N240 L241 H242 S243 H244
F245 I246 L247 V248 D249 D250 G251 T252 V253 G254 K255 Y256 G257 A258 E259 V260 R261 L262 R263 R264 E265 L266 E267 K268 T269 I270 N271 Q272 Q273 R274 I275 H276 A277 R278 I279 G280 Q281 Q282 V283 P284 V285 V286 A287 L288 I289 F290 E291 G292 G293 P294 N295 V296 I297 L298 T299 V300 L301 E302 Y303 L304
Q305 E306 S307 P308 P309 V310 P311 V312 V313 V314 C315 E316 G317 T318 G319 R320 A321 A322 D323 L324 L325 A326 Y327 I328 H329 K330 Q331 T332 E333 E334 G335 G336 N337 L338 P339 D340 A341 A342 E343 P344 D345 I346 I347 S348 T349 I350 K351 K352 T353 F354 N355 F356 G357 Q358 S359 E360 A361 V362 H363 L364
F365 Q366 T367 M368 M369 E370 C371 M372 K373 K374 K375 E376 L377 I378 T379 V380 F381 H382 I383 G384 S385 E386 D387 H388 Q389 D390 I391 D392 V393 A394 I395 L396 T397 A398 L399 L400 K401 G402 T403 N404 A405 S406 A407 F408 D409 Q410 L411 L415 A416 W417 D418 D421 K424 N425 H426 V427 F428
V429 Y430 G431 Q432 Q433 W434 L435 V436 G437 S438 L439 E440 Q441 A442 M443 L444 D445 A446 L447 T459 E460 N461 G462 V463 S464 M465 H466 K467 F468 L469 T470 I471 P472 R473 L474 E475 E476 L477 Y478 N479 T480 K481 Q482 G483 P484 T485 N486 P487 M488 L489 F490 H491 L492 I493 R494 D495 V496 K497 Q498
G499 N500 L501 P502 P503 G504 Y505 K506 L509 I510 D511 I512 G513 L514 V515 I516 E517 T523 Y524 R525 C526 T527 Y528 T529 R530 K531 R532 F533 R534 L535 I536 Y537 N538 S539 L540 GLY GLY ASN ASN ARG ARG SER GLY ARG ASN THR SER SER SER THR PRO GLN LEU ARG LYS SER HIS GLU
THR PHE GLY ASN ARG ALA ASP LYS LYS GLU LYS MET ARG HIS ASN HIS PHE ILE LYS THR ALA GLN PRO TYR ARG PRO LYS MET ASP ALA SER MET GLU GLU GLY LYS LYS LYS ARG THR LYS ASP GLU ILE VAL ASP ILE ASP ASP PRO E614 T615 K616 R617 F618 P619 L622 N623 E624
G645 E646 E647 Y664 E665 A666 K667 Q668 S669 D670 L671 V672 D673 D674 T675 E692 E695 R699 Q700 D701 T710 Y711 E712 L713 K714 N718 H736 Q740 D745 N752 M753 R754 K755 N756 S757 W758 Y759 L763 L766 V767 P768 P769 A770 I771 L772 M773 L774
E775 Y776 K777 T778 K779 A780 E781 M782 Q787 S788 Q789 D790 A791 H792 Q793 M794 T795 M796 E797 ASP SER GLU ASN ASN PHE HIS ASN ILE THR GLU GLU ILE PRO MET GLU VAL PHE LYS GLU VAL LYS ILE LEU ASP SER ASP GLY LYS ASN GLU MET GLU ILE HIS ILE LYS SER K837
K838 L839 P840 I841 T842 R843 K844 F845 Y846 A847 F848 I853 F858 L861 G865 S883 V884 A891 T895 Y896 E899 R902 E903 V904 F905 M906 S907 E908 A909 G910 K911 I912 S913 Q914 K915 V918 S921 S927 D928 I932 F943 G944 A945 K946 W947 N948


Y949 I950 N951 A952 Y953 D954 N955 R962 L963 I964 N968 R975 D978 W1030 K1034 D1054 C1066 G1067 P1068 L1081 L1092 N1097 R1115 H1123 E1124 K1125 P1126 V1127 P1130 P1131 L1132 L1135 S1136 H1137 I1138 V1139 S1140 L1141 F1142 C1143 C1144 V1145 C1146 K1147 ARG
ARG LYS LYS ASP LYS THR SER ASP G1157 L1160 F1161 E1165 D1166 Q1167 K1168 H1171 D1172 E1175 E1179 M1180 Y1181 D1186 Q1210 E1213 V1214 G1215 D1216 R1217 V1218 N1219 Y1220 I1221 K1222 R1223 S1224 L1225 Q1226 S1227 L1228 D1229 S1230 GLN ILE GLY HIS LEU GLN ASP LEU SER ALA LEU
THR VAL ASP THR LEU LYS THR LEU THR ALA ALA GLN LYS ALA SER GLU ALA SER LYS VAL HIS ASN GLU ILE THR ARG GLU LEU SER ILE SER LYS HIS LEU ALA GLN ASN LEU ILE ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.839	Depositor
Minimum map value	-1.124	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.26	Depositor
Map size (Å)	249.0, 249.0, 249.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, ZY8, DU0, POV, CA

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	0.48	0/9162	0.59	0/12409
1	B	0.48	0/9162	0.59	0/12409
1	C	0.48	0/9162	0.59	0/12409
1	D	0.48	0/9162	0.59	0/12409
All	All	0.48	0/36648	0.59	0/49636

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
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	LYS	Peptide
1	A	146	PHE	Peptide
1	A	256	TYR	Peptide
1	A	52	ALA	Peptide
1	A	67	LEU	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	8946	9060	9056	48	0
1	B	8946	9060	9056	48	0
1	C	8946	9060	9056	50	0
1	D	8946	9060	9056	49	0
2	A	672	1062	1056	23	0
2	B	568	898	892	20	0
2	C	620	980	974	21	0
2	D	620	980	974	22	0
3	A	28	46	46	1	0
3	B	28	46	46	1	0
3	C	28	46	46	1	0
3	D	28	46	46	1	0
4	A	37	52	0	0	0
4	B	37	52	0	0	0
4	C	37	52	0	0	0
4	D	37	52	0	0	0
5	A	31	26	0	1	0
5	B	31	26	0	1	0
5	C	31	26	0	1	0
5	D	31	26	0	1	0
6	C	1	0	0	0	0
All	All	38649	40656	40304	234	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 3.

The worst 5 of 234 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:B:903:GLU:OE2	1:B:1125:LYS:NZ	2.16	0.79
1:C:903:GLU:OE2	1:C:1125:LYS:NZ	2.16	0.79
1:A:903:GLU:OE2	1:A:1125:LYS:NZ	2.16	0.78
1:D:903:GLU:OE2	1:D:1125:LYS:NZ	2.16	0.78
1:A:895:THR:OG1	1:A:1130:PRO:O	2.05	0.75

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	1099/1279 (86%)	1009 (92%)	82 (8%)	8 (1%)	19	22
1	B	1099/1279 (86%)	1008 (92%)	83 (8%)	8 (1%)	19	22
1	C	1099/1279 (86%)	1009 (92%)	82 (8%)	8 (1%)	19	22
1	D	1099/1279 (86%)	1008 (92%)	83 (8%)	8 (1%)	19	22
All	All	4396/5116 (86%)	4034 (92%)	330 (8%)	32 (1%)	21	22

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	146	PHE
1	B	67	LEU
1	B	146	PHE
1	C	67	LEU

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	981/1138 (86%)	969 (99%)	12 (1%)	67	79
1	B	981/1138 (86%)	969 (99%)	12 (1%)	67	79
1	C	981/1138 (86%)	969 (99%)	12 (1%)	67	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	981/1138 (86%)	969 (99%)	12 (1%)	67 79
All	All	3924/4552 (86%)	3876 (99%)	48 (1%)	66 79

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	197	ARG
1	C	1222	LYS
1	C	234	LYS
1	C	948	ASN
1	D	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	276	HIS
1	D	955	ASN
1	B	1098	ASN
1	C	3	GLN
1	C	98	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)

Of 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 for Mogul analysis.

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	$\#\|Z\| > 2$
2	POV	C	1302	-	51,51,51	0.34	0	57,59,59	0.38	0
2	POV	B	1308	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	A	1316	-	14,14,51	1.01	1 (7%)	13,13,59	0.58	0
2	POV	D	1301	-	51,51,51	0.37	0	57,59,59	0.49	0
5	ZY8	B	1313	-	34,38,38	1.17	4 (11%)	49,63,63	1.31	6 (12%)
2	POV	B	1305	-	51,51,51	0.32	0	57,59,59	0.37	0
2	POV	C	1306	-	51,51,51	0.32	0	57,59,59	0.37	0
4	DU0	B	1312	-	42,42,42	0.22	0	64,66,66	0.34	0
2	POV	B	1301	-	51,51,51	0.33	0	57,59,59	0.38	0
2	POV	D	1304	-	51,51,51	0.33	0	57,59,59	0.37	0
2	POV	D	1313	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	A	1310	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	B	1314	-	51,51,51	0.36	0	57,59,59	0.49	0
2	POV	A	1303	-	51,51,51	0.38	0	57,59,59	0.65	1 (1%)
2	POV	B	1307	-	51,51,51	0.37	0	57,59,59	0.46	0
2	POV	A	1306	-	51,51,51	0.31	0	57,59,59	0.37	0
2	POV	B	1310	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	B	1315	-	14,14,51	1.01	1 (7%)	13,13,59	0.59	0
2	POV	C	1308	-	51,51,51	0.37	0	57,59,59	0.46	0
2	POV	C	1307	-	51,51,51	0.33	0	57,59,59	0.48	0
2	POV	A	1308	-	51,51,51	0.37	0	57,59,59	0.46	0
2	POV	C	1303	-	51,51,51	0.38	0	57,59,59	0.53	1 (1%)
2	POV	C	1304	-	51,51,51	0.38	0	57,59,59	0.64	1 (1%)
2	POV	B	1309	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	C	1301	-	51,51,51	0.31	0	57,59,59	0.38	0
2	POV	B	1306	-	51,51,51	0.33	0	57,59,59	0.49	0
2	POV	C	1316	-	14,14,51	1.01	1 (7%)	13,13,59	0.58	0
2	POV	D	1308	-	51,51,51	0.32	0	57,59,59	0.37	0
5	ZY8	D	1316	-	34,38,38	1.17	4 (11%)	49,63,63	1.32	5 (10%)
2	POV	A	1305	-	51,51,51	0.32	0	57,59,59	0.37	0
2	POV	D	1305	-	51,51,51	0.37	0	57,59,59	0.53	1 (1%)
2	POV	C	1310	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	C	1315	-	51,51,51	0.37	0	57,59,59	0.48	0
3	CLR	D	1307	-	31,31,31	0.20	0	48,48,48	0.35	0
2	POV	B	1303	-	51,51,51	0.38	0	57,59,59	0.65	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CLR	A	1304	-	31,31,31	0.20	0	48,48,48	0.35	0
3	CLR	C	1305	-	31,31,31	0.20	0	48,48,48	0.35	0
4	DU0	A	1313	-	42,42,42	0.21	0	64,66,66	0.34	0
2	POV	D	1303	-	51,51,51	0.30	0	57,59,59	0.37	0
2	POV	C	1309	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	A	1315	-	51,51,51	0.37	0	57,59,59	0.49	0
2	POV	D	1312	-	51,51,51	0.32	0	57,59,59	0.40	0
2	POV	B	1311	-	51,51,51	0.31	0	57,59,59	0.39	0
2	POV	A	1302	-	51,51,51	0.37	0	57,59,59	0.53	1 (1%)
2	POV	A	1309	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	D	1309	-	51,51,51	0.33	0	57,59,59	0.49	0
2	POV	D	1314	-	51,51,51	0.31	0	57,59,59	0.39	0
3	CLR	B	1304	-	31,31,31	0.20	0	48,48,48	0.35	0
2	POV	C	1311	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	C	1312	-	51,51,51	0.31	0	57,59,59	0.39	0
5	ZY8	A	1314	-	34,38,38	1.17	4 (11%)	49,63,63	1.32	6 (12%)
5	ZY8	C	1314	-	34,38,38	1.17	4 (11%)	49,63,63	1.33	6 (12%)
2	POV	B	1302	-	51,51,51	0.37	0	57,59,59	0.54	1 (1%)
2	POV	D	1310	-	51,51,51	0.37	0	57,59,59	0.46	0
4	DU0	D	1315	-	42,42,42	0.22	0	64,66,66	0.34	0
2	POV	A	1301	-	51,51,51	0.33	0	57,59,59	0.38	0
2	POV	D	1302	-	14,14,51	1.01	1 (7%)	13,13,59	0.58	0
2	POV	D	1311	-	51,51,51	0.35	0	57,59,59	0.50	0
2	POV	A	1311	-	32,32,51	0.41	0	37,38,59	0.37	0
2	POV	D	1306	-	51,51,51	0.38	0	57,59,59	0.64	1 (1%)
2	POV	A	1312	-	51,51,51	0.31	0	57,59,59	0.39	0
4	DU0	C	1313	-	42,42,42	0.24	0	64,66,66	0.36	0
2	POV	A	1307	-	51,51,51	0.32	0	57,59,59	0.48	0
2	POV	A	1317	-	51,51,51	0.31	0	57,59,59	0.37	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
2	POV	C	1302	-	-	26/55/55/55	-
2	POV	B	1308	-	-	21/55/55/55	-
2	POV	A	1316	-	-	6/12/12/55	-
2	POV	D	1301	-	-	23/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ZY8	B	1313	-	-	2/4/60/60	0/1/8/8
2	POV	B	1305	-	-	23/55/55/55	-
2	POV	C	1306	-	-	24/55/55/55	-
4	DU0	B	1312	-	-	3/10/98/98	0/6/6/6
2	POV	B	1301	-	-	26/55/55/55	-
2	POV	D	1304	-	-	26/55/55/55	-
2	POV	D	1313	-	-	13/33/33/55	-
2	POV	A	1310	-	-	20/55/55/55	-
2	POV	B	1314	-	-	24/55/55/55	-
2	POV	A	1303	-	-	25/55/55/55	-
2	POV	B	1307	-	-	20/55/55/55	-
2	POV	A	1306	-	-	20/55/55/55	-
2	POV	B	1310	-	-	13/33/33/55	-
2	POV	B	1315	-	-	6/12/12/55	-
2	POV	C	1308	-	-	20/55/55/55	-
2	POV	C	1307	-	-	27/55/55/55	-
2	POV	A	1308	-	-	20/55/55/55	-
2	POV	C	1303	-	-	24/55/55/55	-
2	POV	C	1304	-	-	25/55/55/55	-
2	POV	B	1309	-	-	20/55/55/55	-
2	POV	C	1301	-	-	18/55/55/55	-
2	POV	B	1306	-	-	27/55/55/55	-
2	POV	C	1316	-	-	6/12/12/55	-
2	POV	D	1308	-	-	24/55/55/55	-
5	ZY8	D	1316	-	-	2/4/60/60	0/1/8/8
2	POV	A	1305	-	-	24/55/55/55	-
2	POV	D	1305	-	-	24/55/55/55	-
2	POV	C	1310	-	-	20/55/55/55	-
2	POV	C	1315	-	-	23/55/55/55	-
3	CLR	D	1307	-	-	4/10/68/68	0/4/4/4
2	POV	B	1303	-	-	25/55/55/55	-
3	CLR	A	1304	-	-	4/10/68/68	0/4/4/4
3	CLR	C	1305	-	-	4/10/68/68	0/4/4/4
4	DU0	A	1313	-	-	3/10/98/98	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	D	1303	-	-	20/55/55/55	-
2	POV	C	1309	-	-	21/55/55/55	-
2	POV	A	1315	-	-	24/55/55/55	-
2	POV	D	1312	-	-	20/55/55/55	-
2	POV	B	1311	-	-	23/55/55/55	-
2	POV	A	1302	-	-	24/55/55/55	-
2	POV	A	1309	-	-	21/55/55/55	-
2	POV	D	1309	-	-	27/55/55/55	-
2	POV	D	1314	-	-	23/55/55/55	-
3	CLR	B	1304	-	-	4/10/68/68	0/4/4/4
2	POV	C	1311	-	-	13/33/33/55	-
2	POV	C	1312	-	-	23/55/55/55	-
5	ZY8	A	1314	-	-	2/4/60/60	0/1/8/8
5	ZY8	C	1314	-	-	2/4/60/60	0/1/8/8
2	POV	B	1302	-	-	24/55/55/55	-
2	POV	D	1310	-	-	20/55/55/55	-
4	DU0	D	1315	-	-	3/10/98/98	0/6/6/6
2	POV	A	1301	-	-	26/55/55/55	-
2	POV	D	1302	-	-	6/12/12/55	-
2	POV	D	1311	-	-	21/55/55/55	-
2	POV	A	1311	-	-	13/33/33/55	-
2	POV	D	1306	-	-	25/55/55/55	-
2	POV	A	1312	-	-	23/55/55/55	-
4	DU0	C	1313	-	-	3/10/98/98	0/6/6/6
2	POV	A	1307	-	-	27/55/55/55	-
2	POV	A	1317	-	-	19/55/55/55	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1314	ZY8	C14-N5	4.37	1.52	1.48
5	A	1314	ZY8	C14-N5	4.35	1.52	1.48
5	B	1313	ZY8	C14-N5	4.34	1.52	1.48
5	D	1316	ZY8	C14-N5	4.32	1.52	1.48
2	D	1302	POV	C29-C210	3.62	1.52	1.31

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1314	ZY8	C13-C14-N5	4.23	109.40	105.41
5	A	1314	ZY8	C13-C14-N5	4.21	109.38	105.41
5	D	1316	ZY8	C13-C14-N5	4.18	109.36	105.41
5	A	1314	ZY8	C15-C14-N5	-4.18	111.16	115.63
5	B	1313	ZY8	C13-C14-N5	4.18	109.35	105.41

There are no chirality outliers.

5 of 1122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	POV	C1-O11-P-O12
2	A	1301	POV	C1-O11-P-O13
2	A	1301	POV	C1-O11-P-O14
2	A	1301	POV	C11-O12-P-O11
2	A	1301	POV	C11-O12-P-O13

There are no ring outliers.

49 monomers are involved in 90 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1301	POV	5	0
5	B	1313	ZY8	1	0
2	B	1305	POV	2	0
2	C	1306	POV	2	0
2	B	1301	POV	1	0
2	D	1313	POV	3	0
2	A	1310	POV	4	0
2	B	1314	POV	5	0
2	A	1303	POV	1	0
2	B	1307	POV	2	0
2	A	1306	POV	2	0
2	B	1310	POV	2	0
2	C	1308	POV	2	0
2	C	1307	POV	2	0
2	A	1308	POV	2	0
2	C	1303	POV	1	0
2	C	1304	POV	1	0
2	B	1309	POV	3	0
2	C	1301	POV	2	0
2	B	1306	POV	2	0
2	D	1308	POV	2	0

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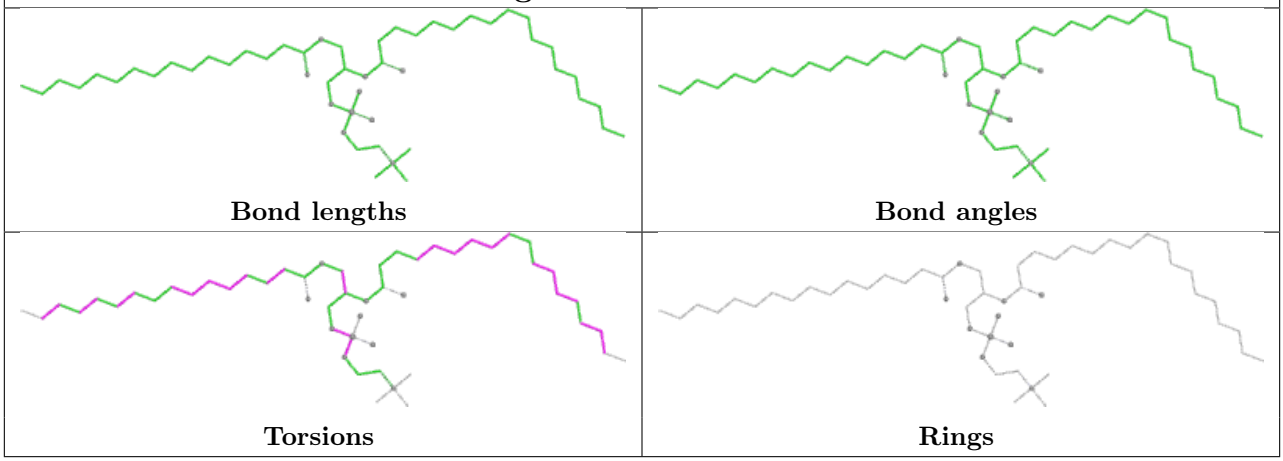
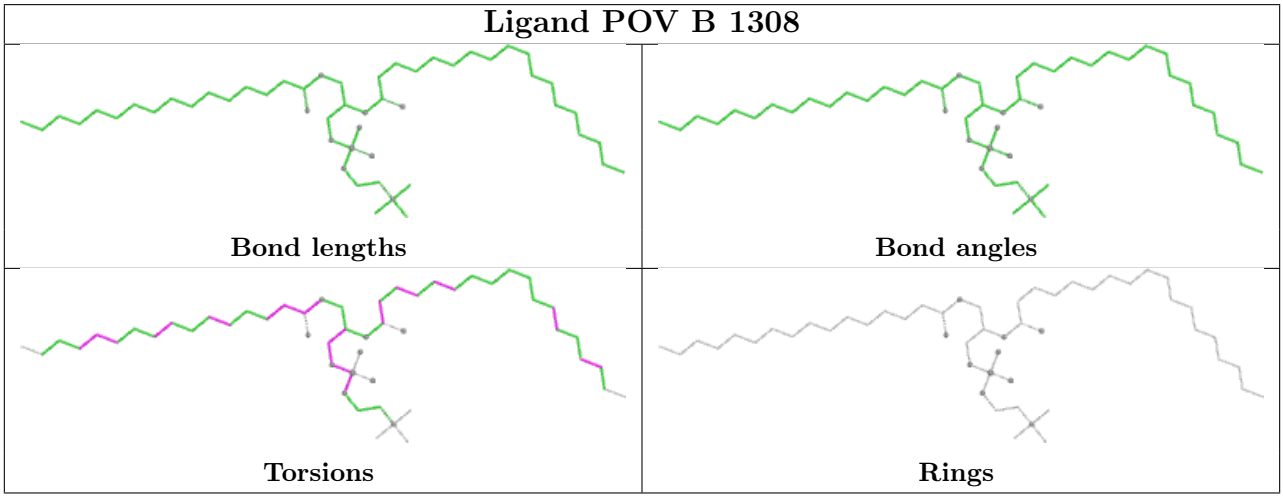
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1316	ZY8	1	0
2	A	1305	POV	2	0
2	D	1305	POV	2	0
2	C	1310	POV	3	0
2	C	1315	POV	5	0
3	D	1307	CLR	1	0
2	B	1303	POV	1	0
3	A	1304	CLR	1	0
3	C	1305	CLR	1	0
2	D	1303	POV	2	0
2	A	1315	POV	5	0
2	D	1312	POV	4	0
2	B	1311	POV	5	0
2	A	1302	POV	1	0
2	D	1309	POV	2	0
2	D	1314	POV	5	0
3	B	1304	CLR	1	0
2	C	1311	POV	2	0
2	C	1312	POV	5	0
5	A	1314	ZY8	1	0
5	C	1314	ZY8	1	0
2	B	1302	POV	1	0
2	D	1310	POV	1	0
2	A	1311	POV	3	0
2	D	1306	POV	1	0
2	A	1312	POV	5	0
2	A	1307	POV	2	0
2	A	1317	POV	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 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.

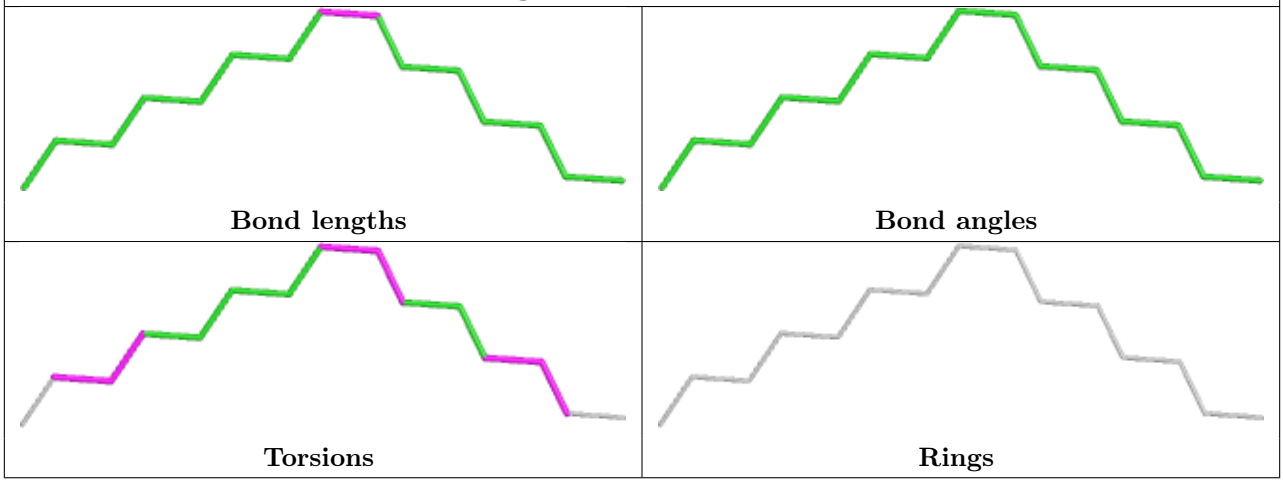
Ligand POV C 1302



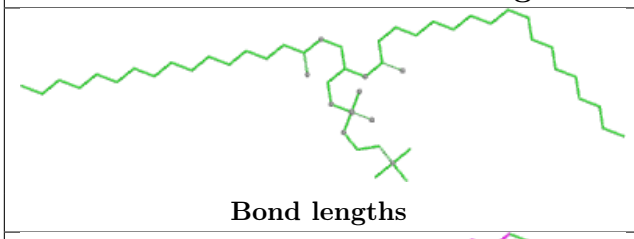
Ligand POV B 1308



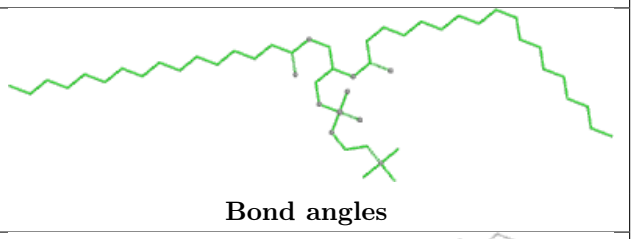
Ligand POV A 1316



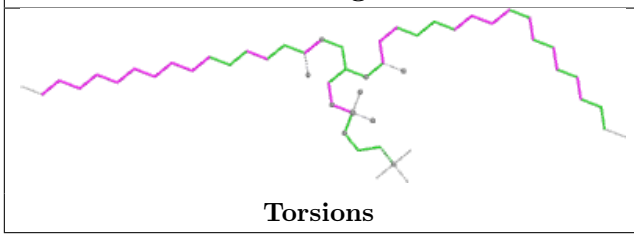
Ligand POV D 1301



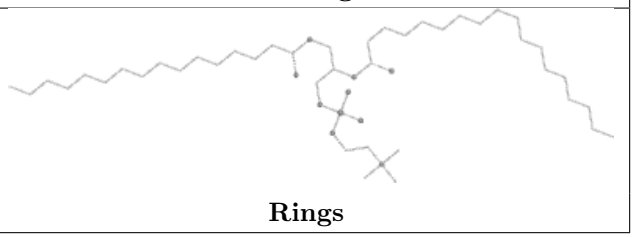
Bond lengths



Bond angles

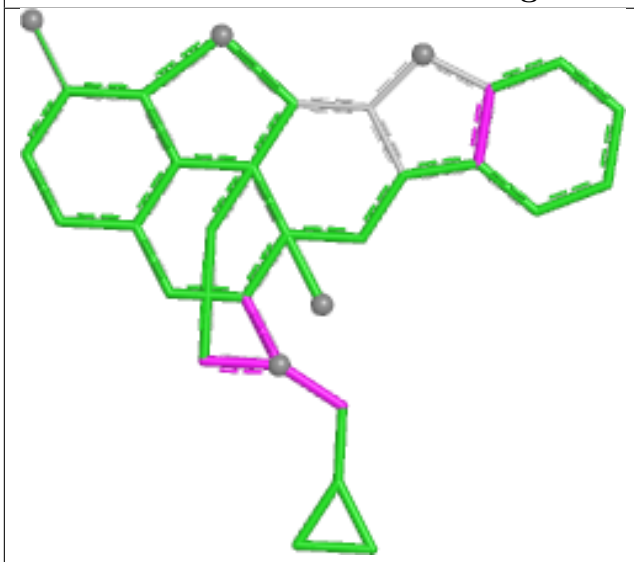


Torsions

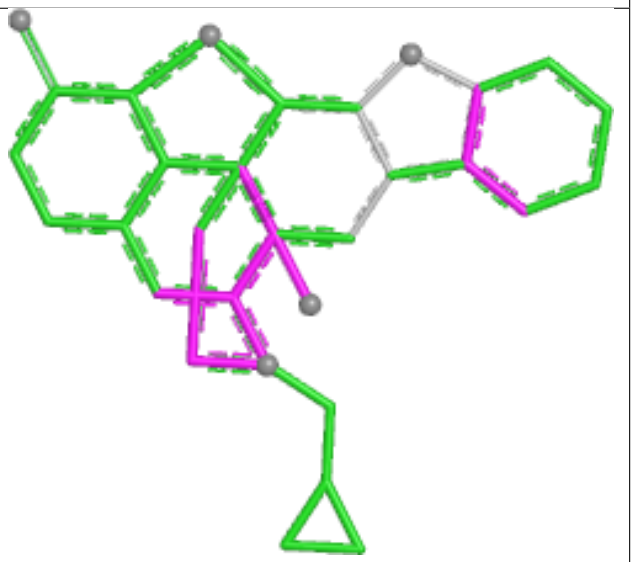


Rings

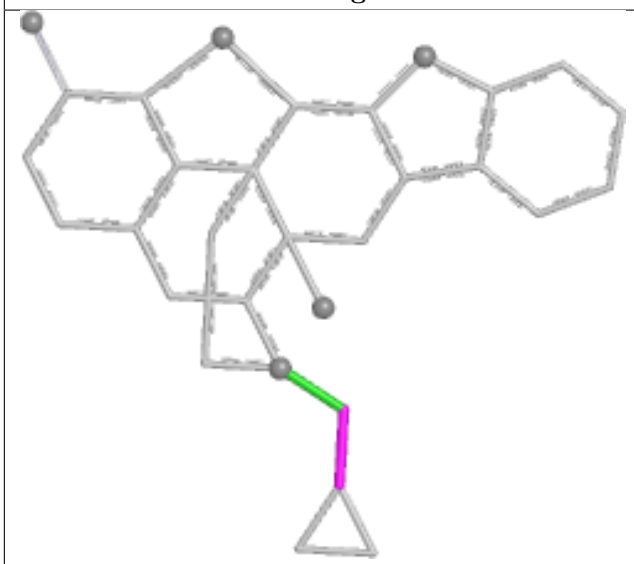
Ligand ZY8 B 1313



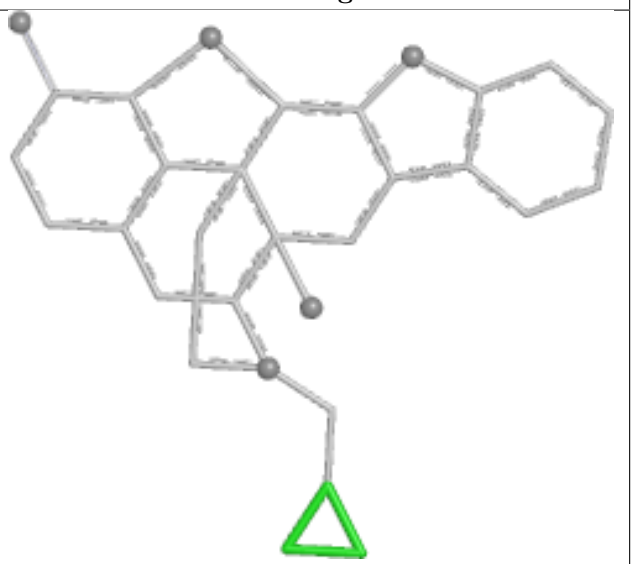
Bond lengths



Bond angles

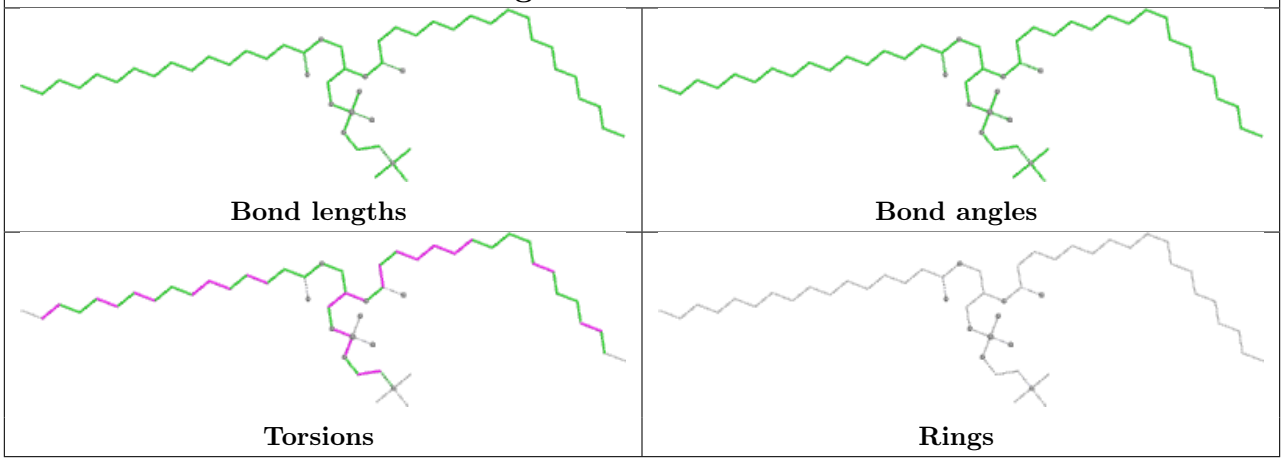


Torsions

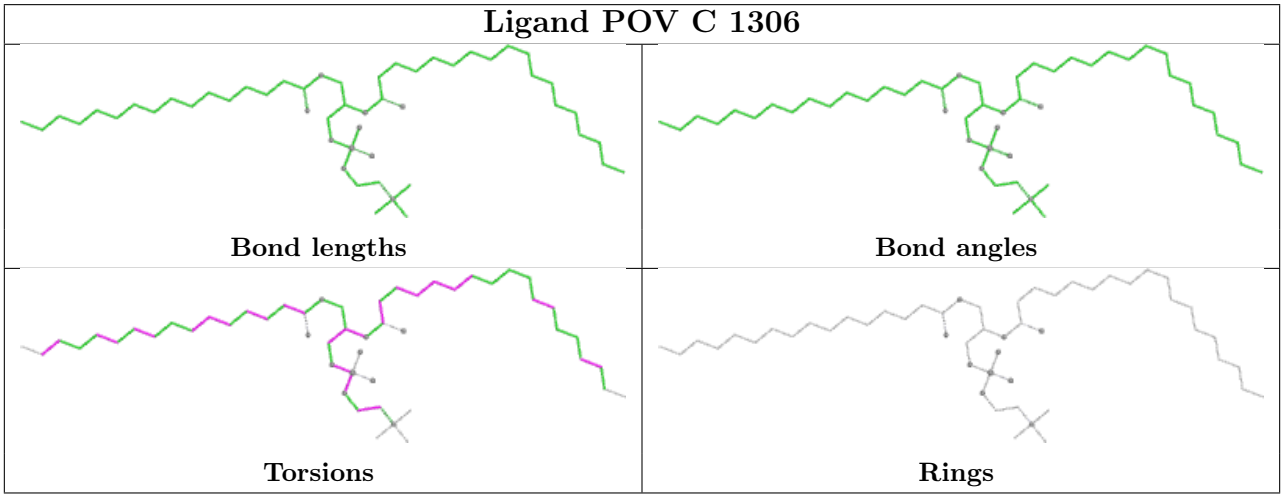


Rings

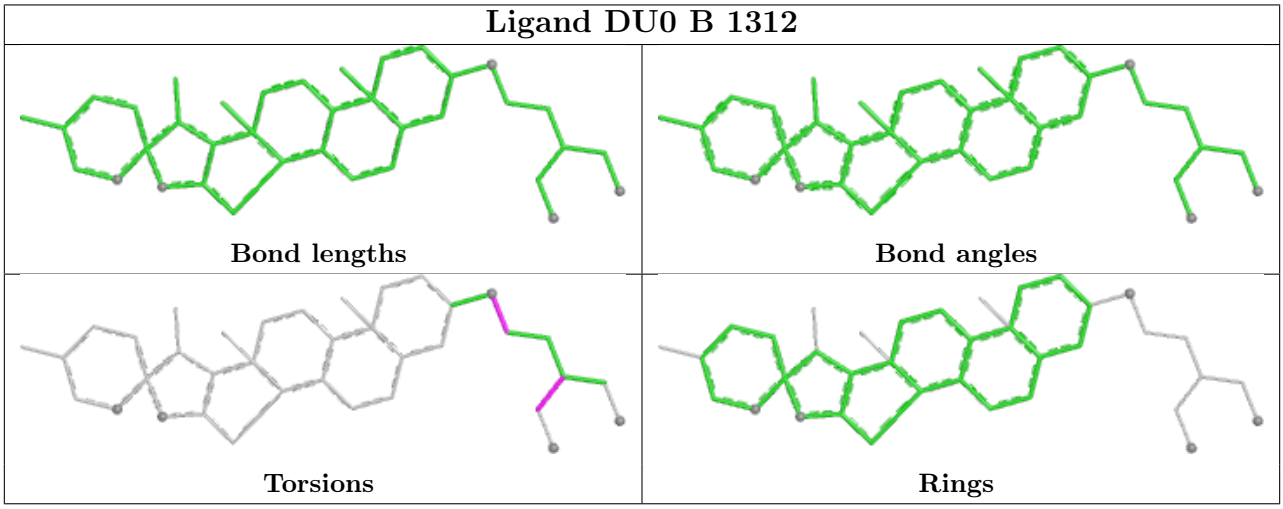
Ligand POV B 1305



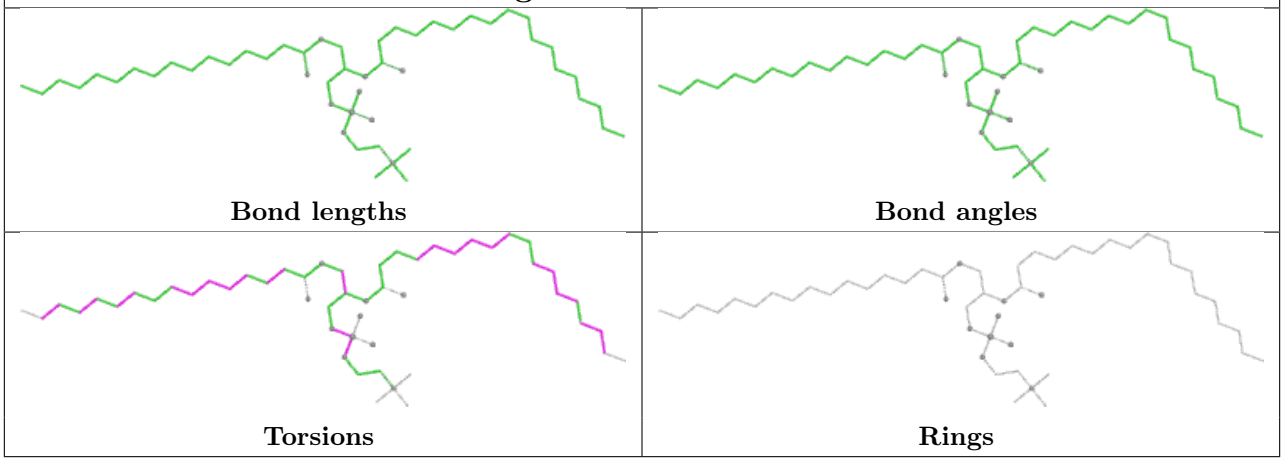
Ligand POV C 1306



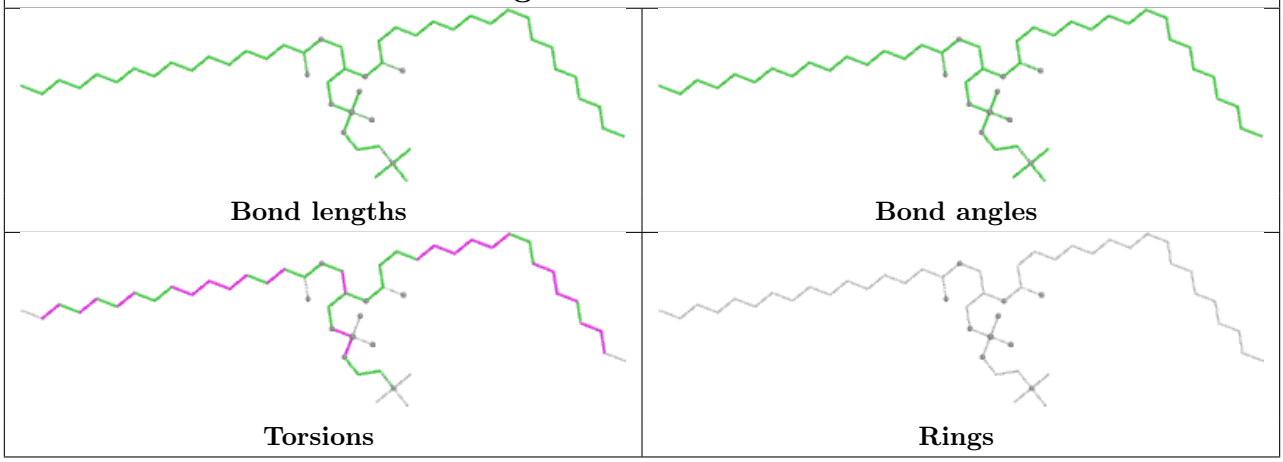
Ligand DU0 B 1312



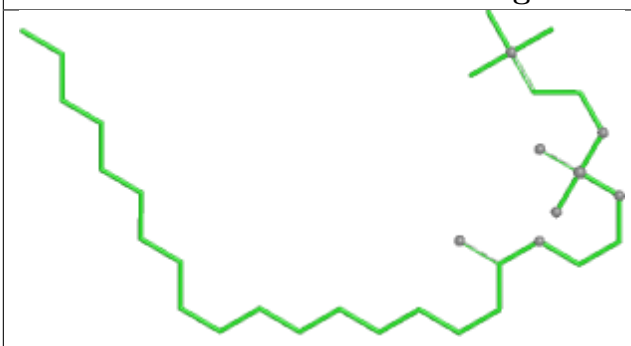
Ligand POV B 1301



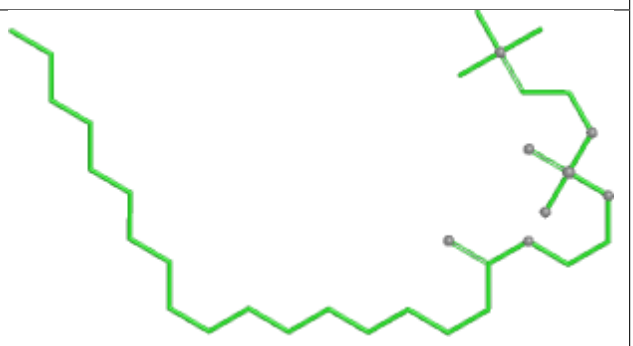
Ligand POV D 1304



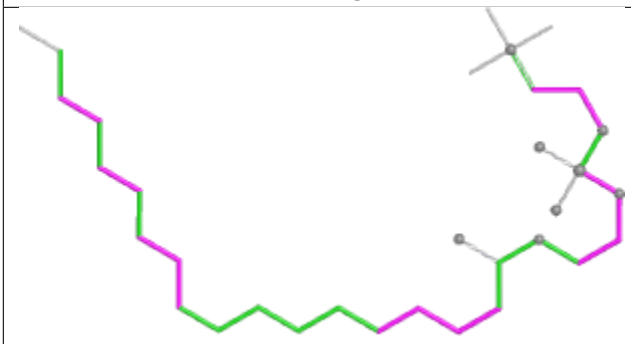
Ligand POV D 1313



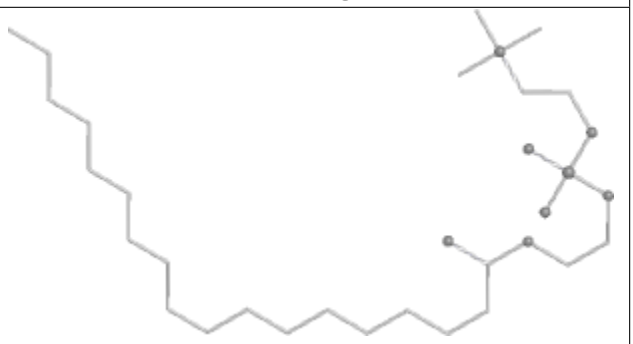
Bond lengths



Bond angles

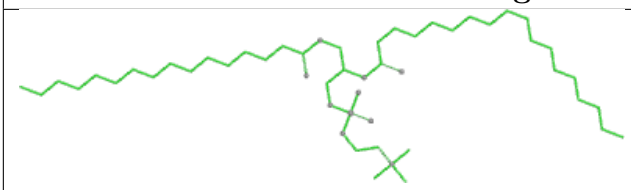


Torsions

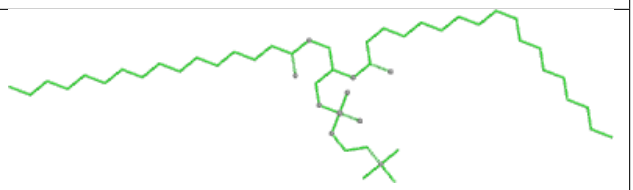


Rings

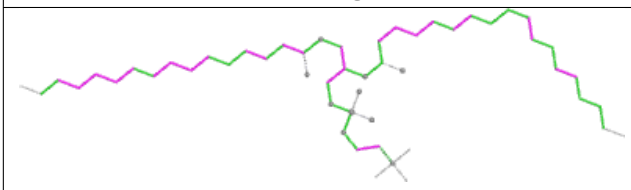
Ligand POV A 1310



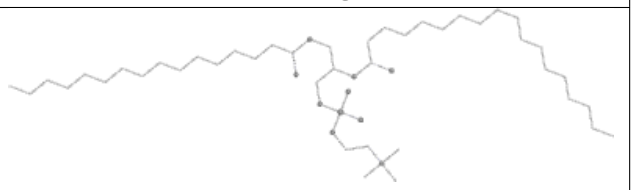
Bond lengths



Bond angles

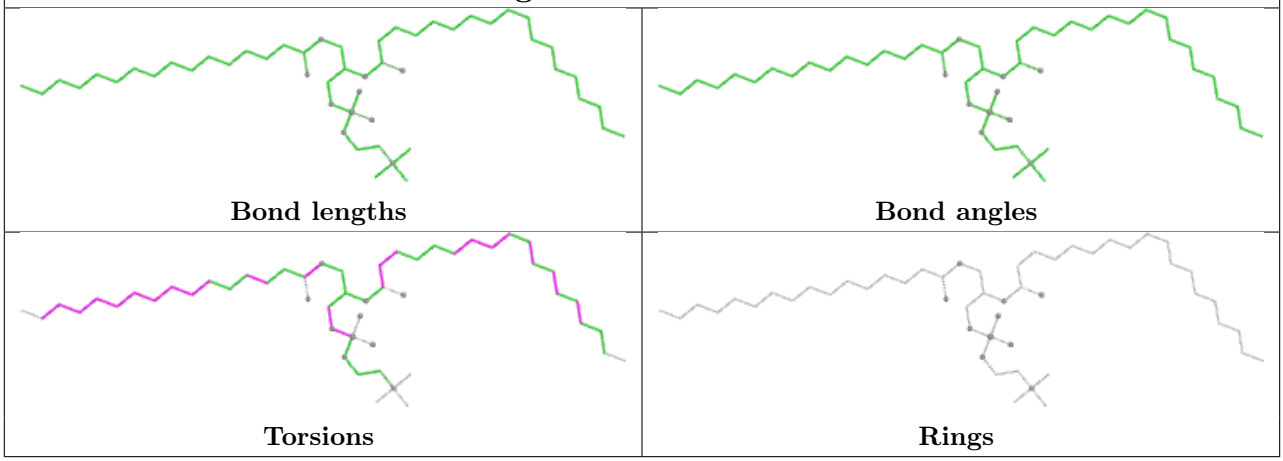


Torsions

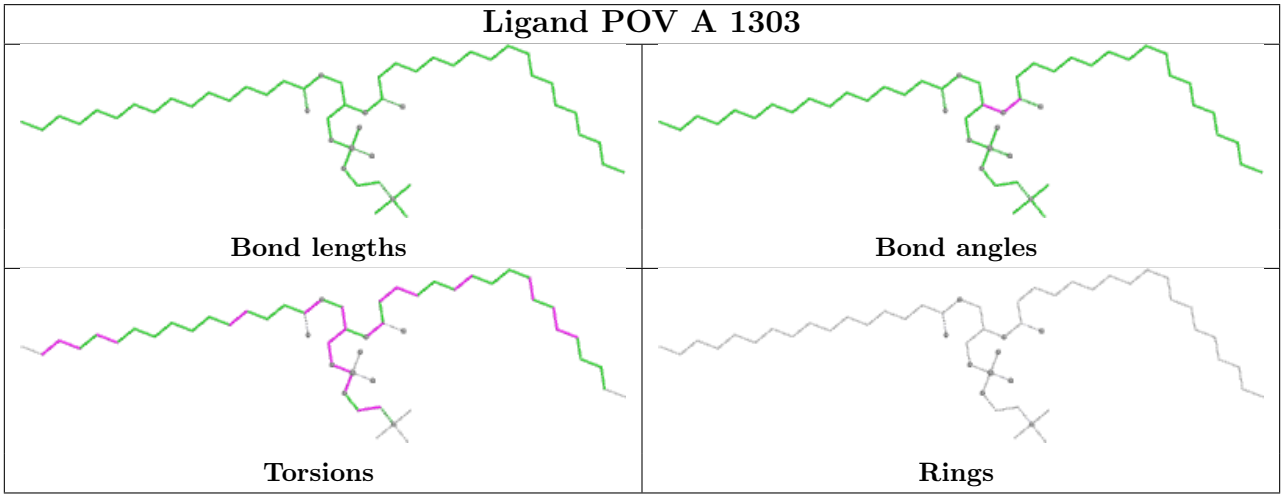


Rings

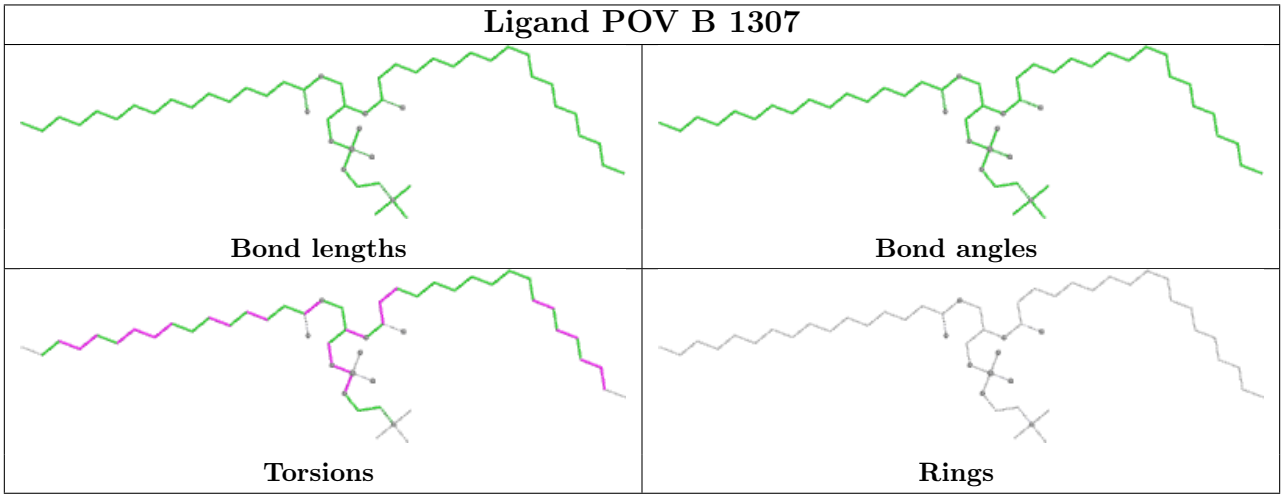
Ligand POV B 1314



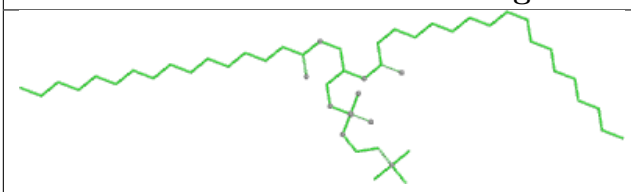
Ligand POV A 1303



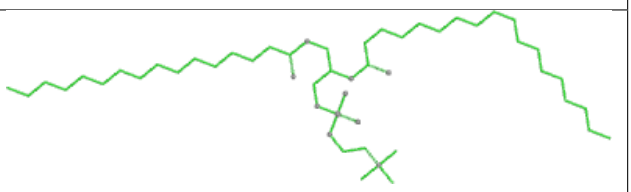
Ligand POV B 1307



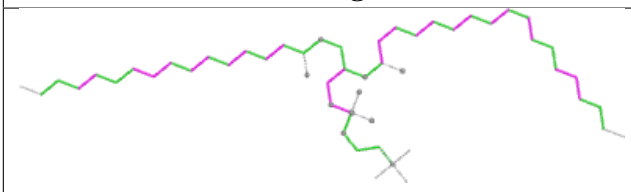
Ligand POV A 1306



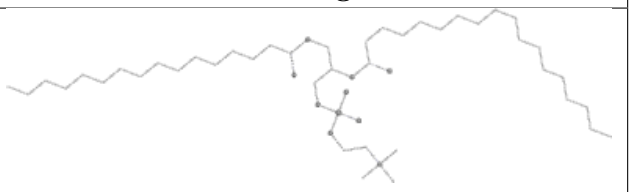
Bond lengths



Bond angles



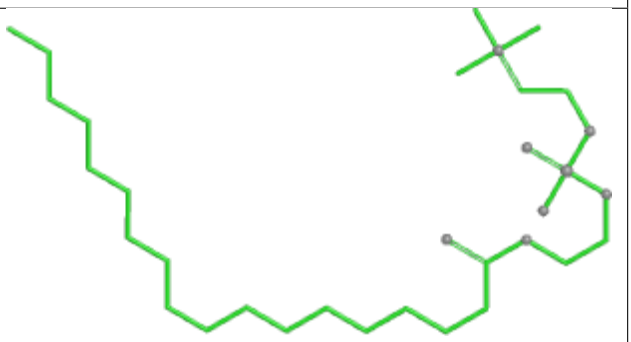
Torsions



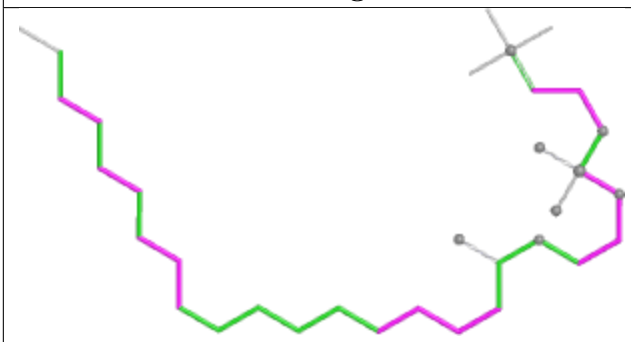
Rings

Ligand POV B 1310

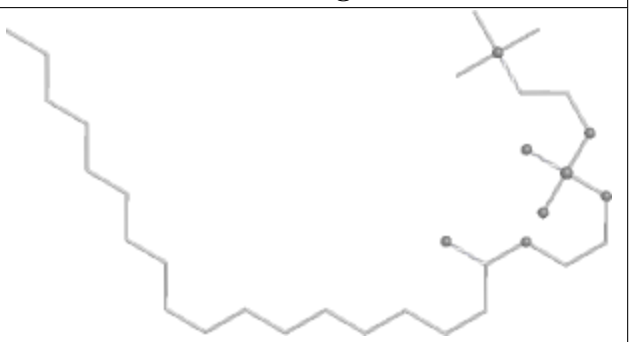
Bond lengths



Bond angles

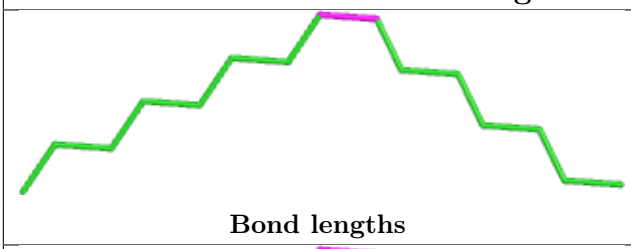


Torsions

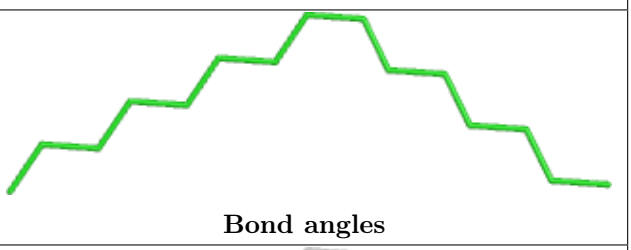


Rings

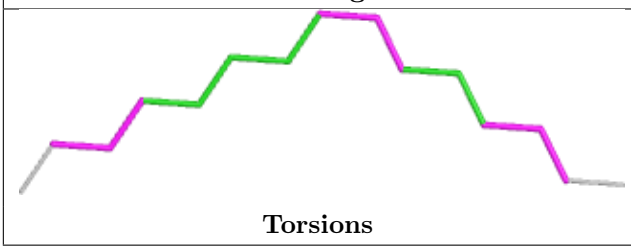
Ligand POV B 1315



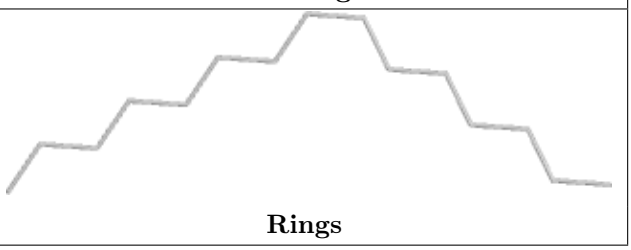
Bond lengths



Bond angles

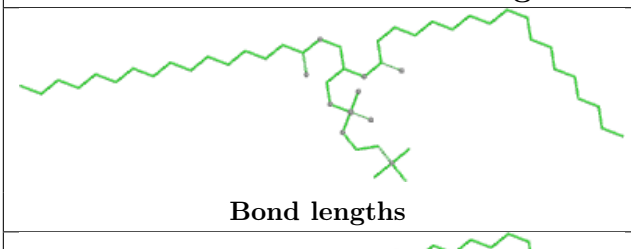


Torsions

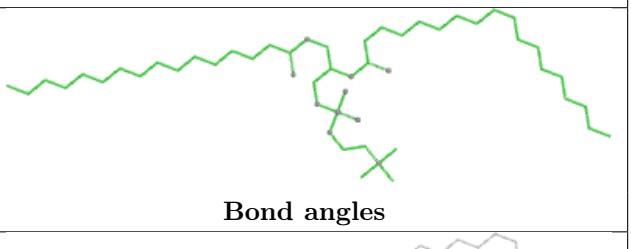


Rings

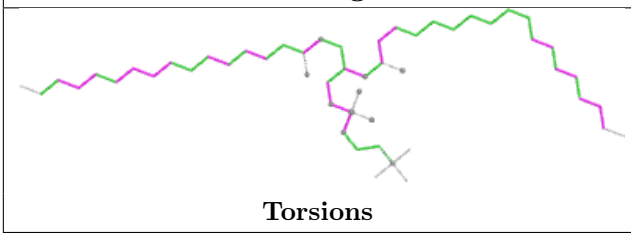
Ligand POV C 1308



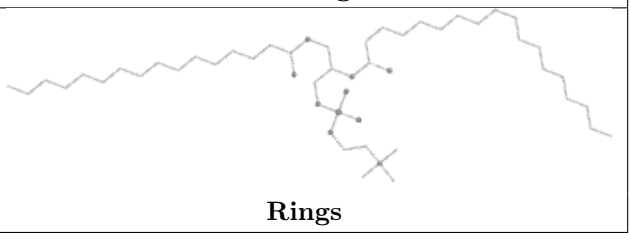
Bond lengths



Bond angles

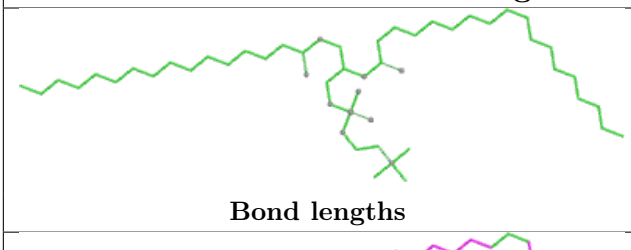


Torsions

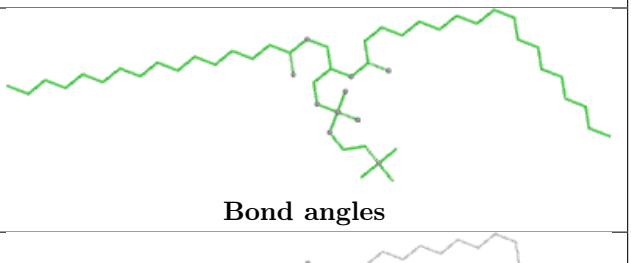


Rings

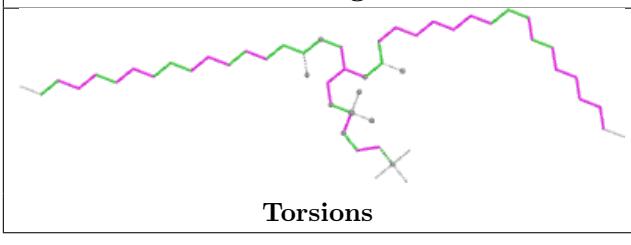
Ligand POV C 1307



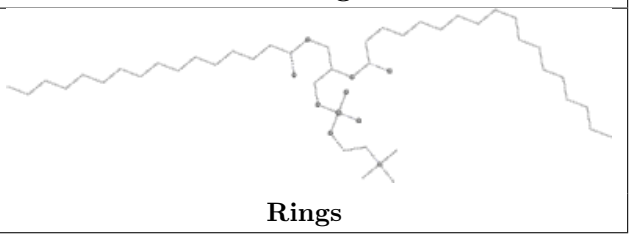
Bond lengths



Bond angles

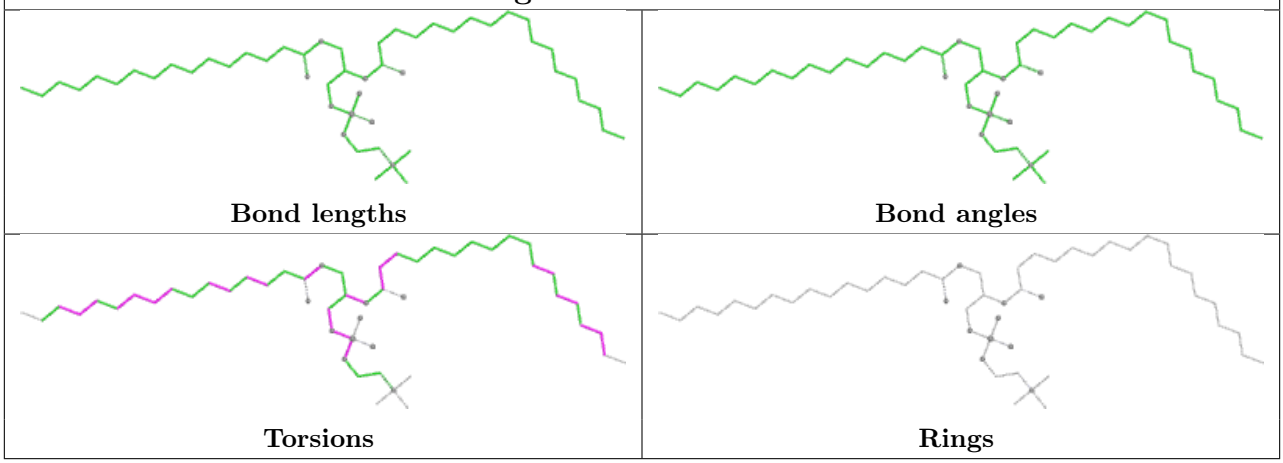


Torsions

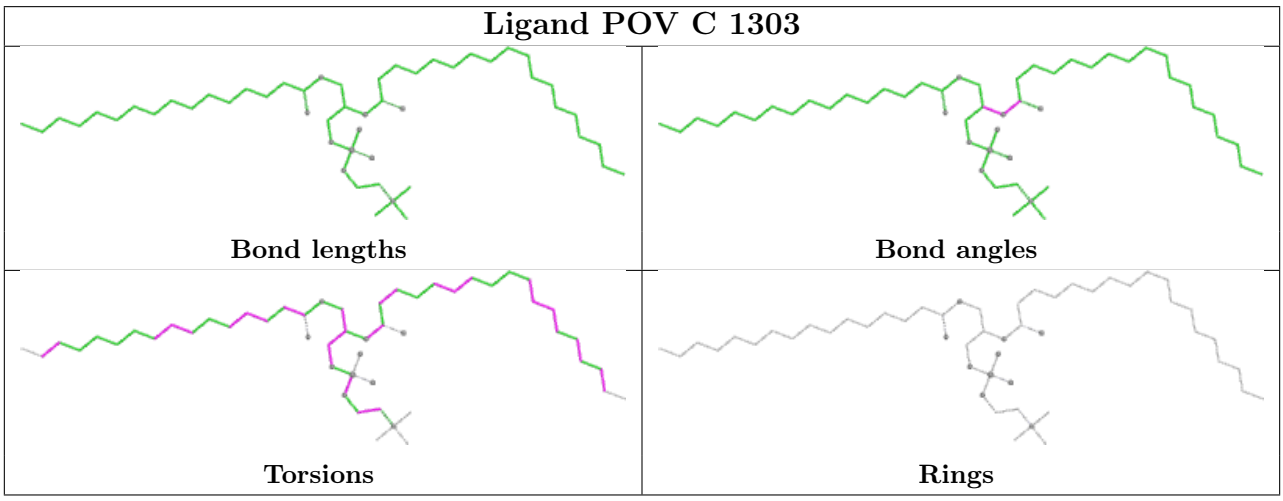


Rings

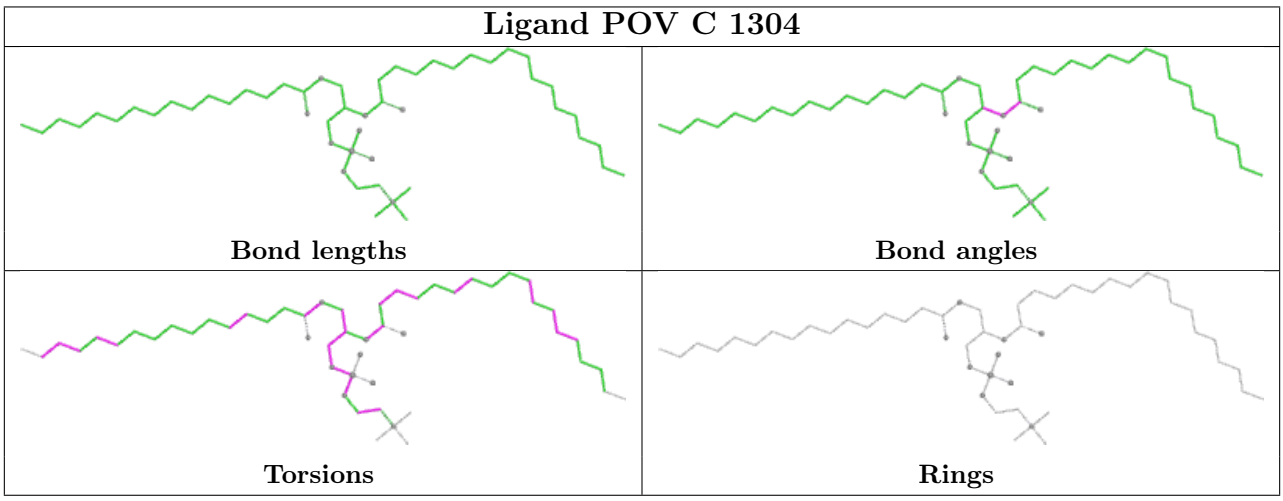
Ligand POV A 1308



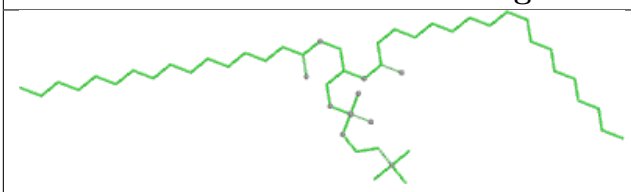
Ligand POV C 1303

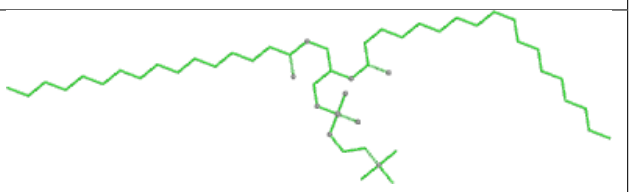


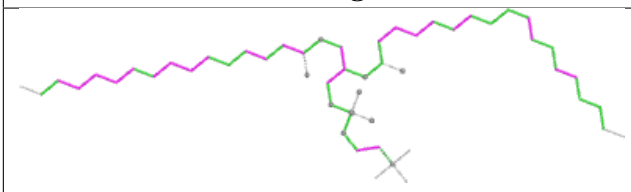
Ligand POV C 1304

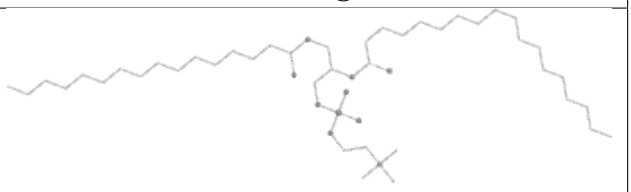


Ligand POV B 1309

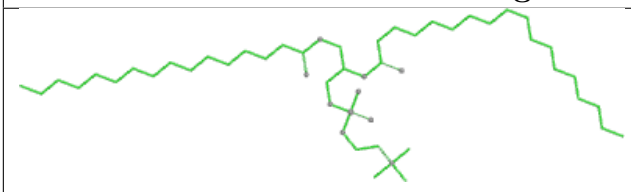

Bond lengths

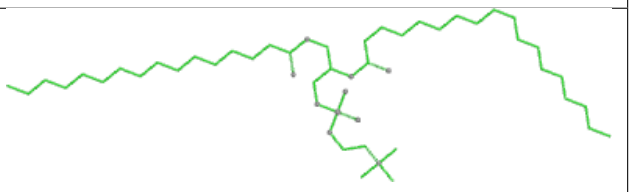

Bond angles

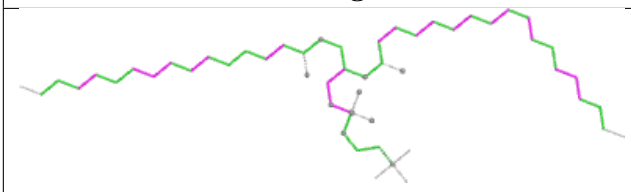

Torsions

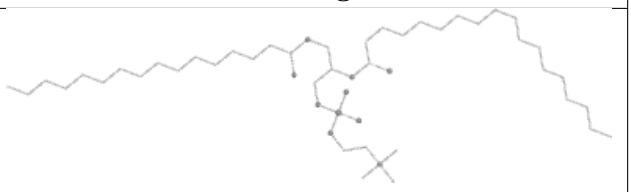

Rings

Ligand POV C 1301

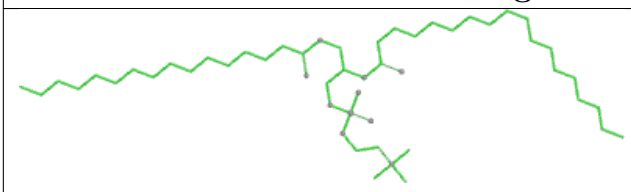

Bond lengths

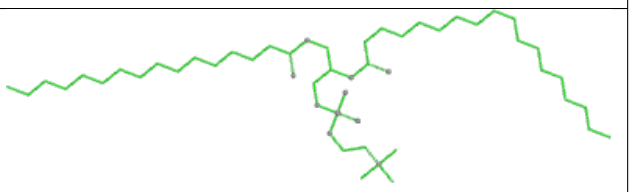

Bond angles

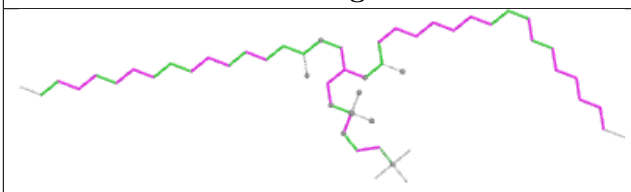

Torsions

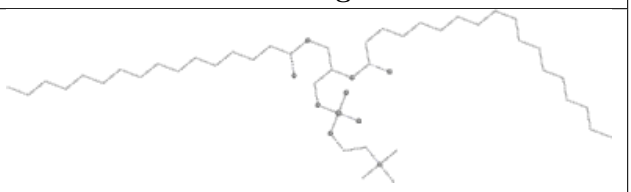

Rings

Ligand POV B 1306

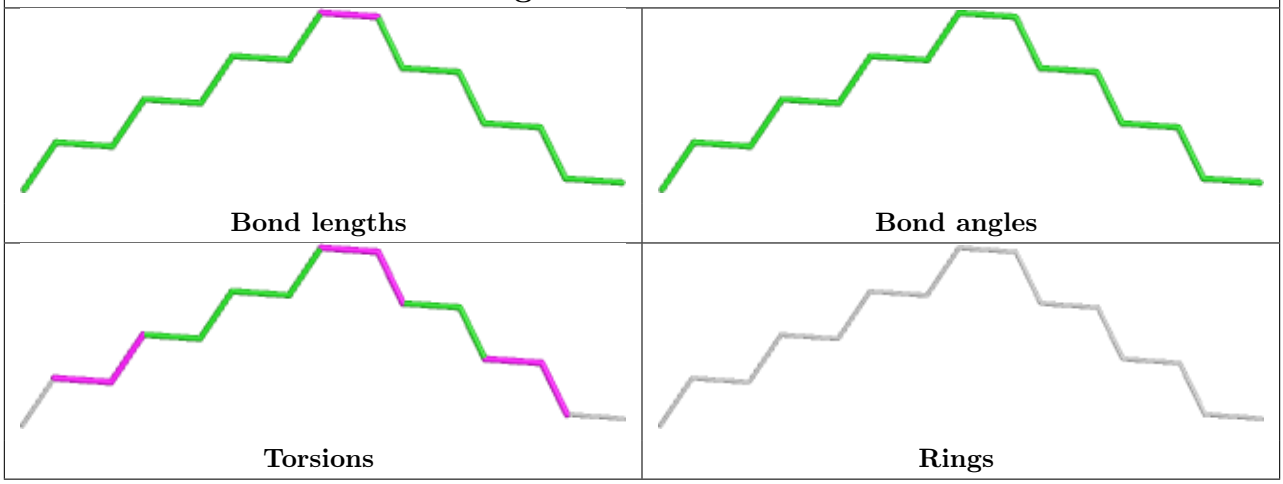

Bond lengths


Bond angles

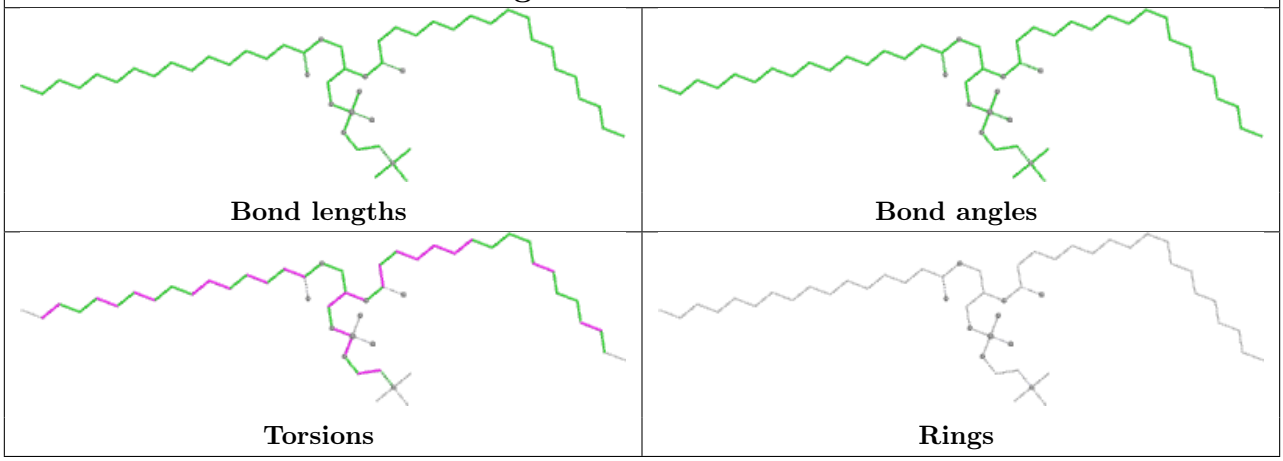

Torsions


Rings

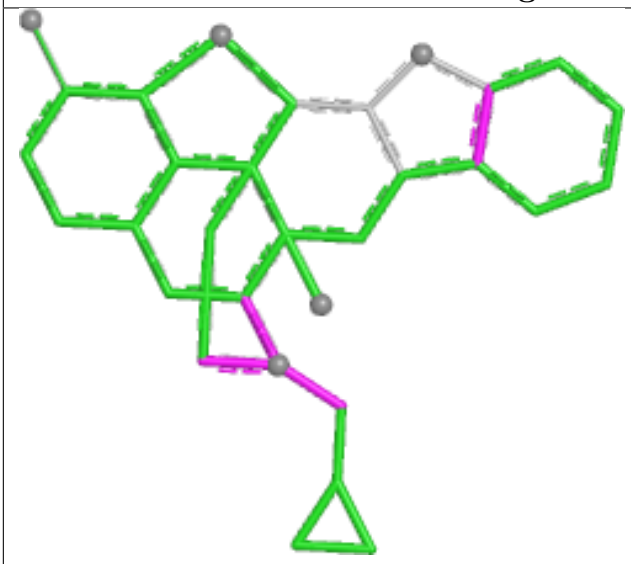
Ligand POV C 1316



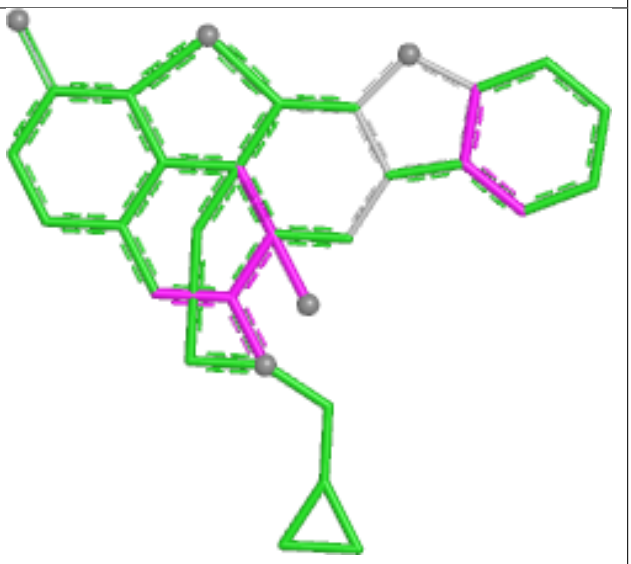
Ligand POV D 1308



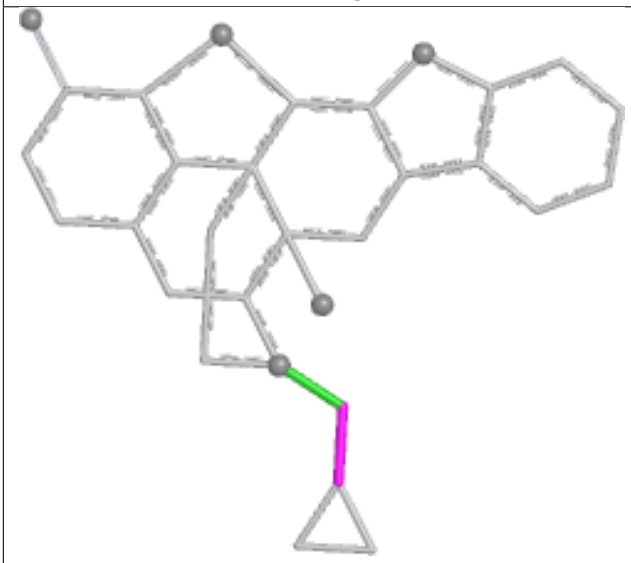
Ligand ZY8 D 1316



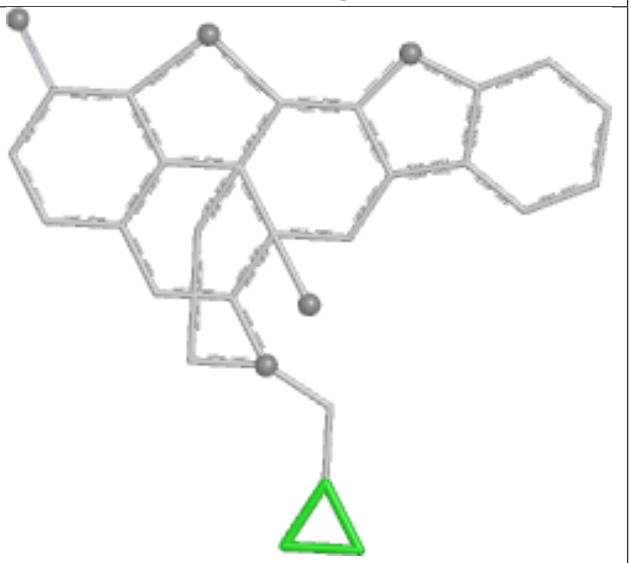
Bond lengths



Bond angles

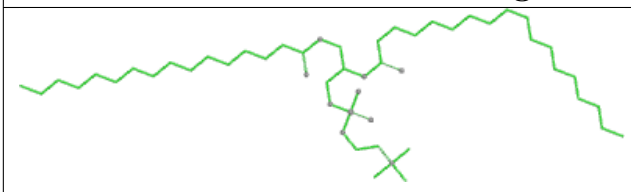


Torsions

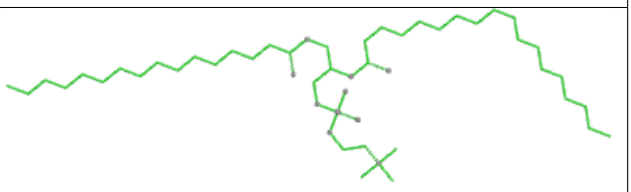


Rings

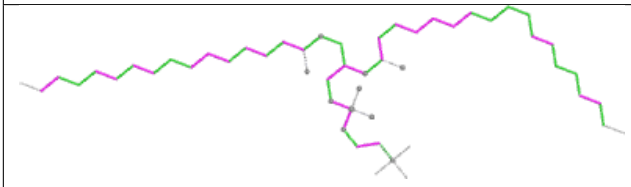
Ligand POV A 1305



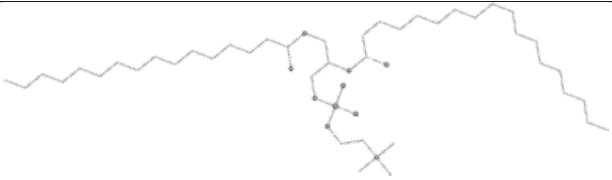
Bond lengths



Bond angles

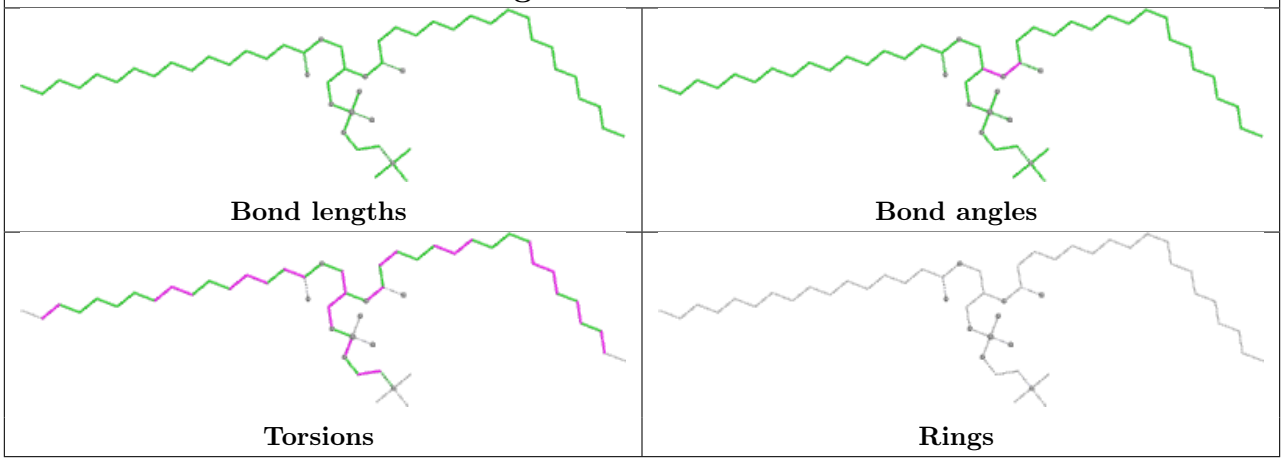


Torsions

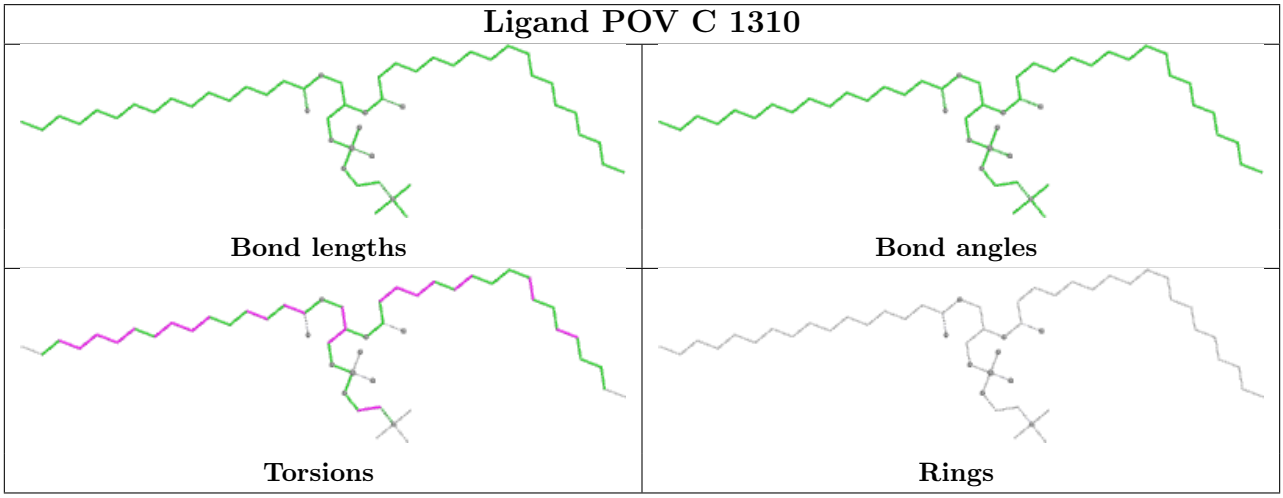


Rings

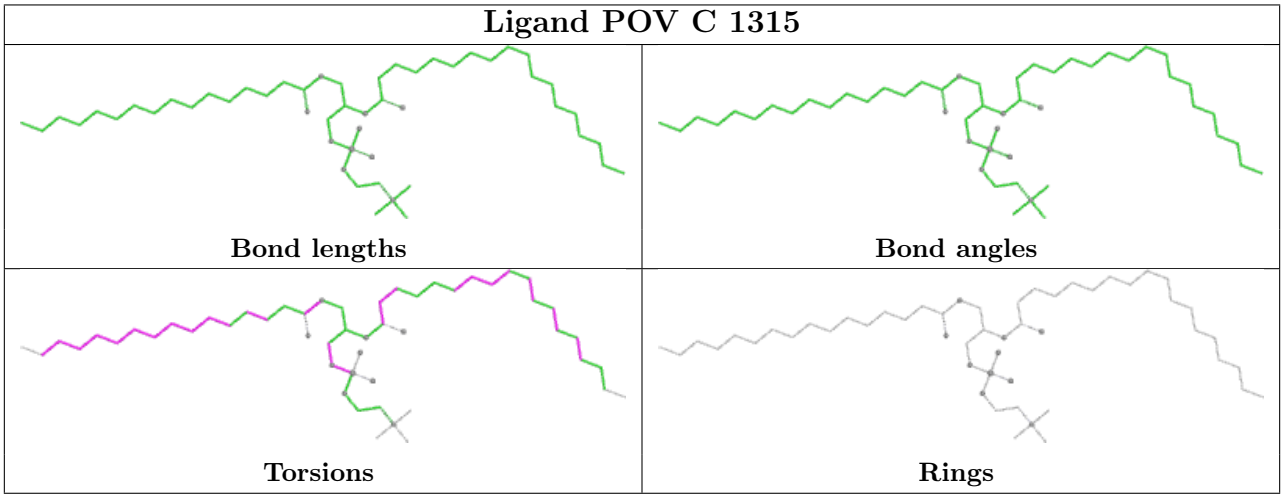
Ligand POV D 1305



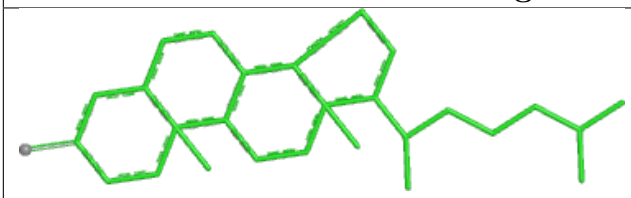
Ligand POV C 1310



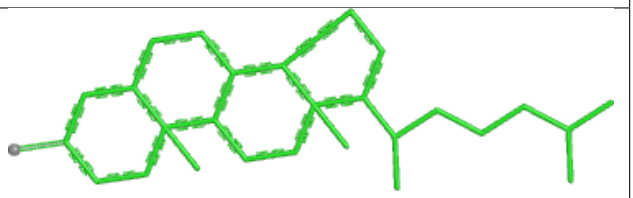
Ligand POV C 1315



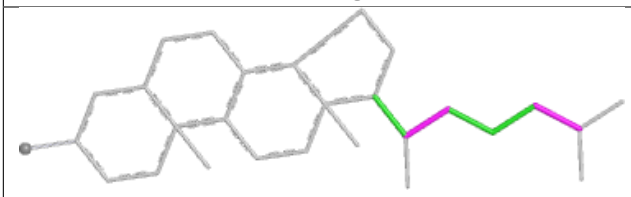
Ligand CLR D 1307



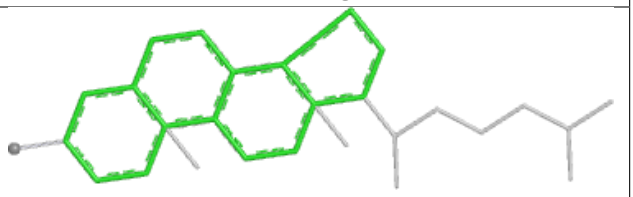
Bond lengths



Bond angles

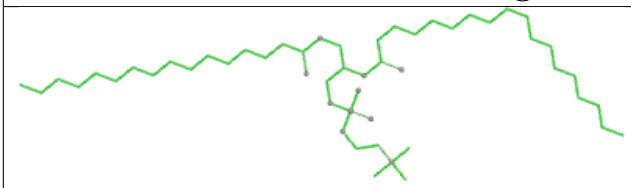


Torsions

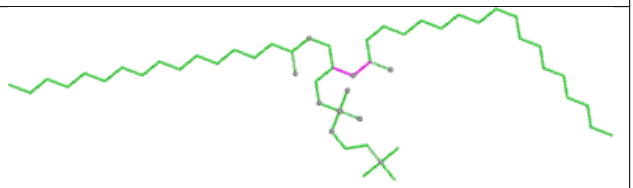


Rings

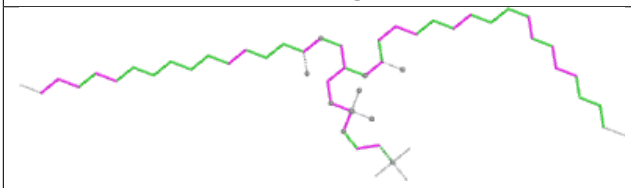
Ligand POV B 1303



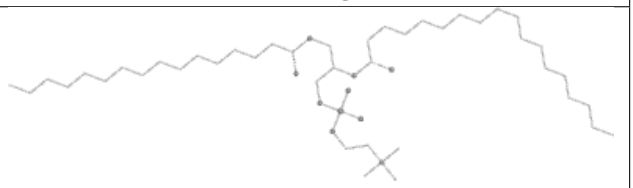
Bond lengths



Bond angles

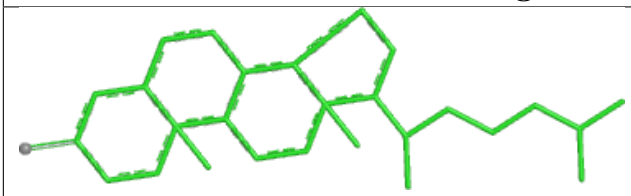


Torsions

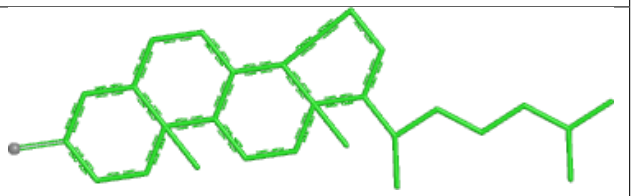


Rings

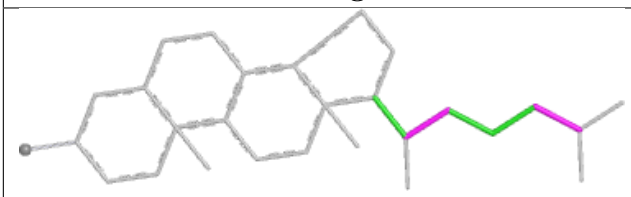
Ligand CLR A 1304



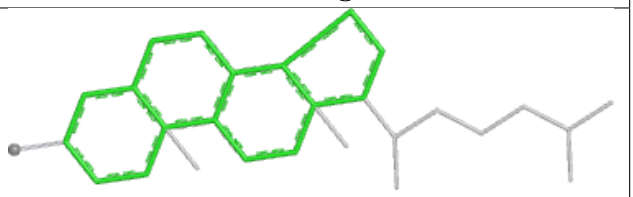
Bond lengths



Bond angles

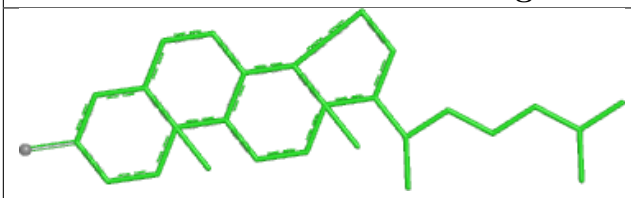


Torsions

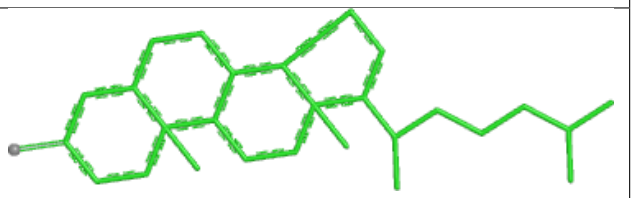


Rings

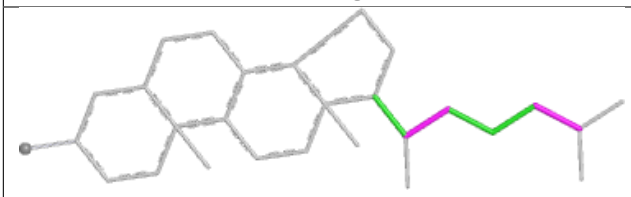
Ligand CLR C 1305



Bond lengths



Bond angles



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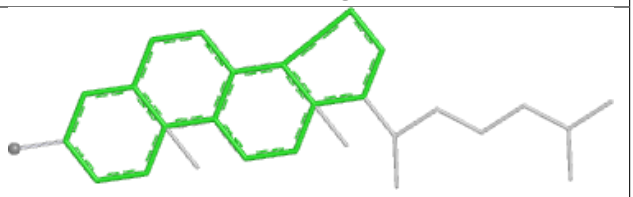
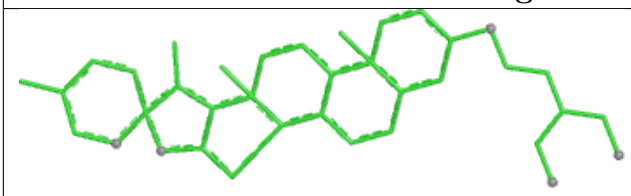
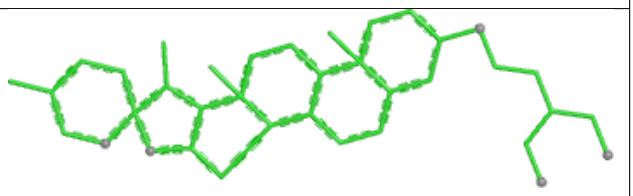


Rings

Ligand DU0 A 1313

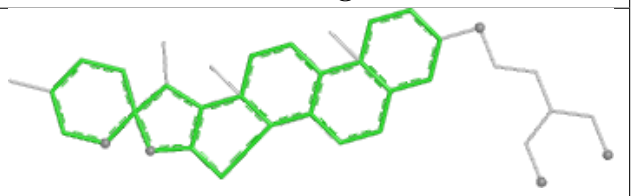


Bond lengths



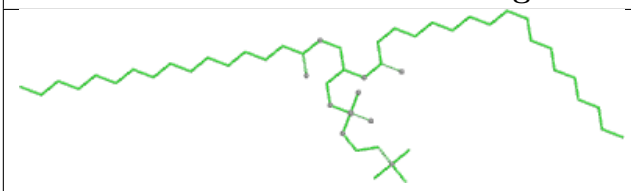
Bond angles

Torsions

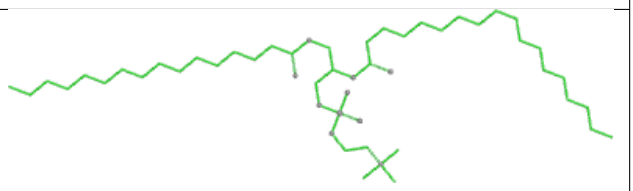


Rings

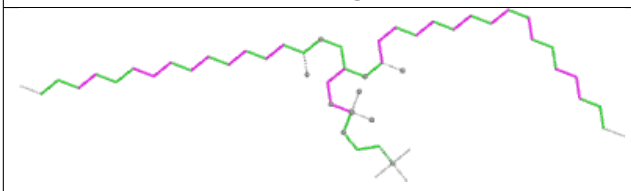
Ligand POV D 1303



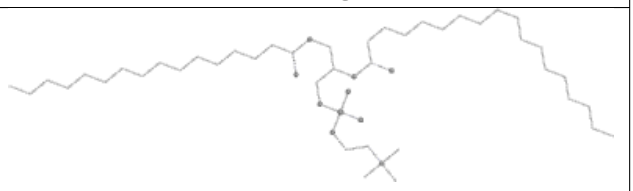
Bond lengths



Bond angles

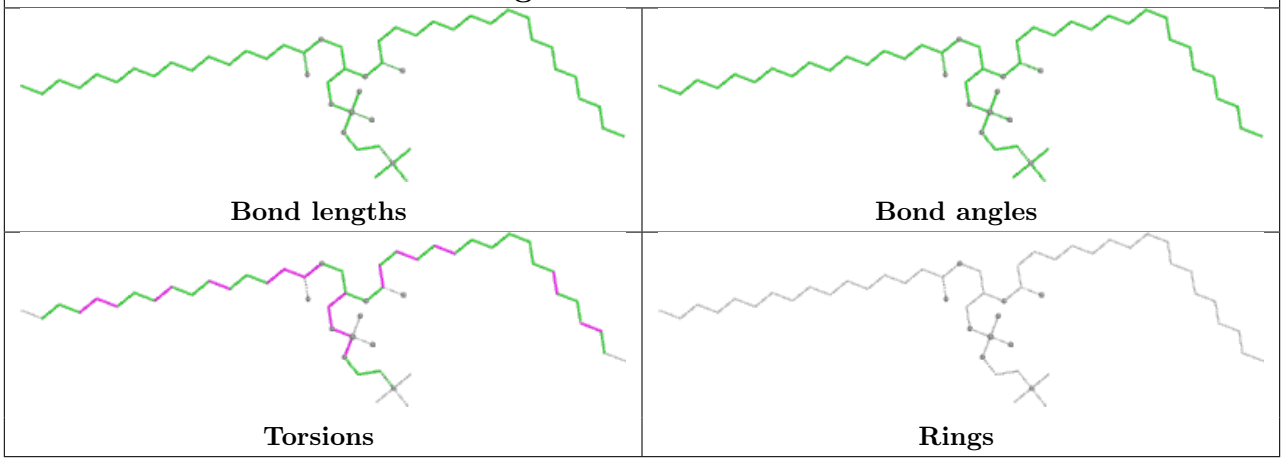


Torsions

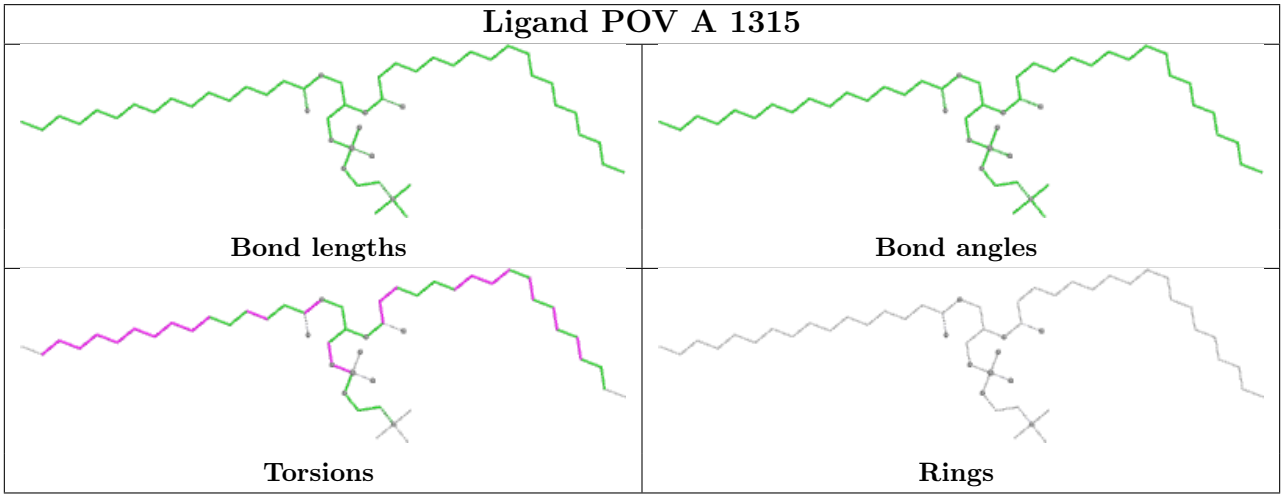


Rings

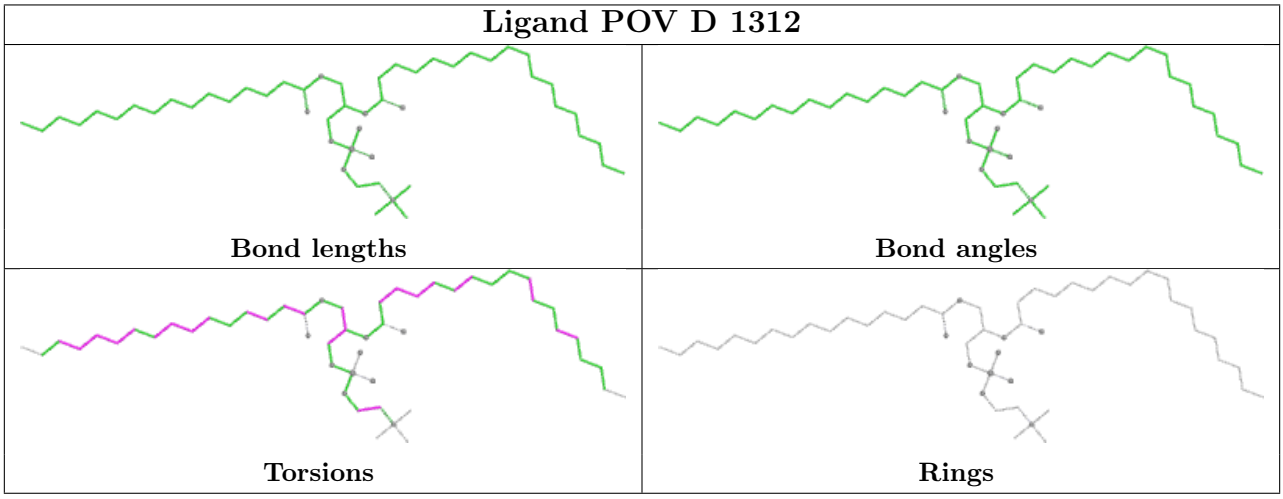
Ligand POV C 1309



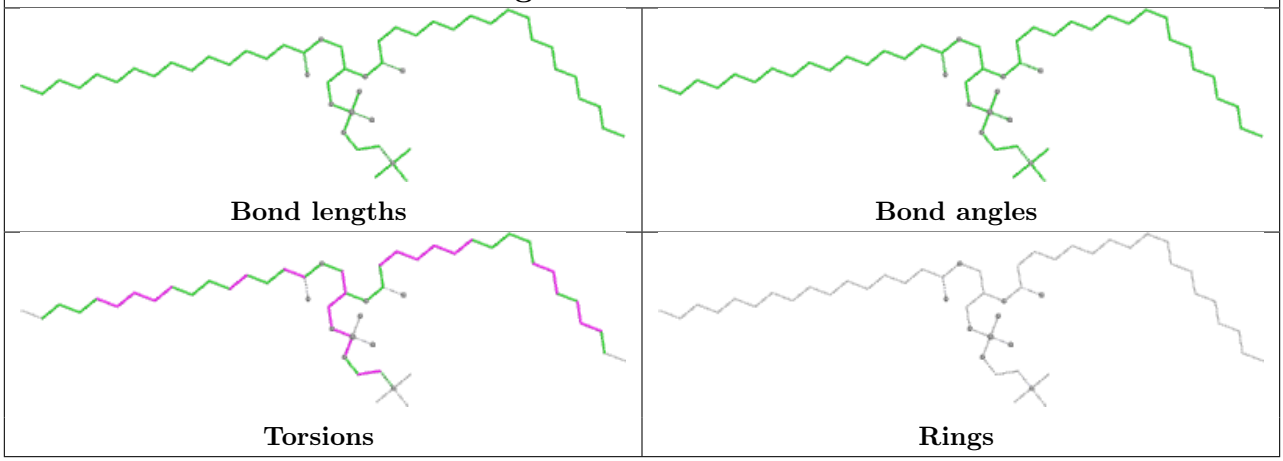
Ligand POV A 1315



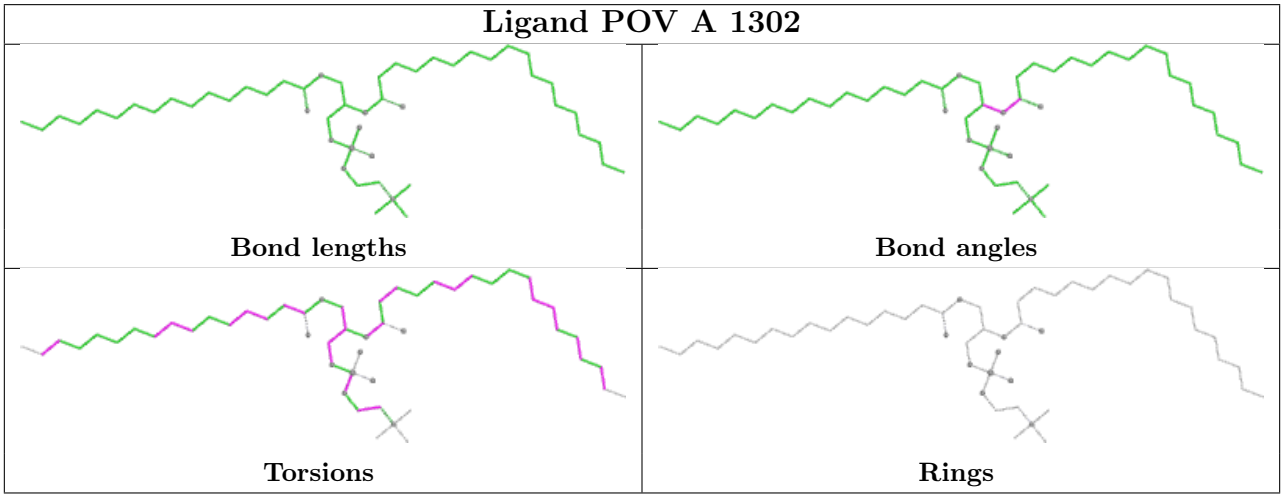
Ligand POV D 1312



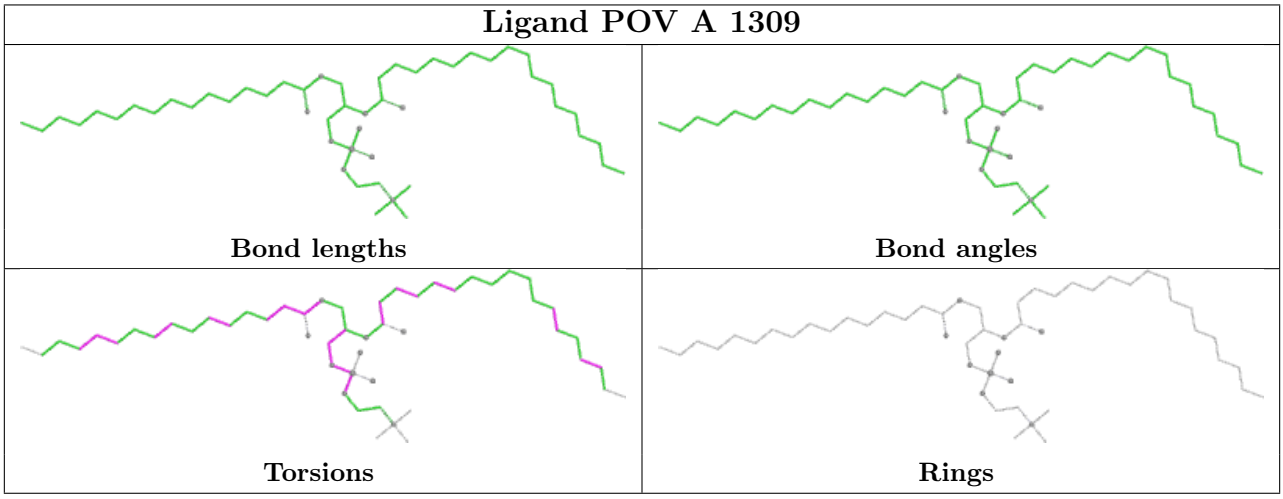
Ligand POV B 1311



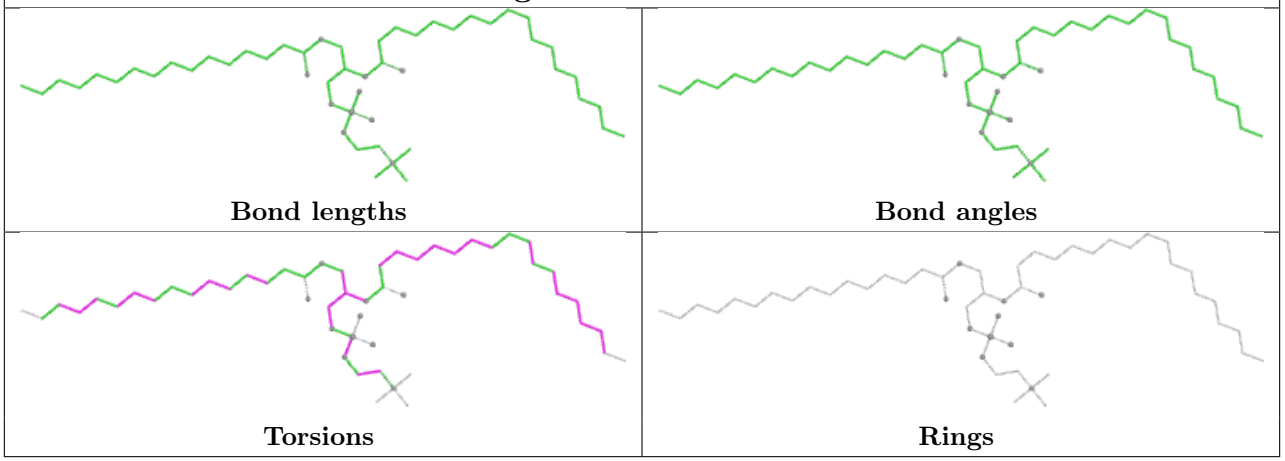
Ligand POV A 1302



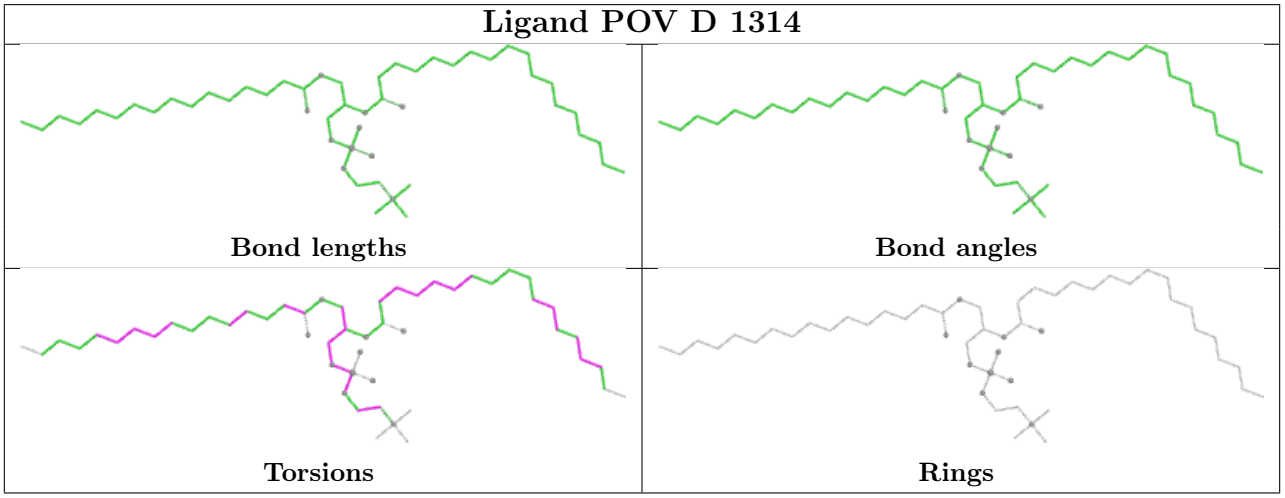
Ligand POV A 1309



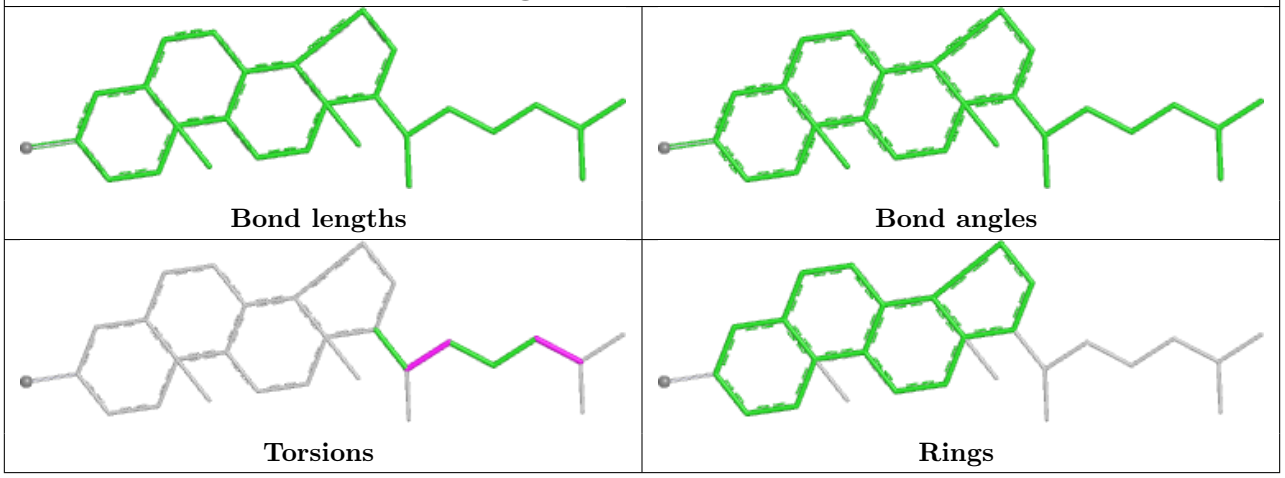
Ligand POV D 1309



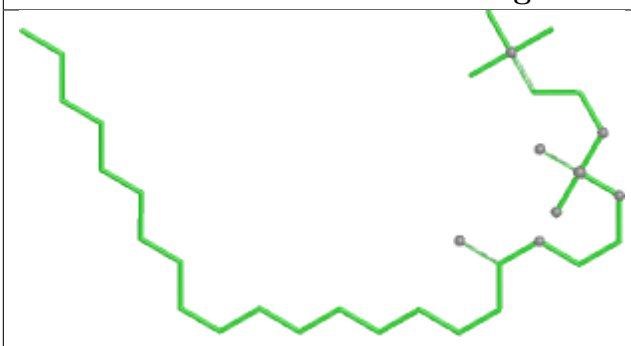
Ligand POV D 1314



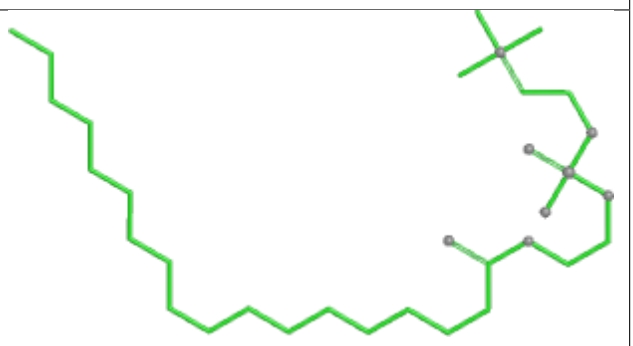
Ligand CLR B 1304



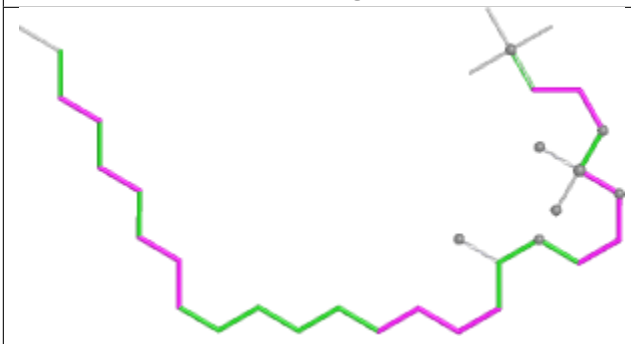
Ligand POV C 1311



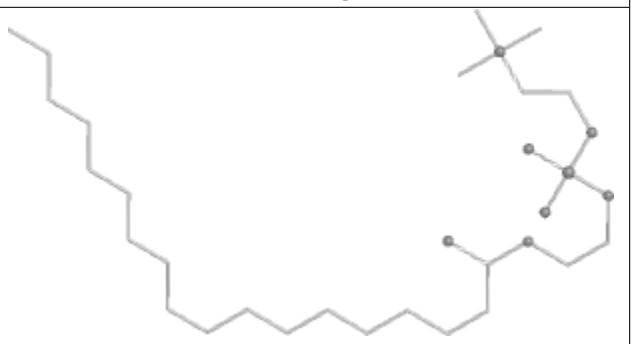
Bond lengths



Bond angles

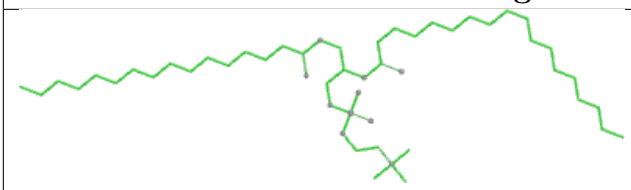


Torsions

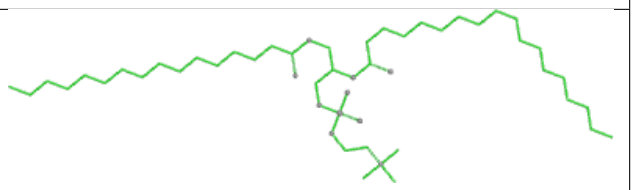


Rings

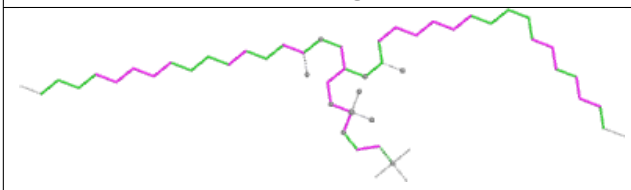
Ligand POV C 1312



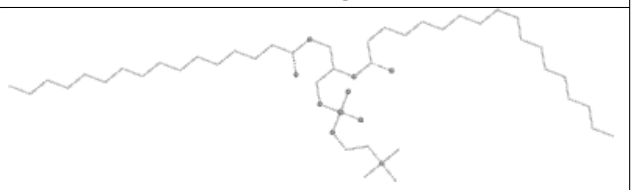
Bond lengths



Bond angles

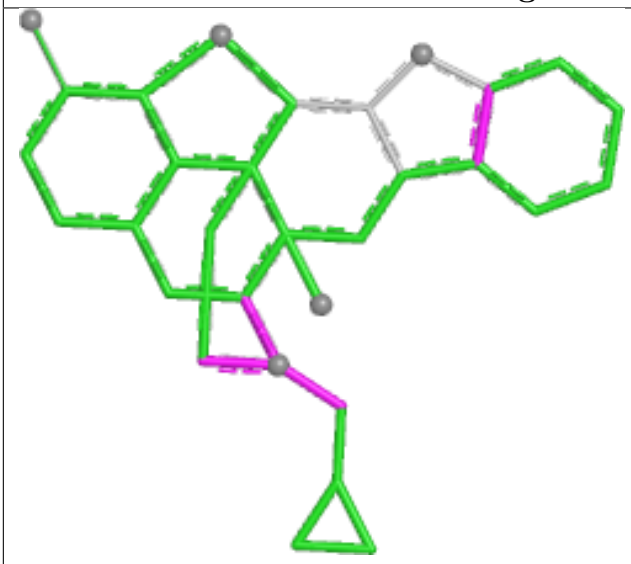


Torsions

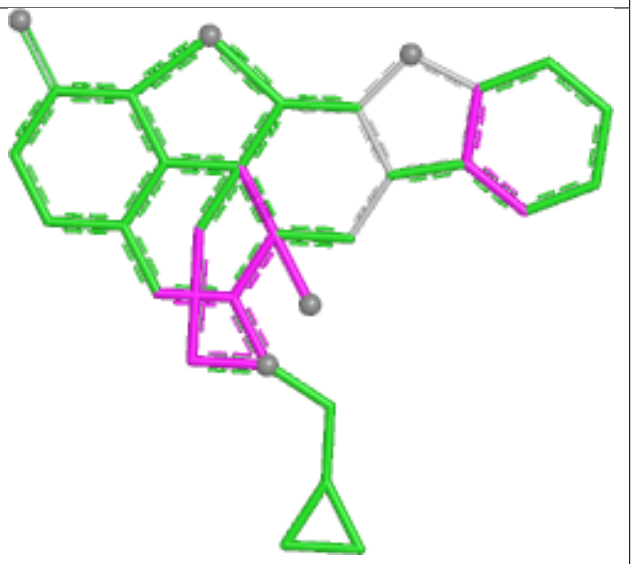


Rings

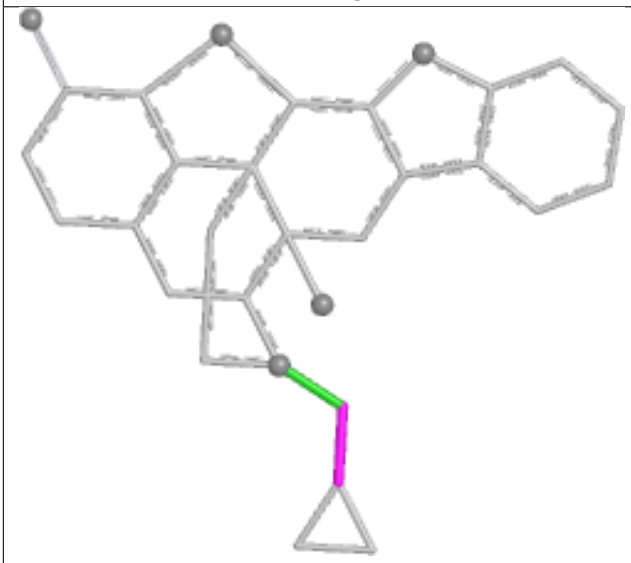
Ligand ZY8 A 1314



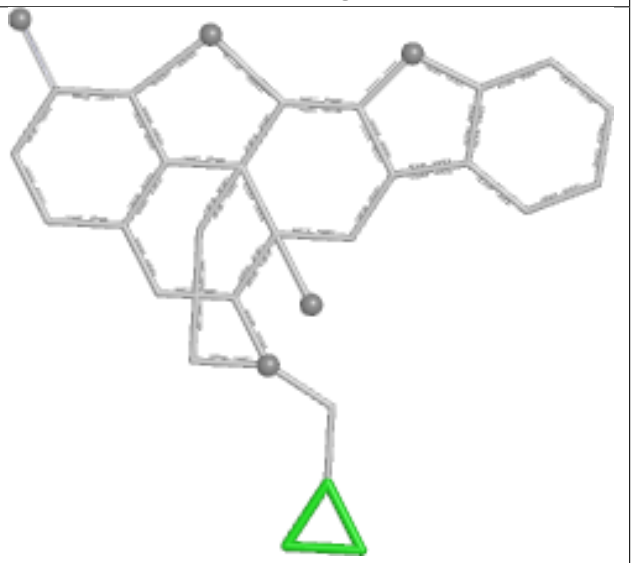
Bond lengths



Bond angles

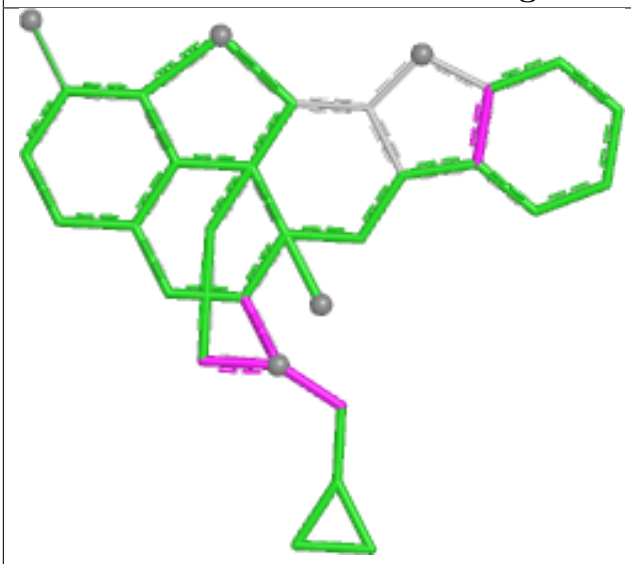


Torsions

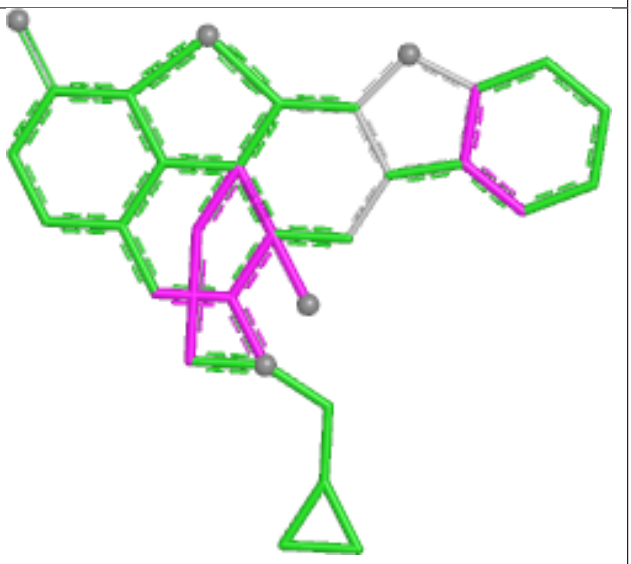


Rings

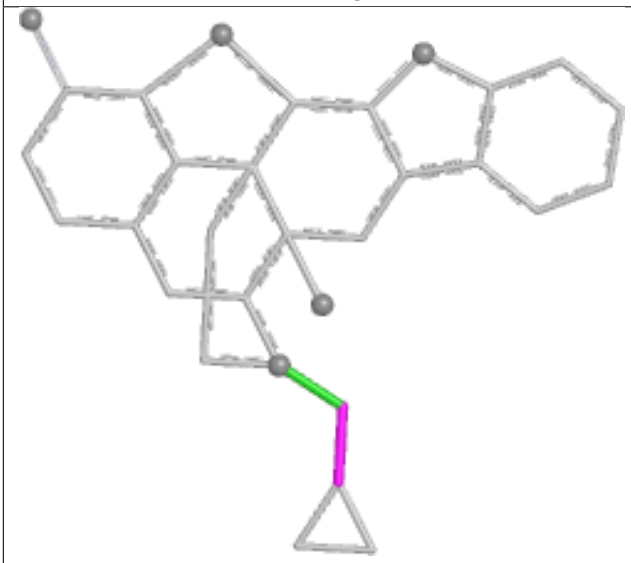
Ligand ZY8 C 1314



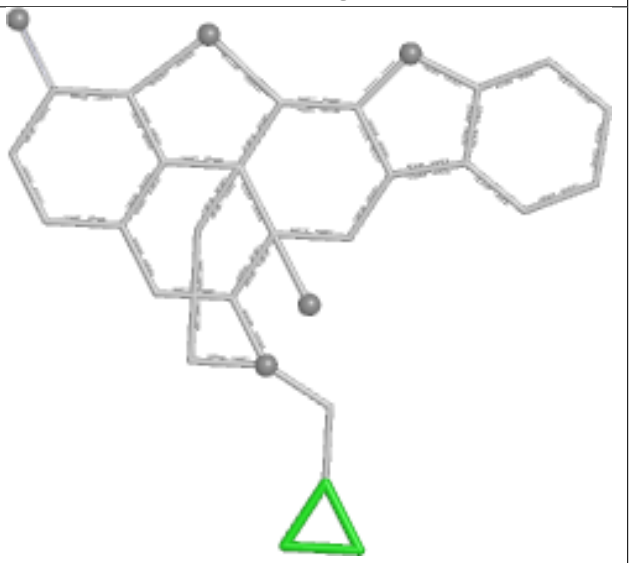
Bond lengths



Bond angles

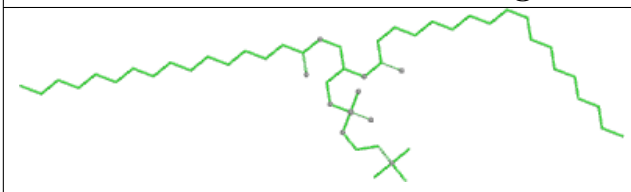


Torsions

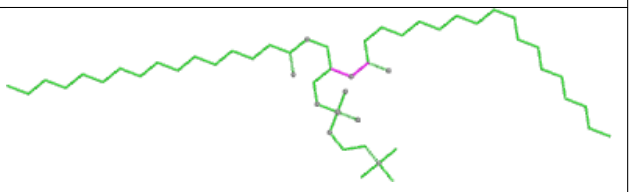


Rings

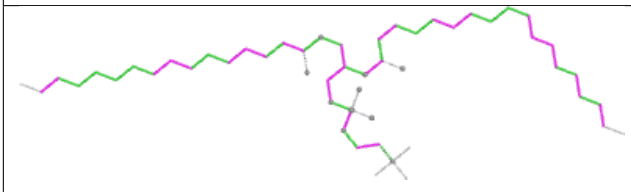
Ligand POV B 1302



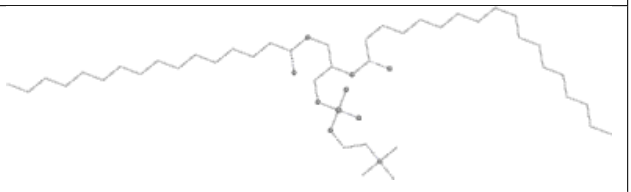
Bond lengths



Bond angles

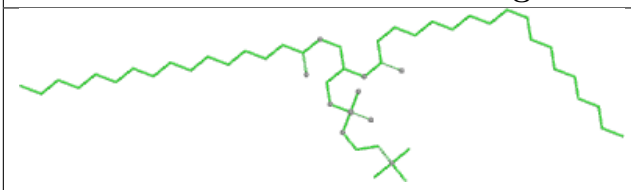


Torsions

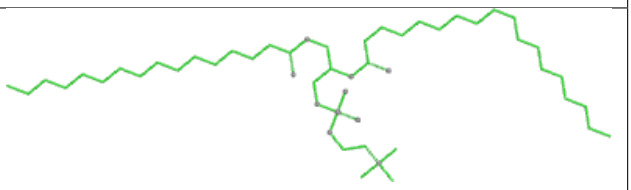


Rings

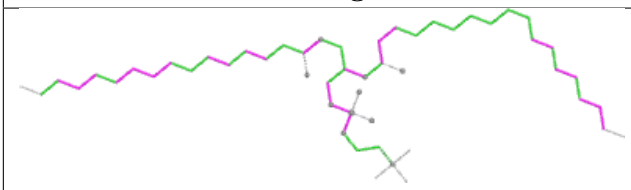
Ligand POV D 1310



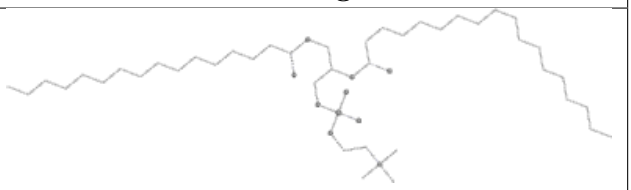
Bond lengths



Bond angles

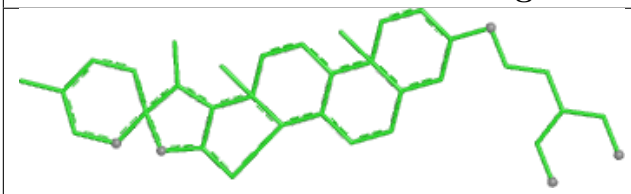


Torsions

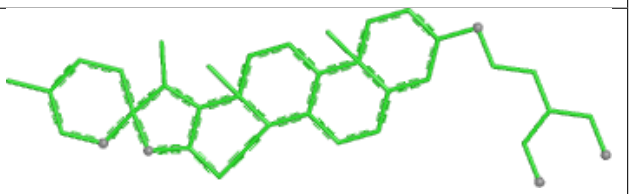


Rings

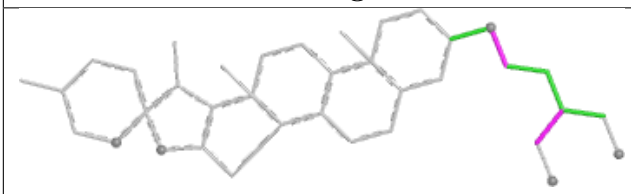
Ligand DU0 D 1315



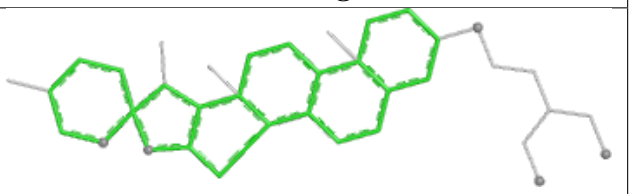
Bond lengths



Bond angles

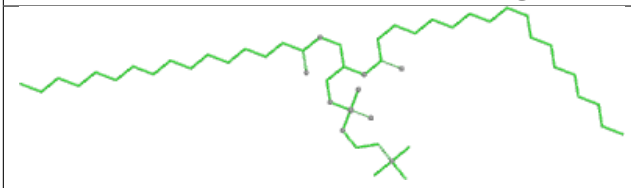


Torsions

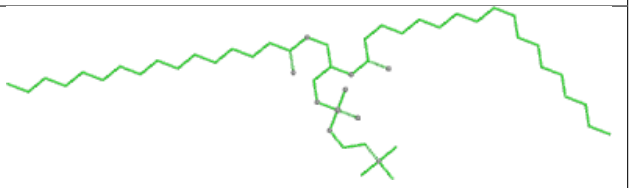


Rings

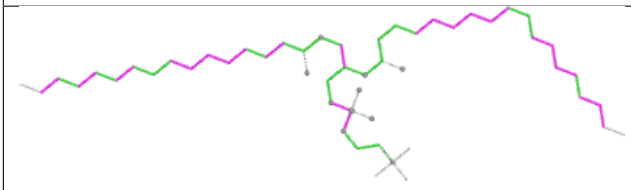
Ligand POV A 1301



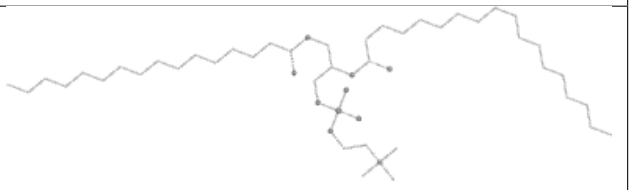
Bond lengths



Bond angles

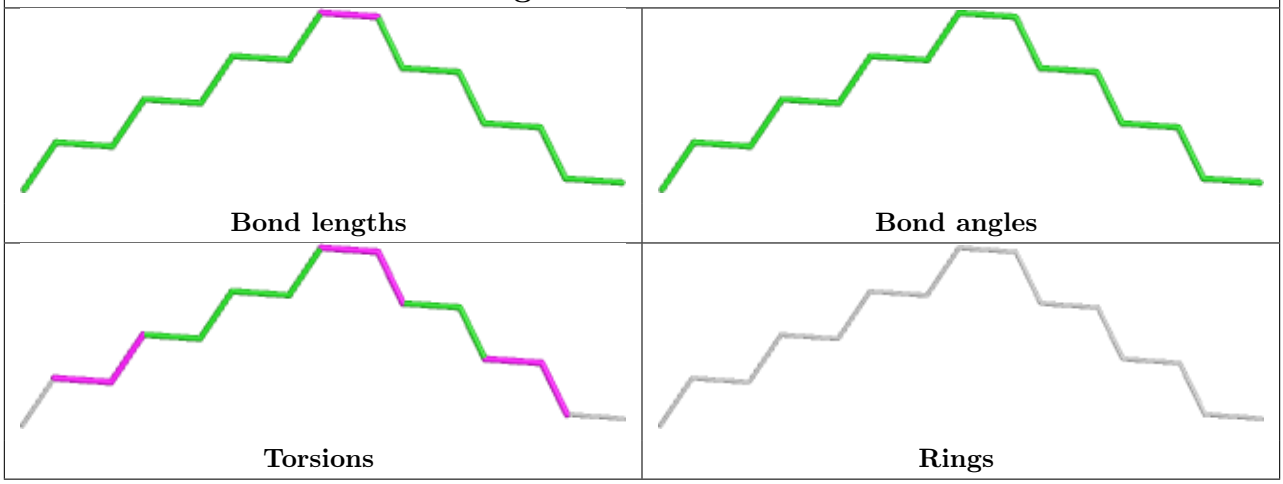


Torsions

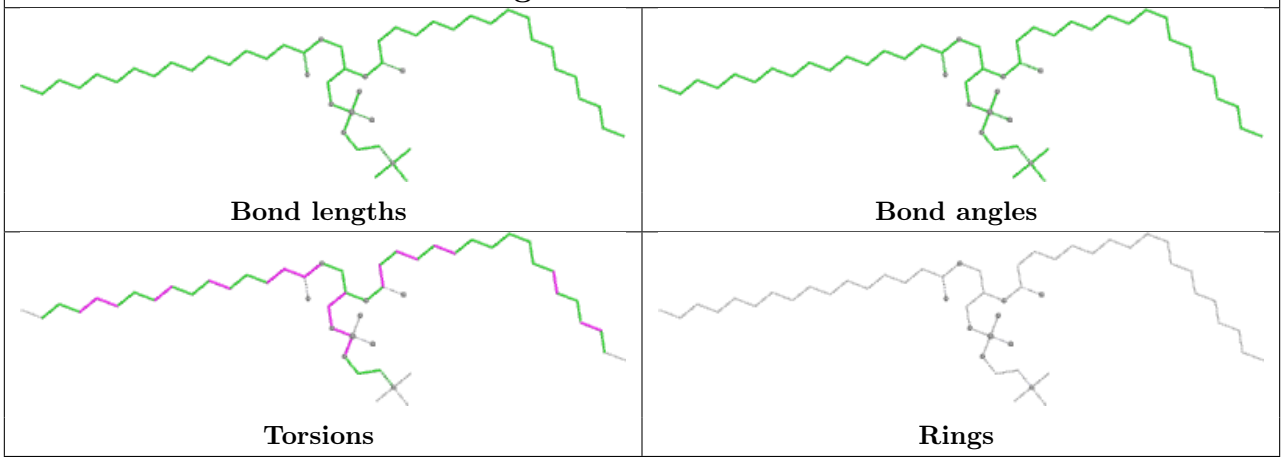


Rings

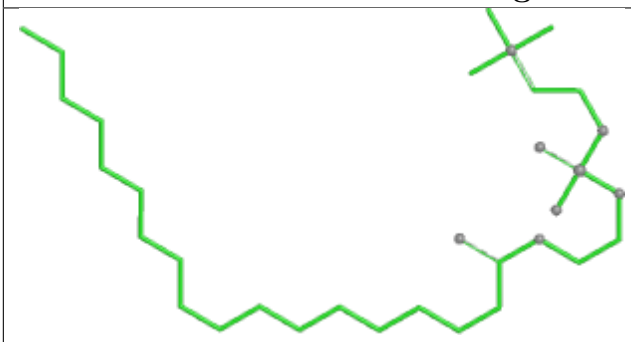
Ligand POV D 1302



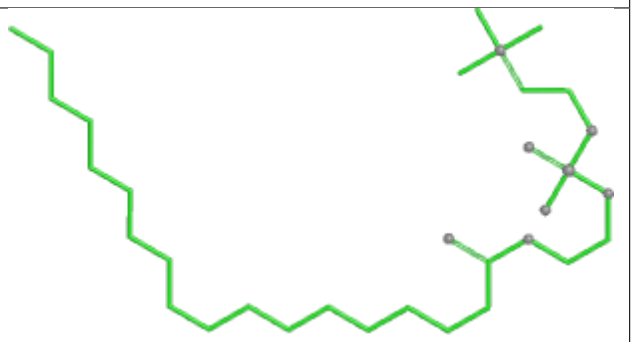
Ligand POV D 1311



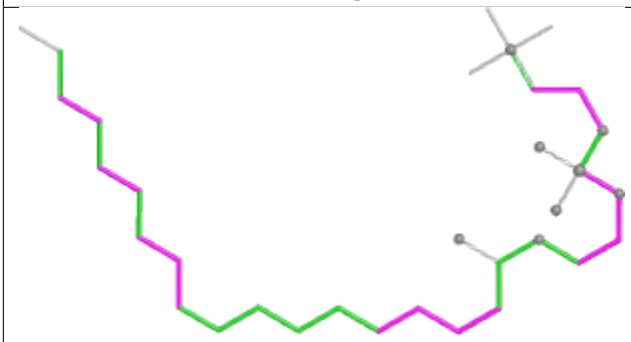
Ligand POV A 1311



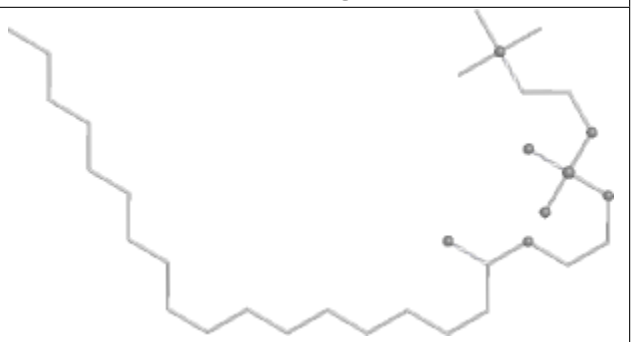
Bond lengths



Bond angles

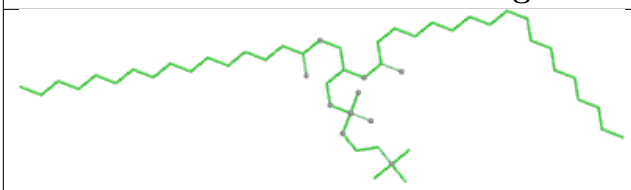


Torsions

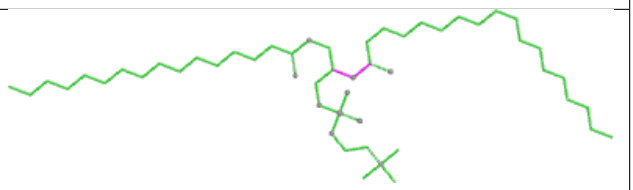


Rings

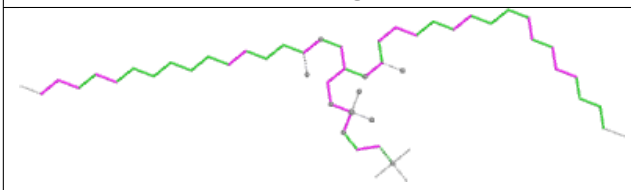
Ligand POV D 1306



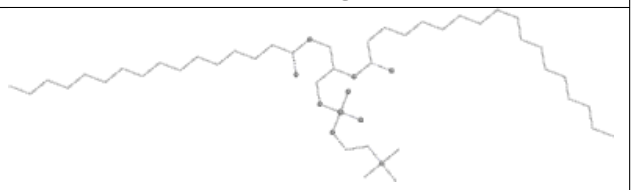
Bond lengths



Bond angles

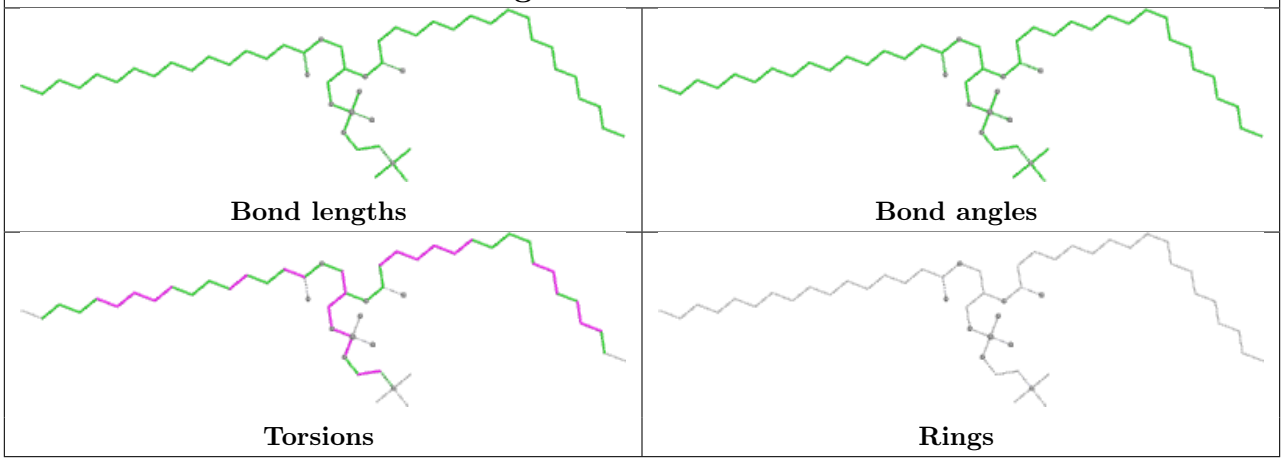


Torsions

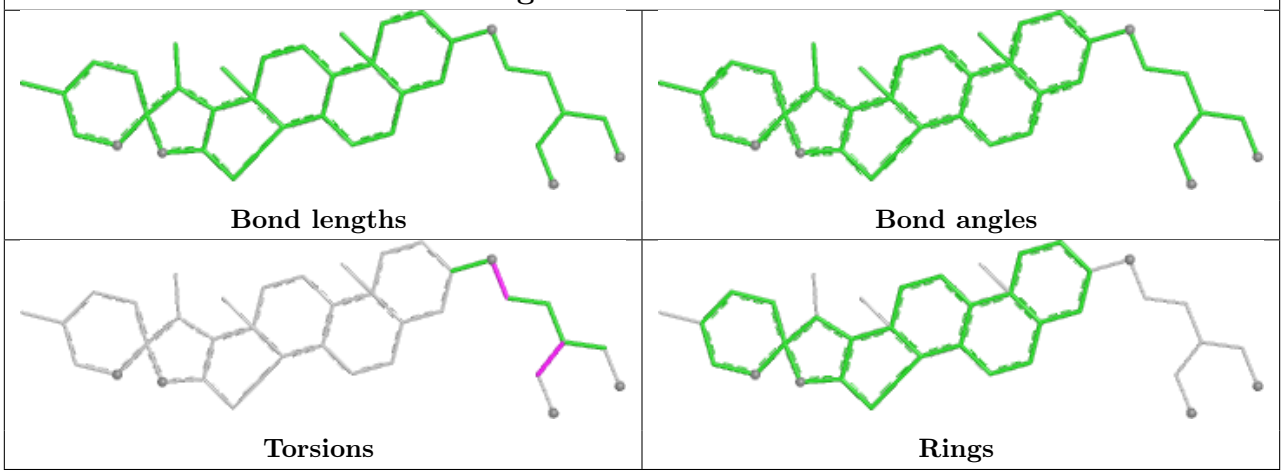


Rings

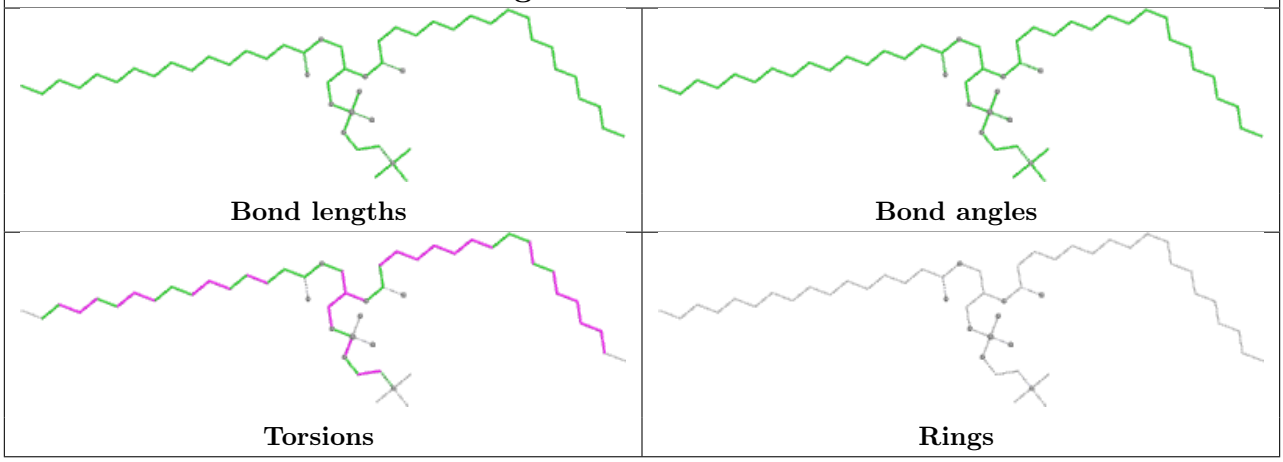
Ligand POV A 1312



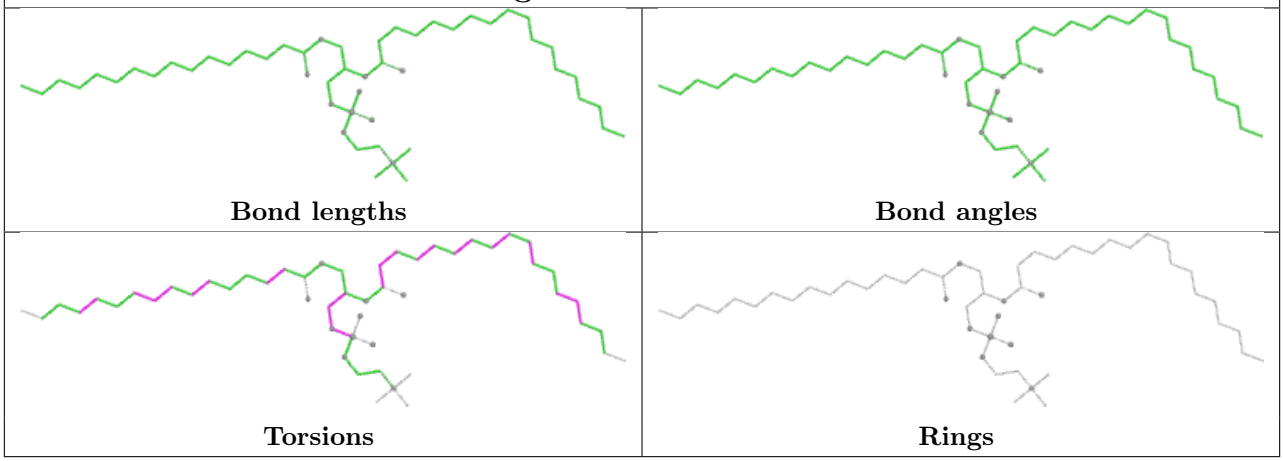
Ligand DU0 C 1313



Ligand POV A 1307



Ligand POV A 1317



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.

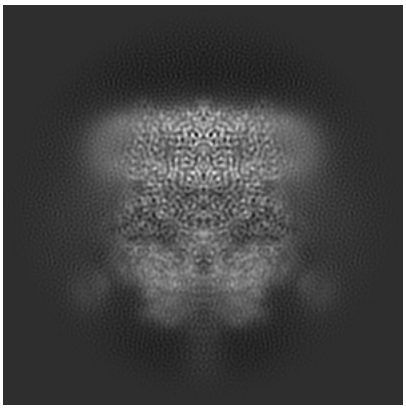
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40500. These allow visual inspection of the internal detail of the map and identification of artifacts.

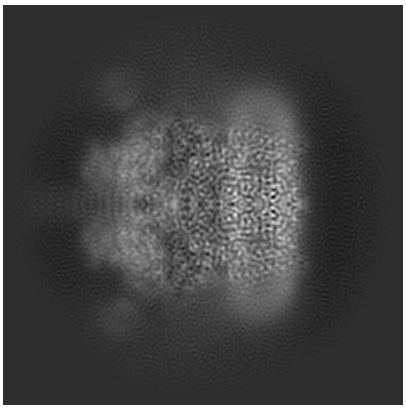
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

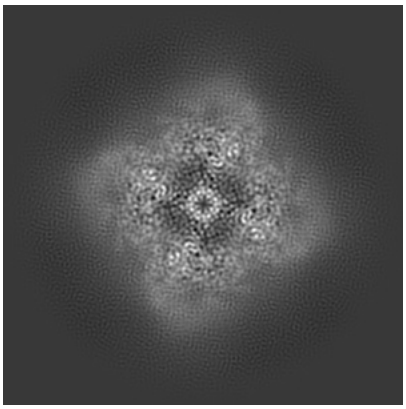
6.1.1 Primary map



X

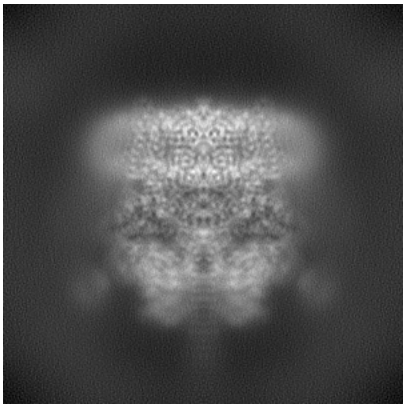


Y

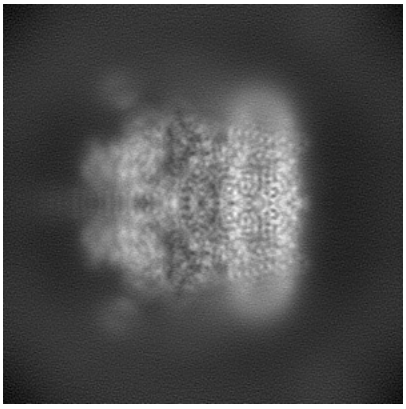


Z

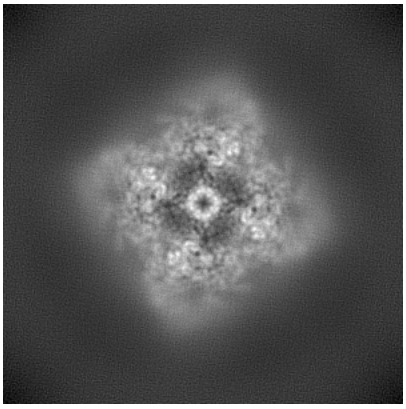
6.1.2 Raw map



X



Y

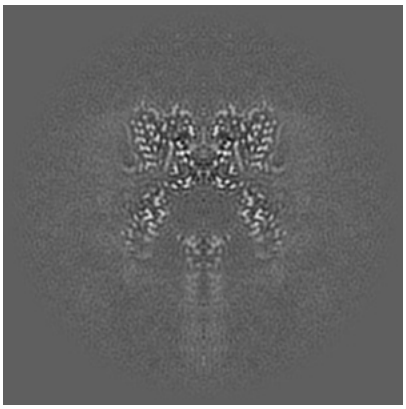


Z

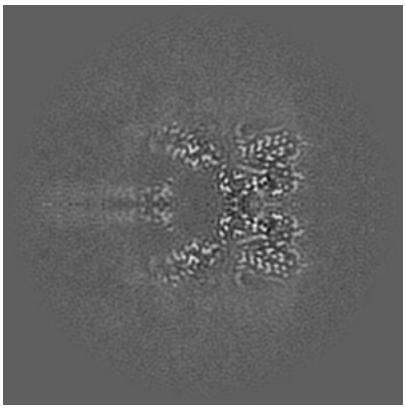
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

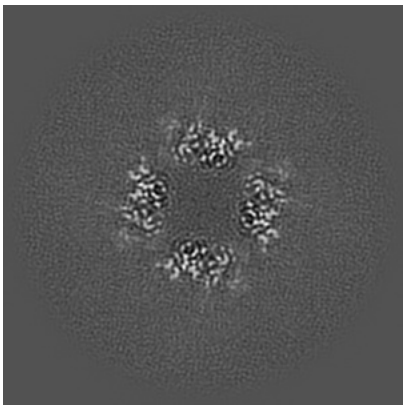
6.2.1 Primary map



X Index: 150

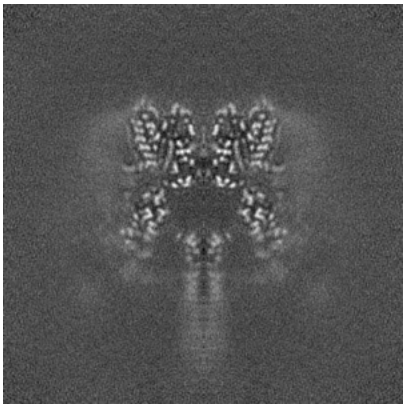


Y Index: 150

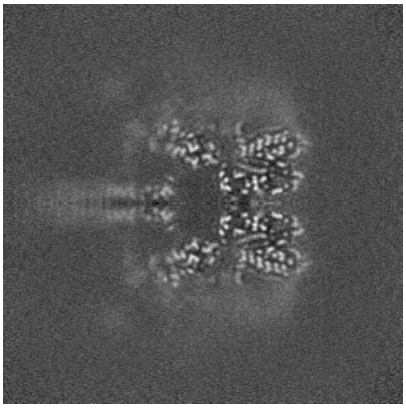


Z Index: 150

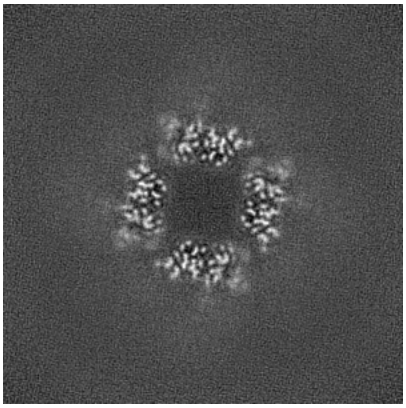
6.2.2 Raw map



X Index: 150



Y Index: 150

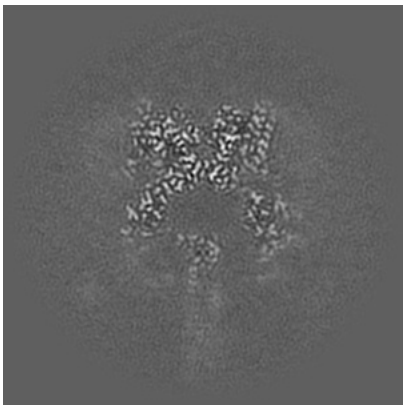


Z Index: 150

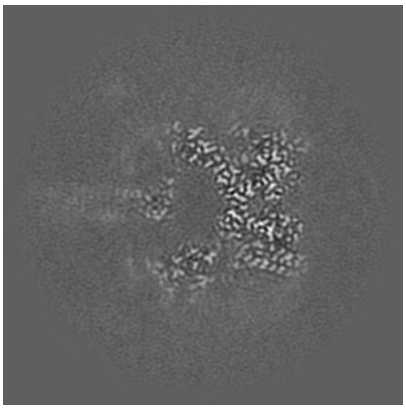
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

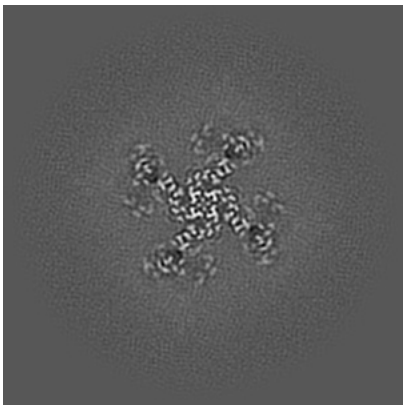
6.3.1 Primary map



X Index: 147

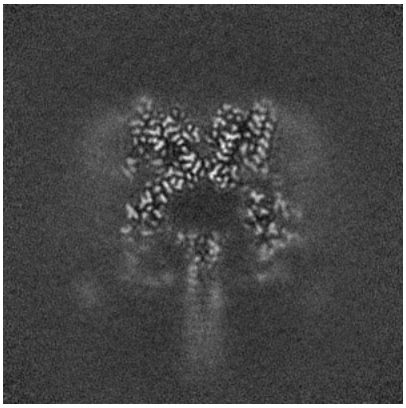


Y Index: 147

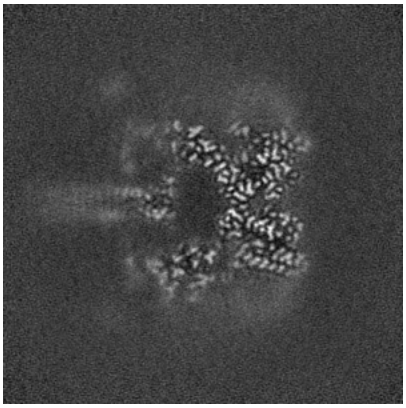


Z Index: 174

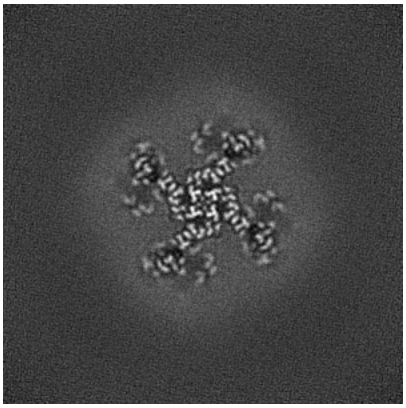
6.3.2 Raw map



X Index: 147



Y Index: 147

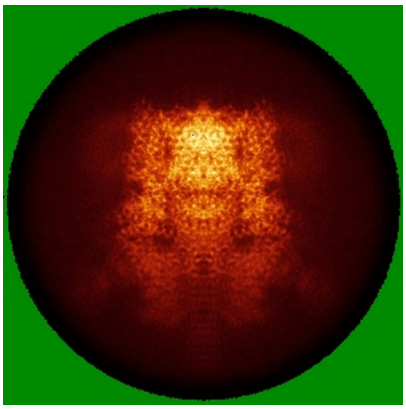


Z Index: 174

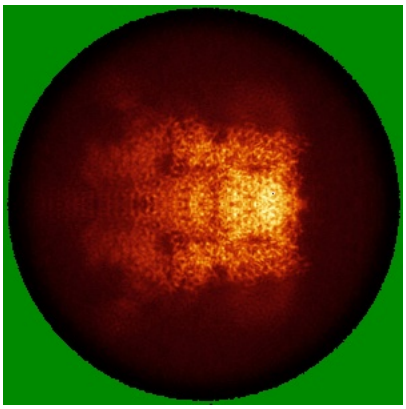
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

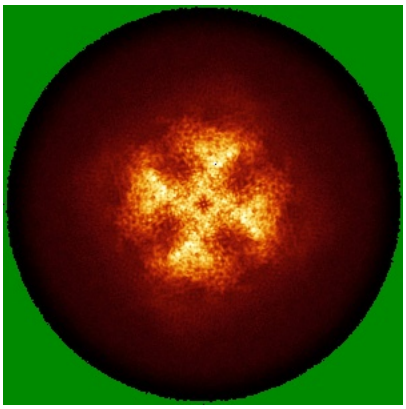
6.4.1 Primary map



X

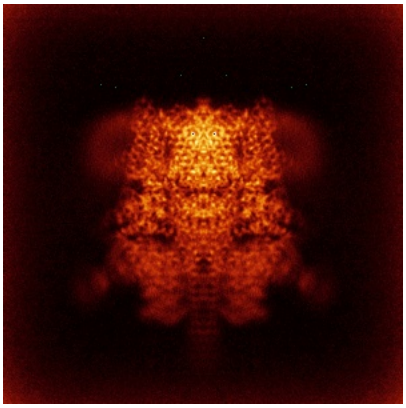


Y

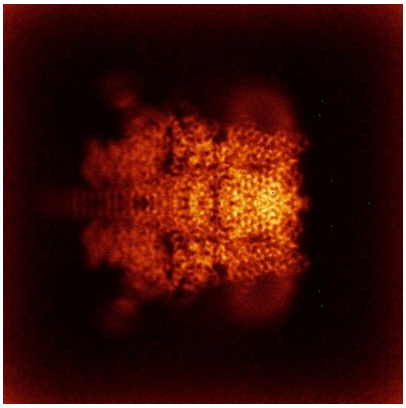


Z

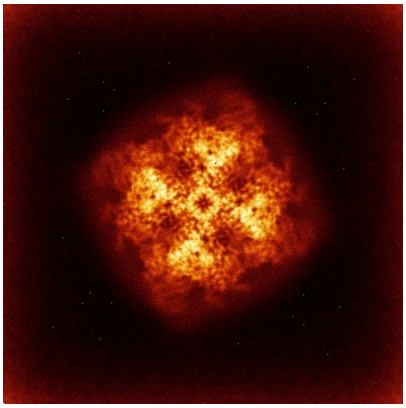
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

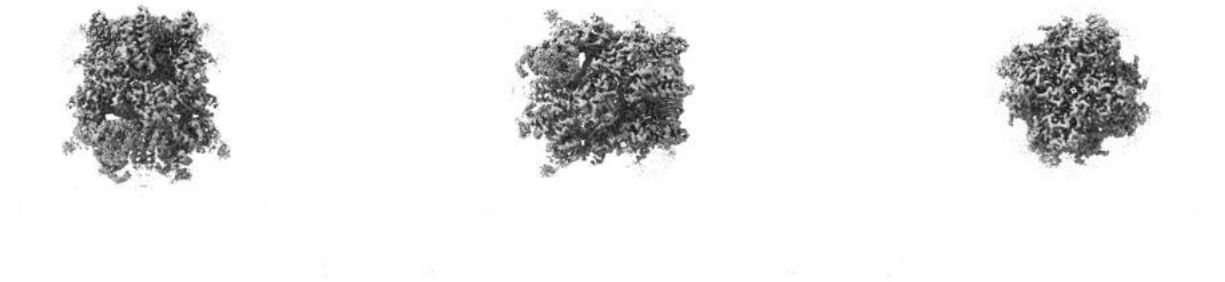
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

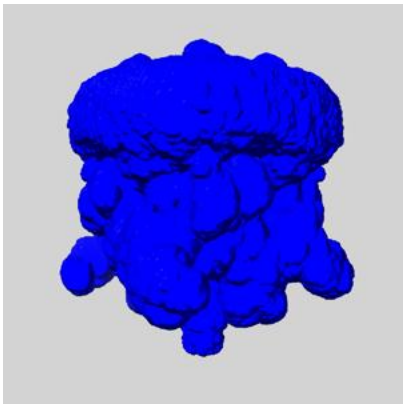
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

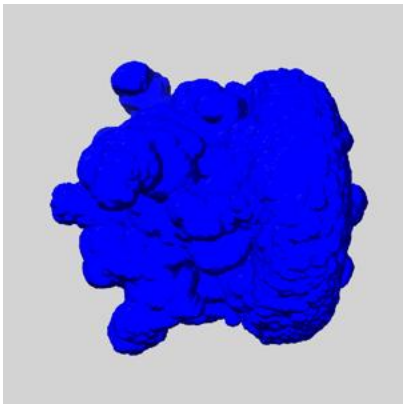
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

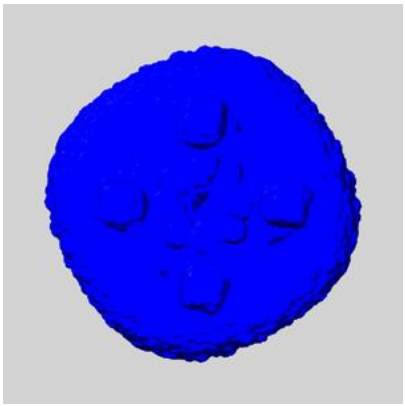
6.6.1 emd_40500_msk_1.map (i)



X



Y

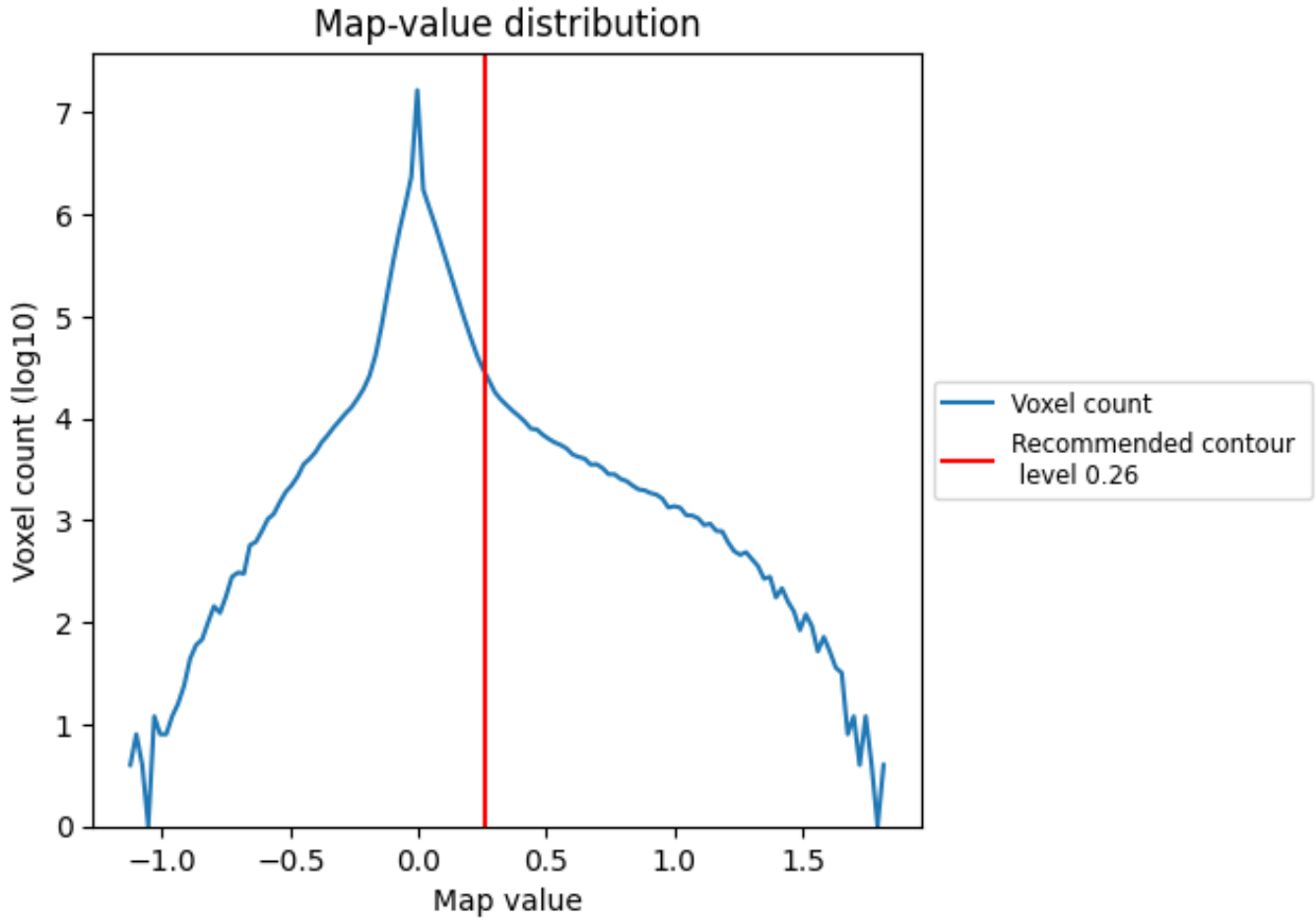


Z

7 Map analysis

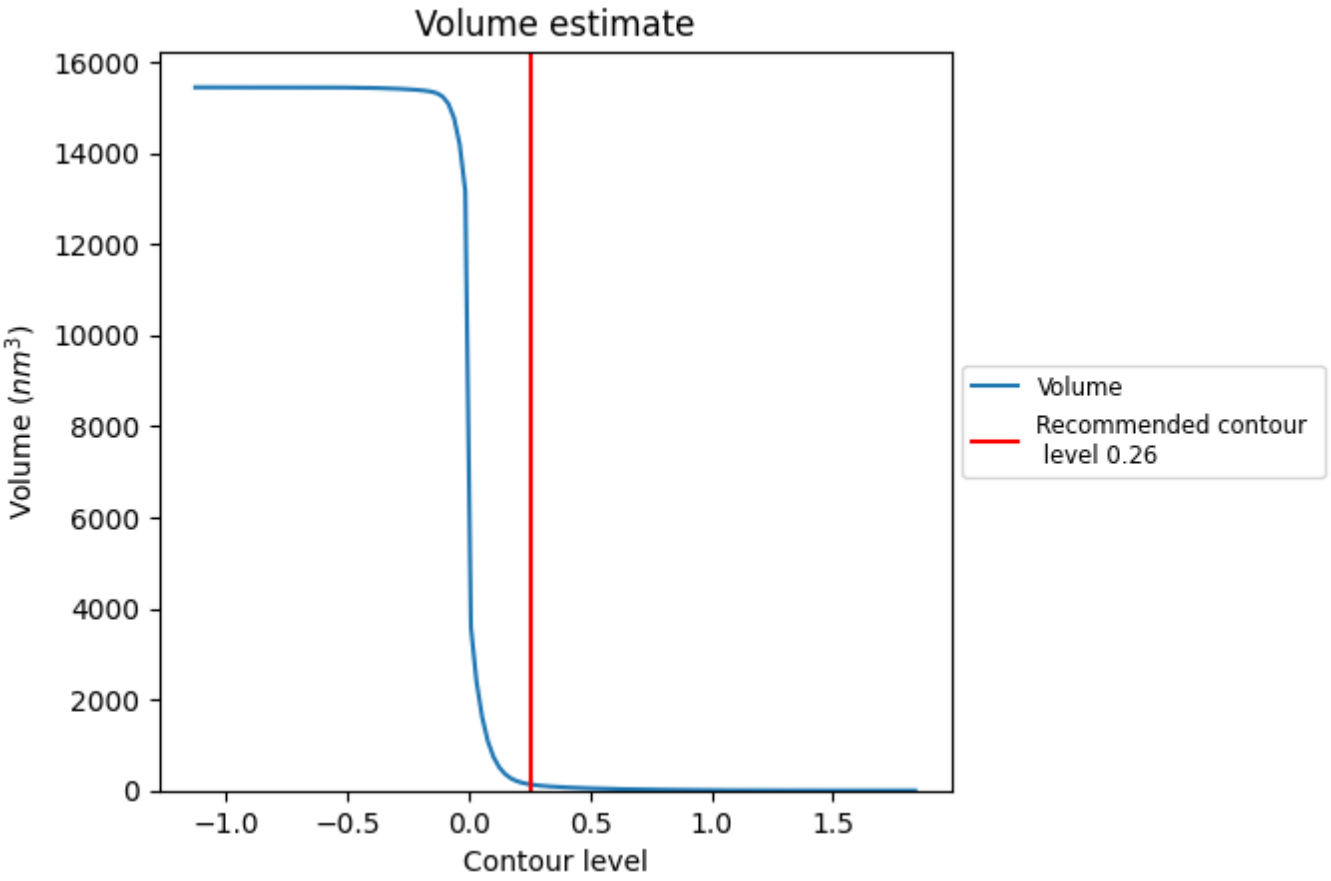
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

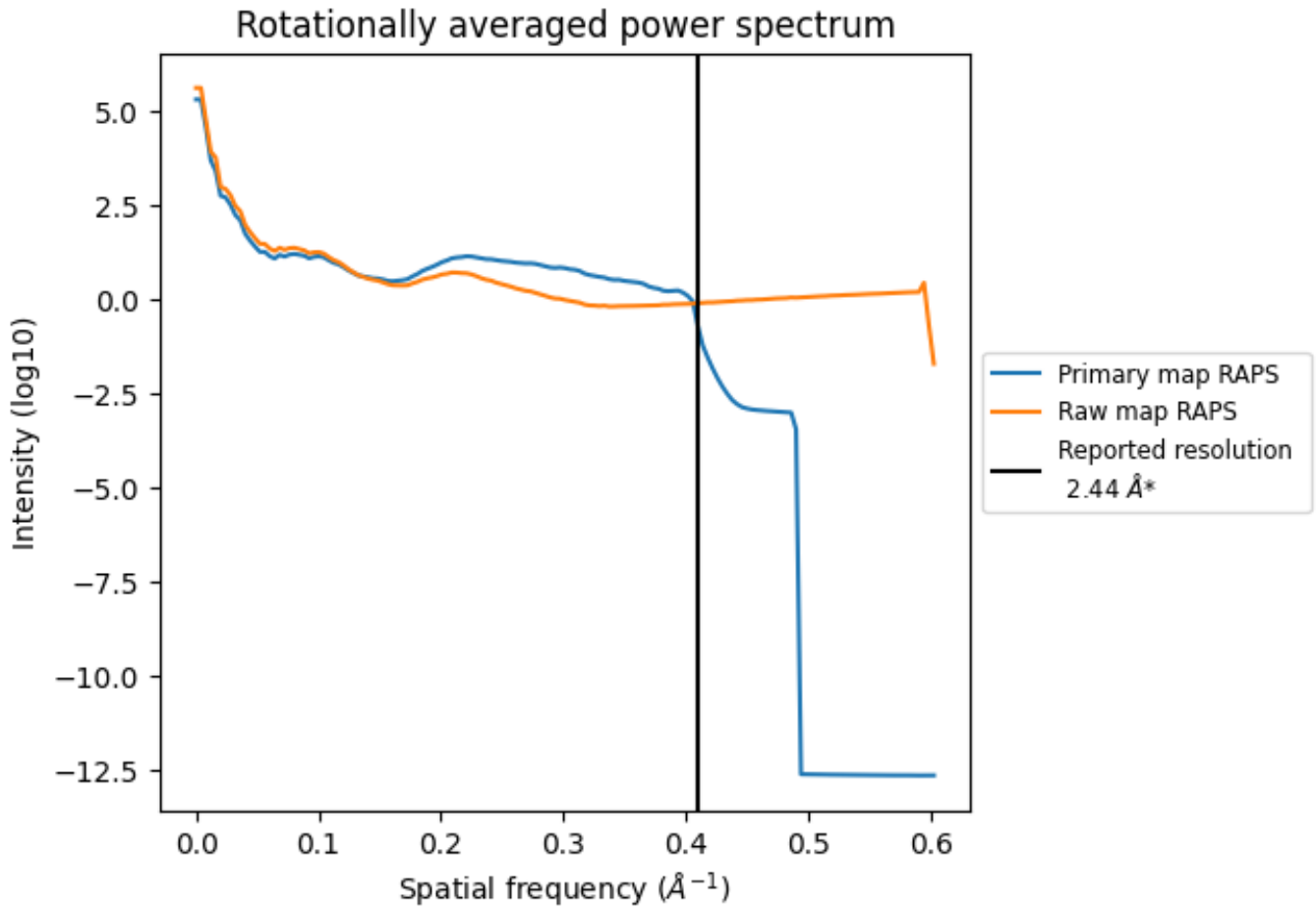
7.2 Volume estimate (i)



The volume at the recommended contour level is 131 nm^3; this corresponds to an approximate mass of 118 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

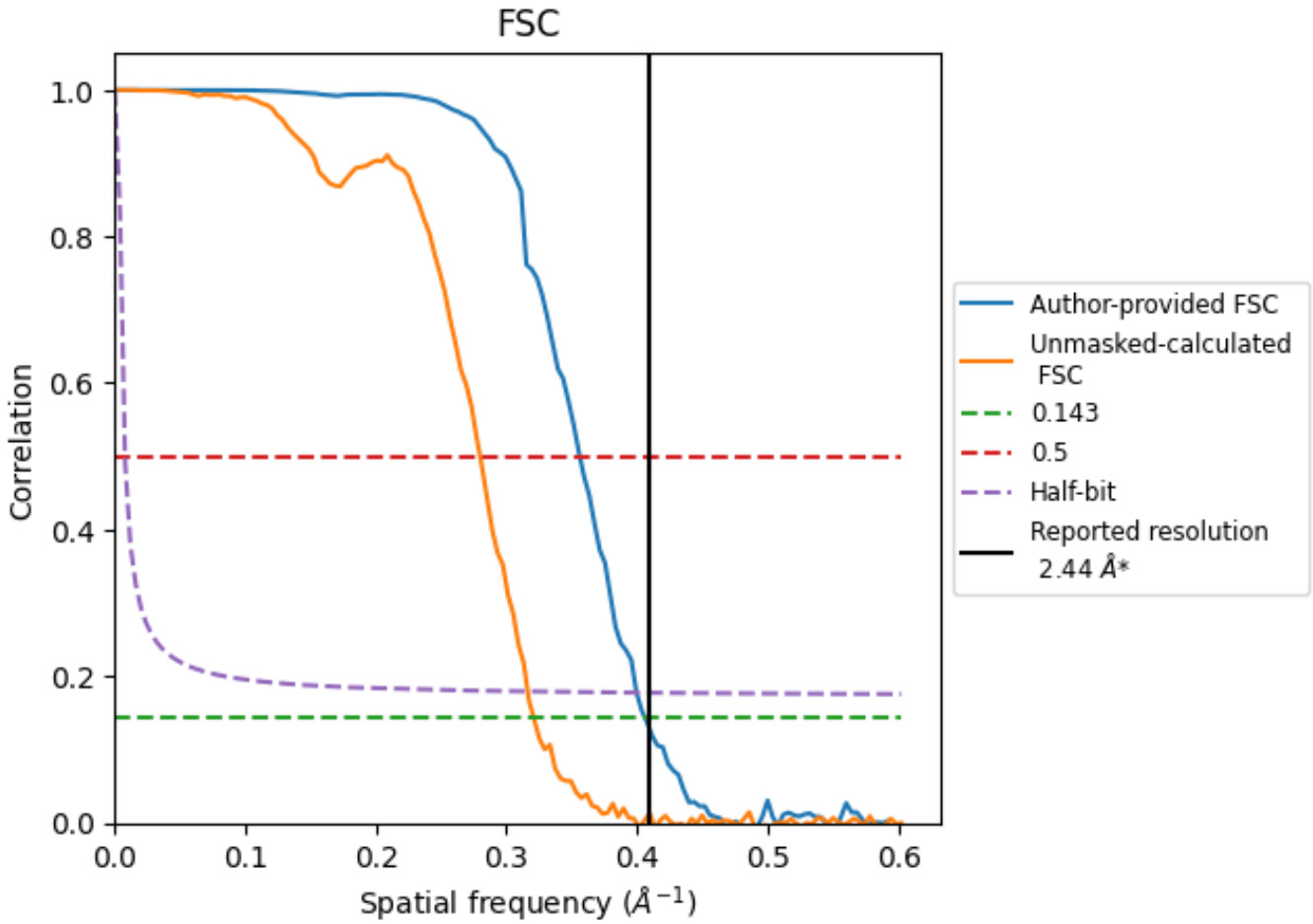


*Reported resolution corresponds to spatial frequency of 0.410 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.410 Å^{-1}

8.2 Resolution estimates (i)

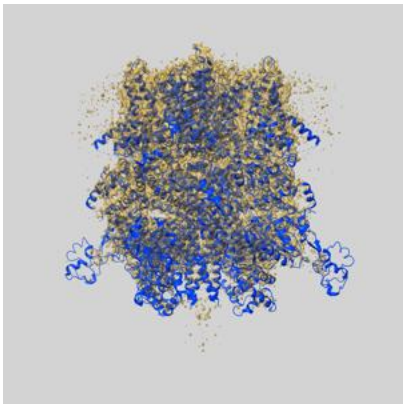
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.46	2.81	2.50
Unmasked-calculated*	3.12	3.57	3.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.44 by more than 10 %

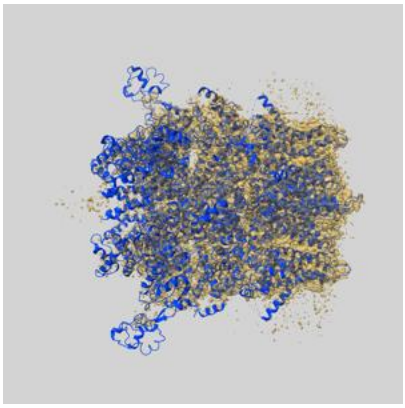
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40500 and PDB model 8SI6. Per-residue inclusion information can be found in section 3 on page 9.

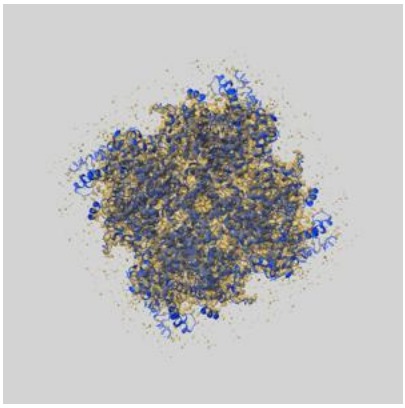
9.1 Map-model overlay



X



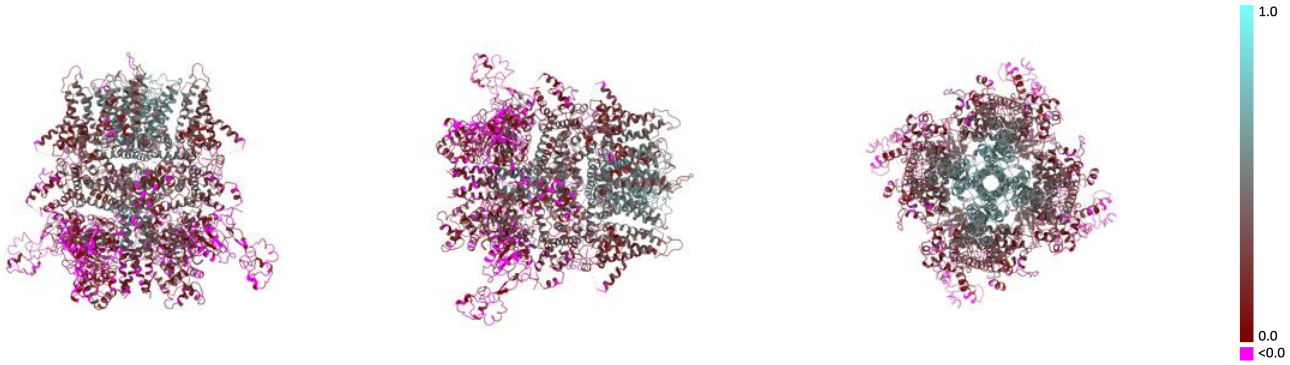
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

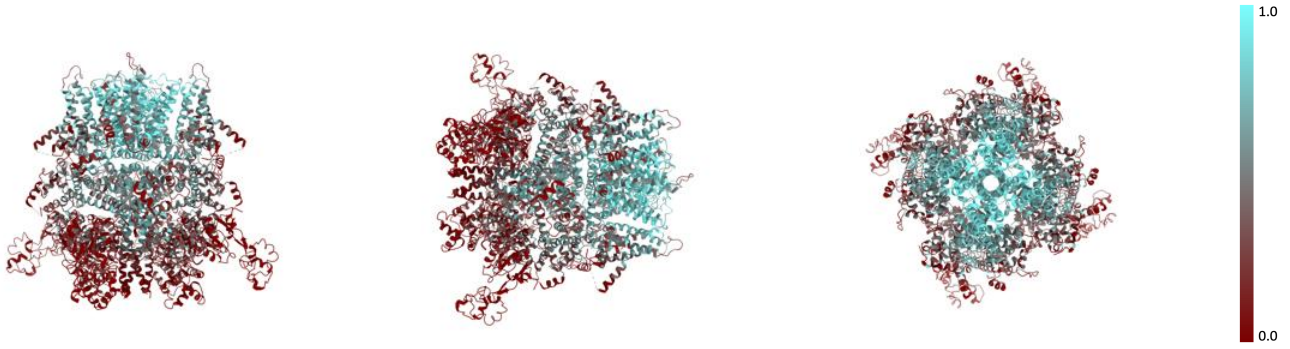
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

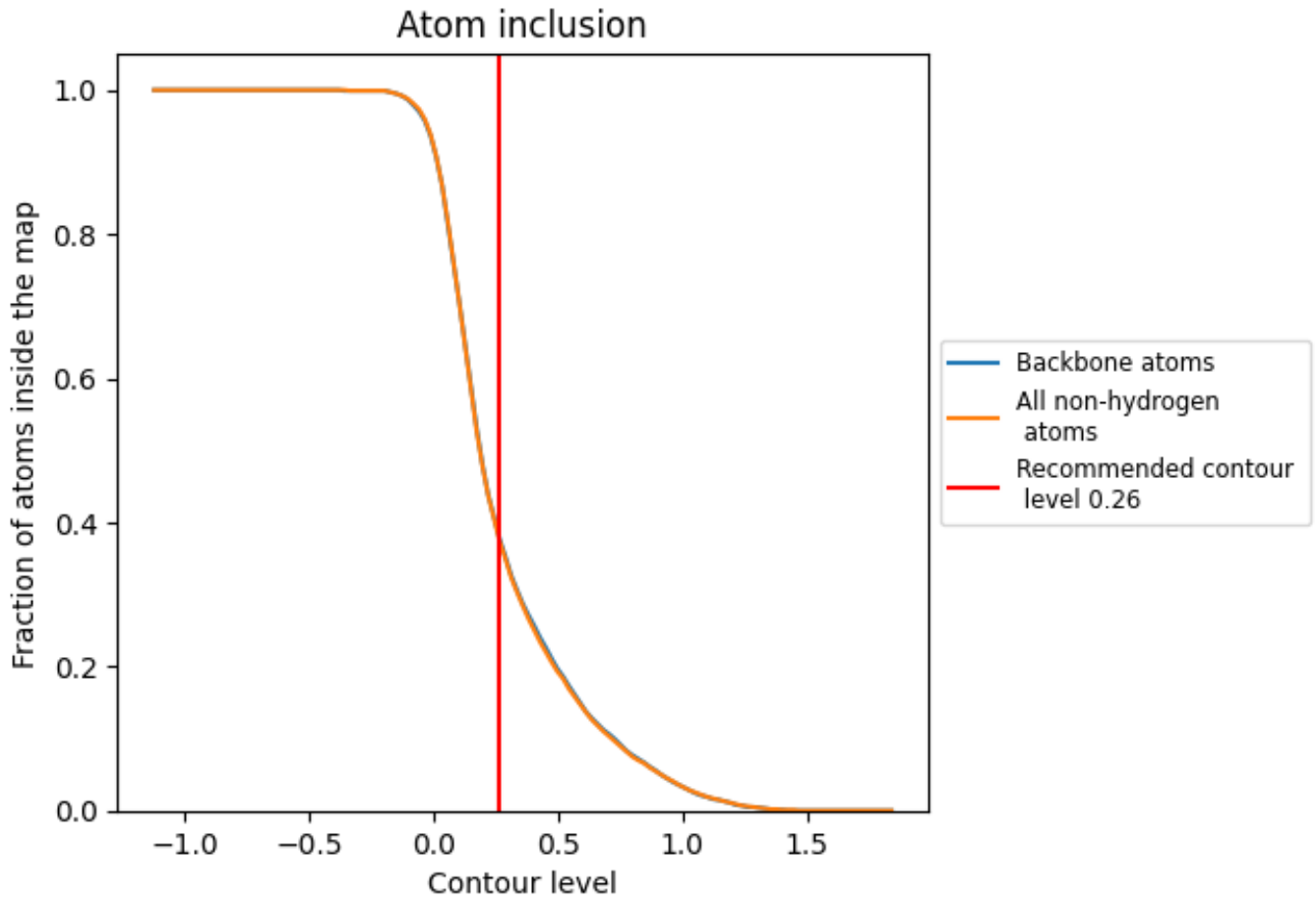
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.26).

9.4 Atom inclusion (i)



At the recommended contour level, 38% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3790	0.2400
A	0.3790	0.2390
B	0.3830	0.2390
C	0.3810	0.2420
D	0.3820	0.2410