wwPDB EM Validation Summary Report (i)

Nov 29, 2022 – 08:13 PM JST

PDB ID	:	7WYV
EMDB ID	:	EMD-32895
Title	:	Cryo-EM structure of Na+,K+-ATPase in the E2P state formed by ATP in the presence of 40 mM Mg2+
Authors	:	Kanai, R.; Cornelius, F.; Vilsen, B.; Toyoshima, C.
Deposited on	:	2022-02-16
Resolution	:	3.70 Å(reported)
Based on initial model	:	7D91

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 (i) 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 (1)) were used in the production of this report:

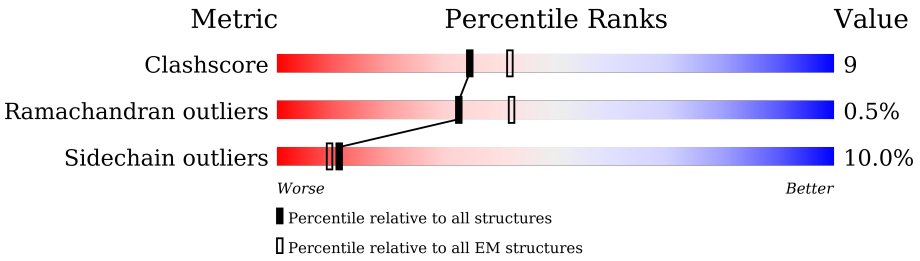
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	1028	20%; 75%; 20%; • •
1	C	1028	20%; 74%; 21%; • •
2	B	305	5%; 61%; 30%; 5%; •
2	D	305	5%; 61%; 30%; 5%; •
3	E	94	7%; 32%; 11%; 57%
3	G	94	7%; 32%; 11%; 57%
4	F	6	50%; 83%; 17%
4	K	6	50%; 17%; 67%; 17%

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Mol	Chain	Length	Quality of chain
5	H	6	83% / 100%
5	L	6	83% / 100%
6	I	5	80% / 100%
6	M	5	80% / 100%
7	J	2	100% / 100%
7	N	2	100% / 100%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 22668 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 Sodium/potassium-transporting ATPase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	A	993	7687	4890	1291	1459	1	46	0	0
1	C	993	7687	4890	1291	1459	1	46	0	0

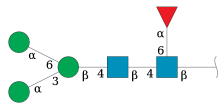
- Molecule 2 is a protein called Na+,K+-ATPase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	294	2399	1551	394	443	11	0	0
2	D	294	2399	1551	394	443	11	0	0

- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	40	311	203	51	55	2	0	0
3	E	40	311	203	51	55	2	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	F	6	71	40	2	29	0	0

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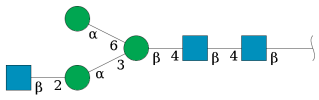
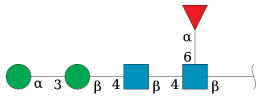
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	K	6	71	40	2	29	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	H	6	75	42	3	30	0	0
5	L	6	75	42	3	30	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	I	5	60	34	2	24	0	0
6	M	5	60	34	2	24	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	J	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	N	2	28	16	2	10	0	0

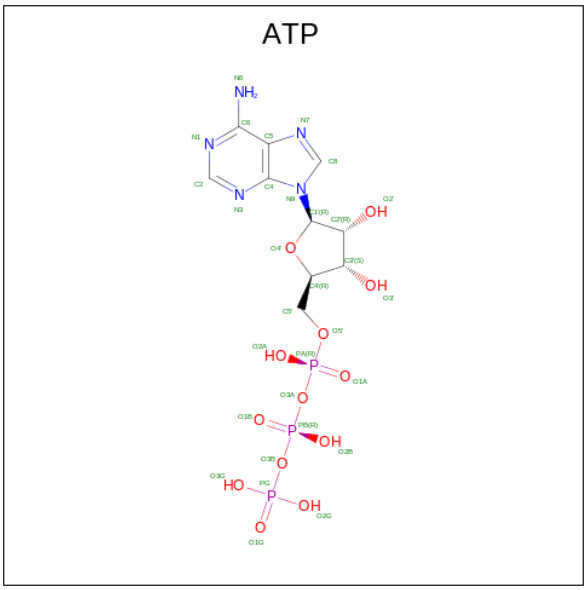
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	A	2	2	2	0
8	C	2	Total	Mg	0
			2	2	

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
9	A	1	1	1	0
9	C	1	Total	Na	0
			1	1	

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	A	1	31	10	5	13	3	0

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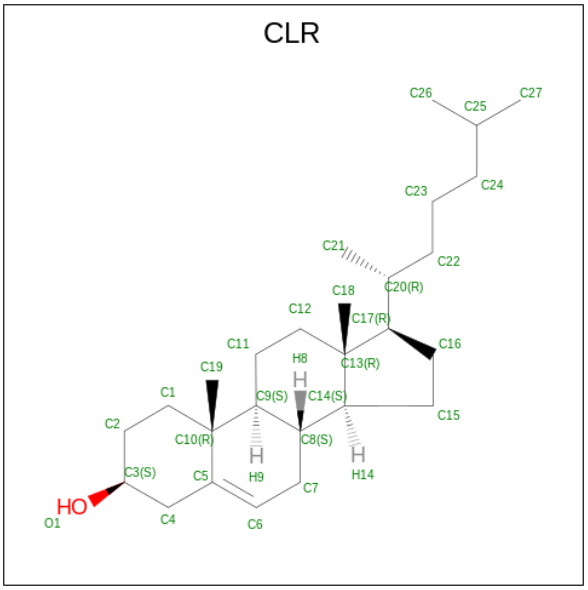
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	C	1	31	10	5	13	3	0

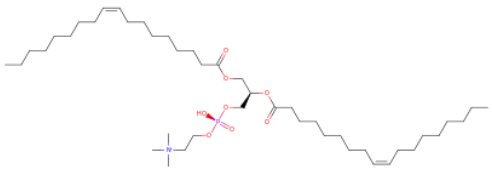
- Molecule 11 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	O			
11	A	1	84	81	3			0
11	A	1	84	81	3			0
11	A	1	84	81	3			0
11	B	1	28	27	1			0
11	C	1	84	81	3			0
11	C	1	84	81	3			0
11	C	1	84	81	3			0
11	D	1	28	27	1			0

- Molecule 12 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

PCW



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	A	1	444	344	10	80	10	0
12	G	1	108	88	2	16	2	0
12	G	1	108	88	2	16	2	0
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0
12	C	1	444	344	10	80	10	0
12	E	1	108	88	2	16	2	0
12	E	1	108	88	2	16	2	0

- Molecule 13 is water.

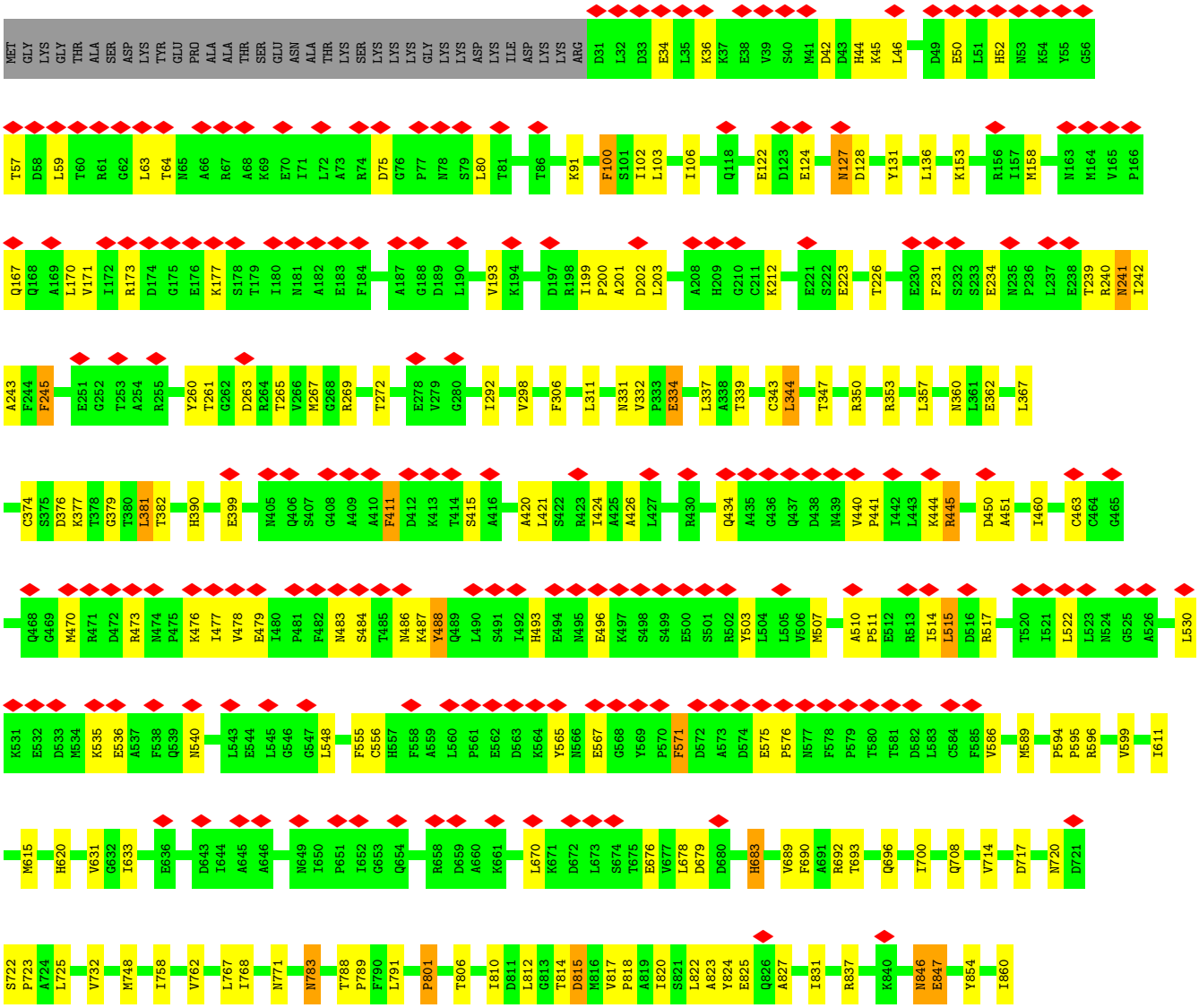
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
13	A	5	5	5	0
13	C	5	5	5	0

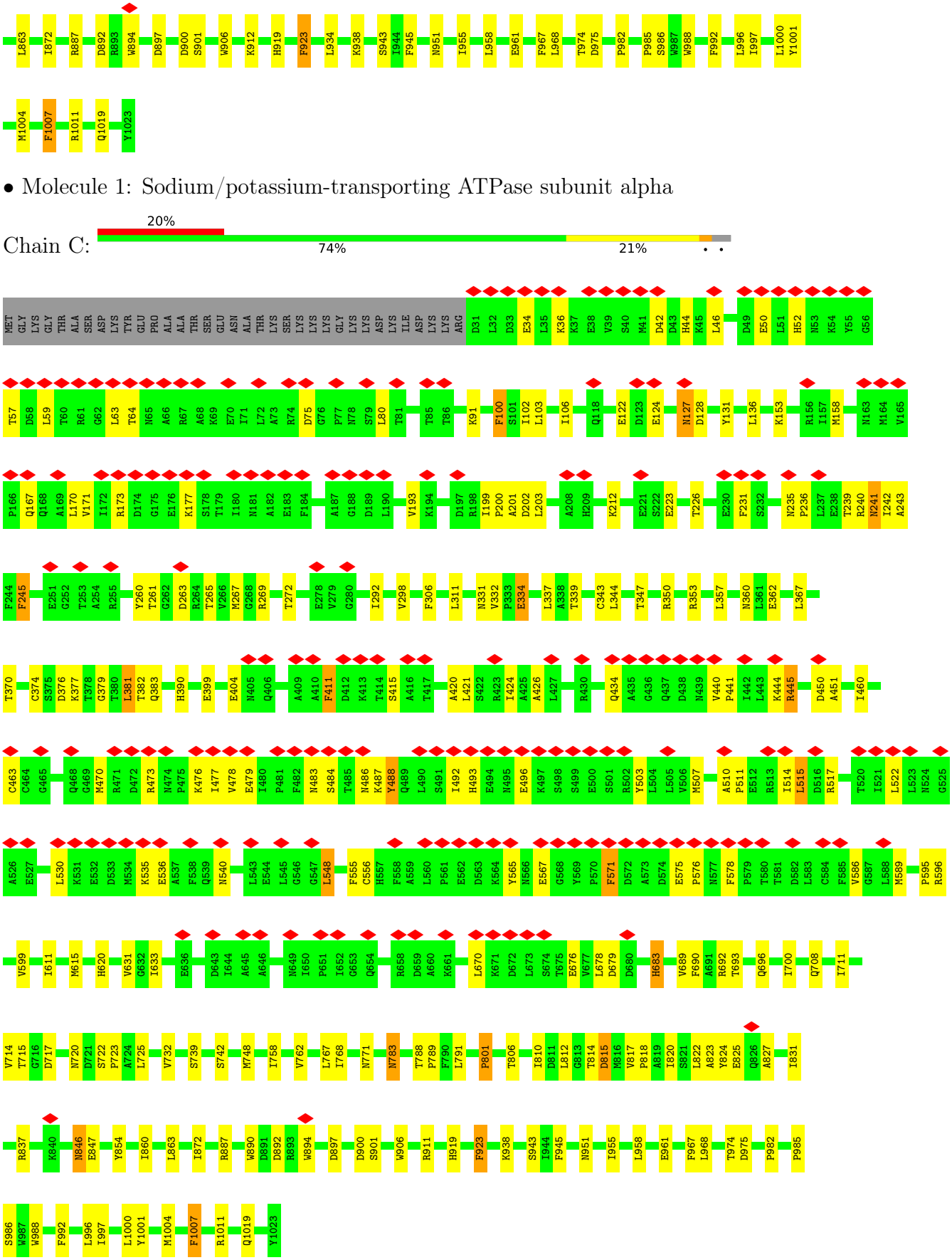
3 Residue-property plots (i)

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: Sodium/potassium-transporting ATPase subunit alpha

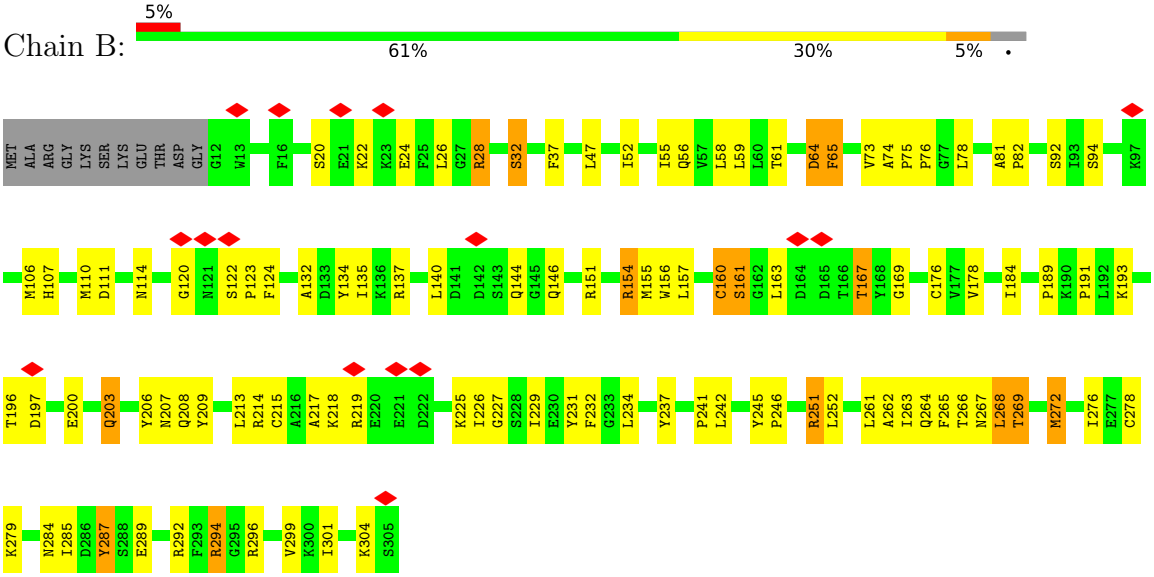
Chain A:




L863 I872 R887 D892 R893 W894 D897 D900 S901 W906 K912 H919 F923 L934 K938 S943 I944 F945 N951 I955 L958 E961 F967 L968 T974 D975 P982 P985 S986 W987 W988 F992 L996 I997 L1000 Y1001
M1004 F1007 R1011 Q1019 Y1023
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha
Chain C:
20%
74%
21%
MET GLY LYS GLY THR ALA SER ASP LYS TYR GLU PRO ALA ALA THR SER GLU ASN ALA THR LYS SER LYS LYS LYS GLY LYS LYS ASP LYS ILE ASP LYS LYS ARG D31 L32 D33 E34 L35 K36 K37 E38 V39 S40 M41 D42 D43 H44 K45 L46 D49 E50 L51 H52 N53 K54 Y55 G56
T57 D58 L59 T60 R61 G62 L63 T64 N65 A66 R67 A68 K69 E70 I71 L72 A73 R74 D75 G76 P77 N78 S79 L80 T81 T85 T86 K91 F100 S101 I102 L103 I106 Q118 E122 D123 E124 N127 D128 Y131 L136 K153 R156 I157 M158 N163 M164 V165
P166 Q167 Q168 A169 L170 V171 I172 R173 D174 G175 E176 K177 S178 T179 I180 N181 A182 E183 F184 A187 G188 D189 L190 V193 K194 D197 R198 I199 P200 A201 D202 L203 A208 H209 K212 E221 S222 E223 T226 E230 F231 S232 N235 P236 L237 E238 T239 R240 N241 I242 A243
F244 F245 E251 G252 T253 A254 R255 Y260 T261 G262 D263 R264 T265 V266 M267 G268 R269 T272 E278 V279 G280 I292 V298 F306 L311 N331 V332 P333 E334 L337 A338 T339 C343 L344 T347 R350 R353 L357 N360 L361 E362 L367
T370 C374 S375 D376 K377 T378 G379 T380 L381 T382 Q383 H390 E399 E404 N405 Q406 A409 A410 F411 D412 K413 T414 S415 A416 T417 A420 L421 S422 R423 I424 A425 A426 L427 R430 Q434 A435 G436 Q437 D438 N439 V440 P441 I442 L443 K444 R445 D450 A451 I460
C463 C464 G465 Q468 G469 M470 R471 D472 R473 N474 P475 K476 I477 V478 E479 I480 P481 F482 N483 S484 T485 N486 K487 Y488 Q489 L490 S491 I492 H493 E494 N495 E496 K497 S498 S499 E500 S501 R502 Y503 L504 L505 V506 M507 A510 P511 E512 R513 I514 L515 D516 R517 T520 I521 L522 L523 N524 G525
A526 E527 L530 K531 E532 D533 M534 K535 E536 A537 F538 Q539 N540 L543 E544 L545 G546 G547 L548 F555 C556 H557 F558 A559 L560 P561 E562 D563 K564 Y565 N566 E567 G568 Y569 P570 F571 D572 A573 D574 E575 P576 N577 F578 P579 T580 T581 D582 L583 C584 F585 V586 G587 L588 M589 P595 R596
V599 I611 M615 H620 V631 G632 I633 E636 D643 I644 A645 A646 N649 I650 P651 I652 G653 Q654 R658 D659 A660 K661 L670 K671 D672 L673 S674 T675 E676 V677 L678 D679 D680 H683 V689 F690 A691 R692 T693 Q696 I700 Q708 I711
V714 T715 G716 D717 N720 D721 S722 P723 A724 L725 V732 S739 S742 M748 I758 V762 L767 I768 N771 N783 T788 P789 F790 L791 P801 T806 I810 D811 L812 G813 T814 D815 M816 V817 P818 A819 I820 S821 L822 A823 Y824 E825 Q826 A827 I831
R837 K840 N846 E847 Y854 I860 L863 I872 R887 W890 D891 D892 R893 W894 D897 D900 S901 W906 R911 H919 F923 K938 S943 I944 F945 N951 I955 L958 E961 F967 L968 T974 D975 P982 P985
S986 W987 W988 F992 L996 I997 L1000 Y1001 M1004 F1007 R1011 Q1019 Y1023

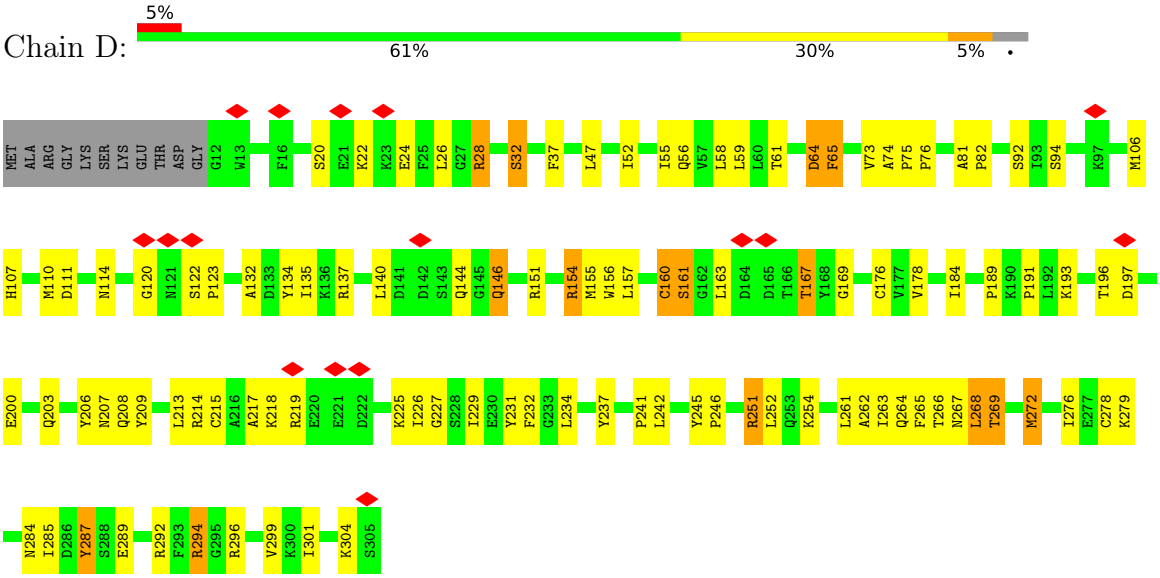
• Molecule 2: Na+,K+-ATPase beta subunit

Chain B:



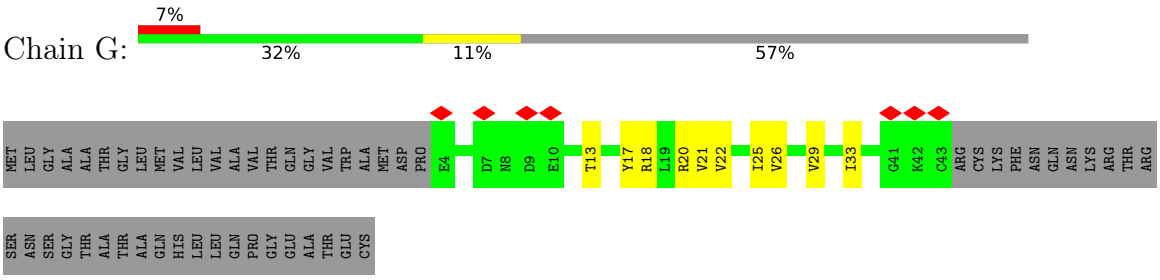
• Molecule 2: Na+,K+-ATPase beta subunit

Chain D:



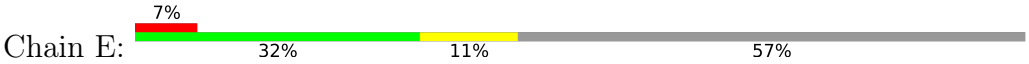
• Molecule 3: FXYD domain-containing ion transport regulator

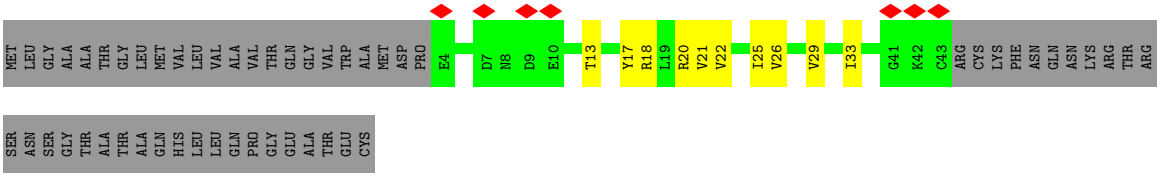
Chain G:



• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:

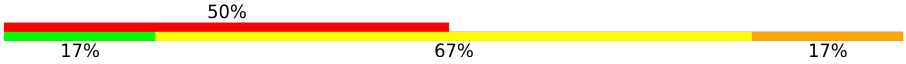


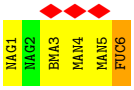


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

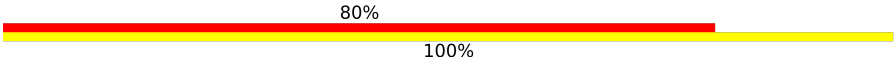
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	31645	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	258.24, 258.24, 258.24	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, PHD, NAG, CLR, FUC, NA, MG, MAN, BMA, ATP

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	0.28	0/7824	0.57	0/10613
1	C	0.28	0/7824	0.57	0/10613
2	B	0.29	0/2462	0.65	0/3317
2	D	0.29	0/2462	0.64	0/3317
3	E	0.26	0/315	0.52	0/427
3	G	0.27	0/315	0.52	0/427
All	All	0.28	0/21202	0.59	0/28714

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7687	0	7703	117	0
1	C	7687	0	7703	121	0
2	B	2399	0	2354	61	0
2	D	2399	0	2354	58	0
3	E	311	0	323	6	0
3	G	311	0	323	6	0
4	F	71	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	71	0	61	1	0
5	H	75	0	64	0	0
5	L	75	0	64	0	0
6	I	60	0	52	0	0
6	M	60	0	52	0	0
7	J	28	0	25	0	0
7	N	28	0	25	0	0
8	A	2	0	0	0	0
8	C	2	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	31	0	12	1	0
10	C	31	0	12	1	0
11	A	84	0	138	9	0
11	B	28	0	46	2	0
11	C	84	0	138	9	0
11	D	28	0	46	2	0
12	A	444	0	642	40	0
12	C	444	0	642	40	0
12	E	108	0	168	6	0
12	G	108	0	168	5	0
13	A	5	0	0	0	0
13	C	5	0	0	0	0
All	All	22668	0	23176	405	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 9.

The worst 5 of 405 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:THR:HB	1:A:961:GLU:HG3	1.62	0.82
11:C:1105:CLR:H273	12:C:1110:PCW:H442	1.62	0.81
11:A:1105:CLR:H273	12:A:1110:PCW:H442	1.62	0.81
1:C:814:THR:HB	1:C:961:GLU:HG3	1.62	0.81
12:A:1114:PCW:H462	11:C:1105:CLR:H241	1.64	0.78

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	990/1028 (96%)	918 (93%)	67 (7%)	5 (0%)	29	66
1	C	990/1028 (96%)	918 (93%)	67 (7%)	5 (0%)	29	66
2	B	292/305 (96%)	257 (88%)	34 (12%)	1 (0%)	41	74
2	D	292/305 (96%)	257 (88%)	34 (12%)	1 (0%)	41	74
3	E	38/94 (40%)	33 (87%)	5 (13%)	0	100	100
3	G	38/94 (40%)	33 (87%)	5 (13%)	0	100	100
All	All	2640/2854 (92%)	2416 (92%)	212 (8%)	12 (0%)	32	66

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	988	TRP
1	C	988	TRP
1	A	985	PRO
2	B	155	MET
1	C	985	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	A	840/868 (97%)	766 (91%)	74 (9%)	10	38
1	C	840/868 (97%)	766 (91%)	74 (9%)	10	38
2	B	258/266 (97%)	221 (86%)	37 (14%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	258/266 (97%)	221 (86%)	37 (14%)	3	19
3	E	33/75 (44%)	31 (94%)	2 (6%)	18	50
3	G	33/75 (44%)	31 (94%)	2 (6%)	18	50
All	All	2262/2418 (94%)	2036 (90%)	226 (10%)	11	32

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	63	LEU
2	D	289	GLU
1	C	367	LEU
2	D	285	ILE
2	D	146	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	241	ASN
1	C	474	ASN
1	C	434	GLN
1	C	540	ASN
1	A	540	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PHD	C	376	1,8	9,11,12	1.98	1 (11%)	10,15,17	1.17	2 (20%)
1	PHD	A	376	1,8	9,11,12	1.97	1 (11%)	10,15,17	1.17	2 (20%)

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
1	PHD	C	376	1,8	-	2/8/11/13	-
1	PHD	A	376	1,8	-	2/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	PHD	P-OD1	-5.24	1.51	1.59
1	A	376	PHD	P-OD1	-5.22	1.51	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	376	PHD	OD1-CG-CB	2.16	117.05	111.11
1	A	376	PHD	OD1-CG-CB	2.15	117.04	111.11
1	A	376	PHD	CA-CB-CG	2.14	117.35	112.86
1	C	376	PHD	CA-CB-CG	2.13	117.33	112.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	376	PHD	CA-CB-CG-OD1
1	C	376	PHD	CA-CB-CG-OD1
1	A	376	PHD	CA-CB-CG-OD2
1	C	376	PHD	CA-CB-CG-OD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

38 monosaccharides 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	$\#\|Z\| > 2$
4	NAG	F	1	4,2	14,14,15	1.14	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	F	2	4	14,14,15	0.21	0	17,19,21	0.58	1 (5%)
4	BMA	F	3	4	11,11,12	0.76	0	15,15,17	1.35	2 (13%)
4	MAN	F	4	4	11,11,12	0.74	0	15,15,17	0.98	2 (13%)
4	MAN	F	5	4	11,11,12	0.70	0	15,15,17	0.92	2 (13%)
4	FUC	F	6	4	10,10,11	1.06	1 (10%)	14,14,16	0.74	0
5	NAG	H	1	5,2	14,14,15	0.57	0	17,19,21	1.14	2 (11%)
5	NAG	H	2	5	14,14,15	0.33	0	17,19,21	1.48	2 (11%)
5	BMA	H	3	5	11,11,12	1.26	1 (9%)	15,15,17	1.08	1 (6%)
5	MAN	H	4	5	11,11,12	1.44	3 (27%)	15,15,17	1.40	2 (13%)
5	NAG	H	5	5	14,14,15	0.66	0	17,19,21	0.80	1 (5%)
5	MAN	H	6	5	11,11,12	0.73	0	15,15,17	0.95	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.79	1 (7%)	17,19,21	1.57	1 (5%)
6	NAG	I	2	6	14,14,15	0.19	0	17,19,21	0.61	1 (5%)
6	BMA	I	3	6	11,11,12	0.58	0	15,15,17	1.30	2 (13%)
6	MAN	I	4	6	11,11,12	0.68	0	15,15,17	0.96	2 (13%)
6	FUC	I	5	6	10,10,11	1.02	1 (10%)	14,14,16	0.71	0
7	NAG	J	1	2,7	14,14,15	0.55	0	17,19,21	0.61	0
7	NAG	J	2	7	14,14,15	0.18	0	17,19,21	0.37	0
4	NAG	K	1	4,2	14,14,15	1.15	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	K	2	4	14,14,15	0.21	0	17,19,21	0.58	0
4	BMA	K	3	4	11,11,12	0.76	0	15,15,17	1.35	2 (13%)
4	MAN	K	4	4	11,11,12	0.74	0	15,15,17	0.99	2 (13%)
4	MAN	K	5	4	11,11,12	0.69	0	15,15,17	0.92	2 (13%)
4	FUC	K	6	4	10,10,11	1.07	1 (10%)	14,14,16	0.74	0
5	NAG	L	1	5,2	14,14,15	0.57	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	L	2	5	14,14,15	0.33	0	17,19,21	1.48	2 (11%)
5	BMA	L	3	5	11,11,12	1.26	1 (9%)	15,15,17	1.08	1 (6%)
5	MAN	L	4	5	11,11,12	1.44	3 (27%)	15,15,17	1.40	2 (13%)
5	NAG	L	5	5	14,14,15	0.65	0	17,19,21	0.81	1 (5%)
5	MAN	L	6	5	11,11,12	0.75	0	15,15,17	0.95	2 (13%)
6	NAG	M	1	6,2	14,14,15	0.78	1 (7%)	17,19,21	1.56	1 (5%)
6	NAG	M	2	6	14,14,15	0.19	0	17,19,21	0.61	1 (5%)
6	BMA	M	3	6	11,11,12	0.58	0	15,15,17	1.29	2 (13%)
6	MAN	M	4	6	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
6	FUC	M	5	6	10,10,11	1.02	1 (10%)	14,14,16	0.71	0
7	NAG	N	1	2,7	14,14,15	0.55	0	17,19,21	0.61	0
7	NAG	N	2	7	14,14,15	0.18	0	17,19,21	0.38	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
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	FUC	F	6	4	-	-	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	BMA	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	-	4/6/23/26	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	1/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	FUC	I	5	6	-	-	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	1/2/19/22	0/1/1/1
4	MAN	K	4	4	-	0/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
4	FUC	K	6	4	-	-	0/1/1/1
5	NAG	L	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	3/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	0/2/19/22	0/1/1/1
5	NAG	L	5	5	-	4/6/23/26	0/1/1/1
5	MAN	L	6	5	-	2/2/19/22	0/1/1/1
6	NAG	M	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	BMA	M	3	6	-	1/2/19/22	0/1/1/1
6	MAN	M	4	6	-	0/2/19/22	0/1/1/1
6	FUC	M	5	6	-	-	0/1/1/1
7	NAG	N	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1	NAG	O5-C1	3.85	1.49	1.43
4	F	1	NAG	O5-C1	3.83	1.49	1.43
5	H	4	MAN	O2-C2	3.04	1.49	1.43
5	L	4	MAN	O2-C2	3.04	1.49	1.43
4	K	6	FUC	O5-C1	-2.81	1.39	1.43

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	1	NAG	C1-O5-C5	5.99	120.31	112.19
6	M	1	NAG	C1-O5-C5	5.95	120.25	112.19
4	K	1	NAG	C1-O5-C5	4.68	118.54	112.19
4	F	1	NAG	C1-O5-C5	4.68	118.53	112.19
5	L	2	NAG	C1-O5-C5	4.46	118.23	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C3-C2-N2-C7
5	L	2	NAG	C3-C2-N2-C7
5	L	5	NAG	O5-C5-C6-O6
5	H	5	NAG	O5-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6

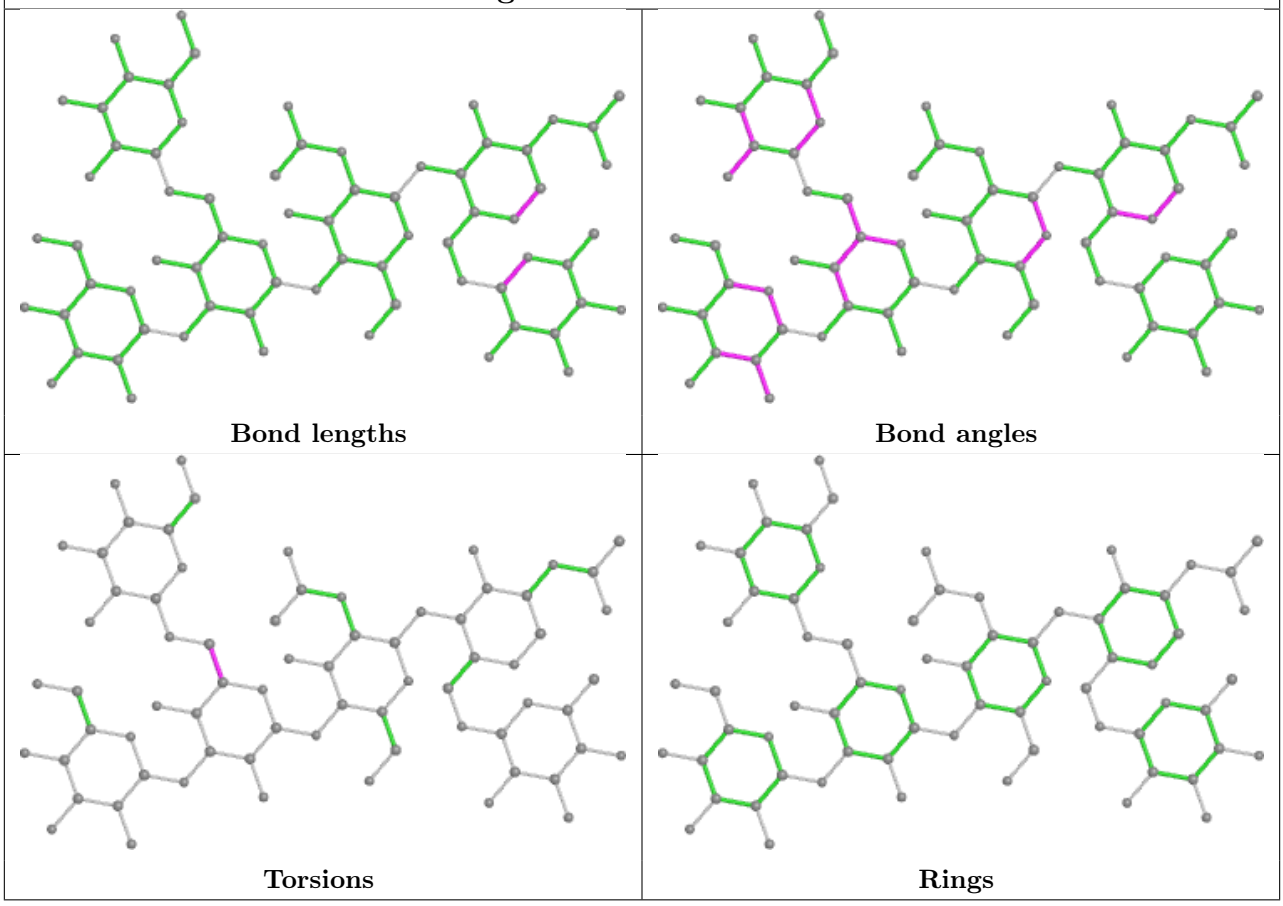
There are no ring outliers.

2 monomers are involved in 2 short contacts:

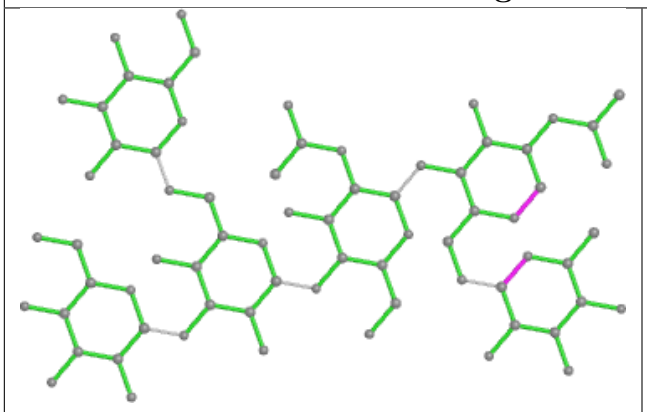
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6	FUC	1	0
4	K	6	FUC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

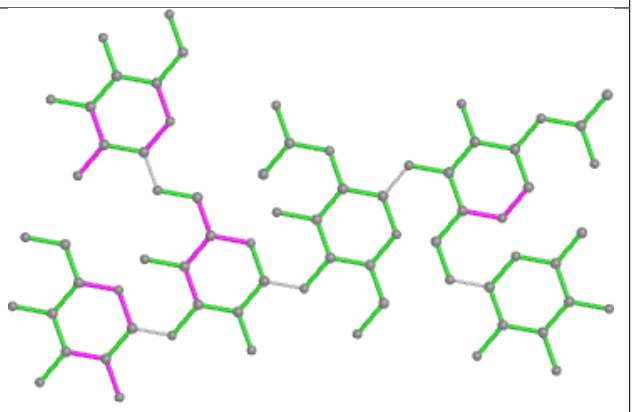
Oligosaccharide Chain F



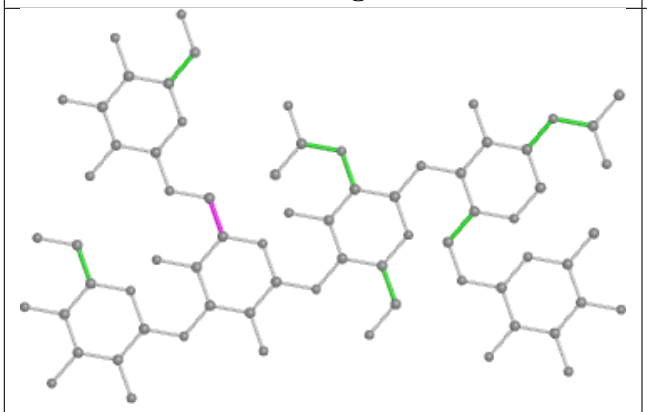
Oligosaccharide Chain K



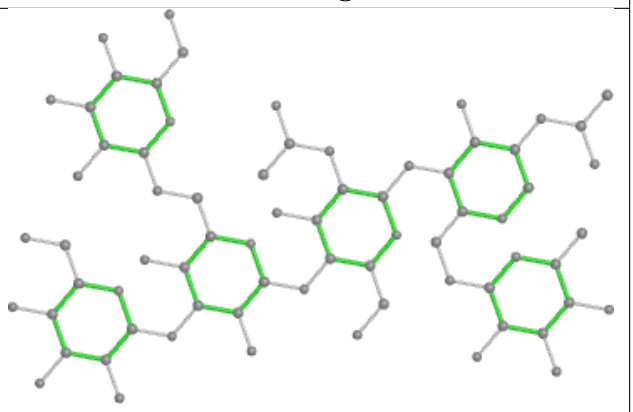
Bond lengths



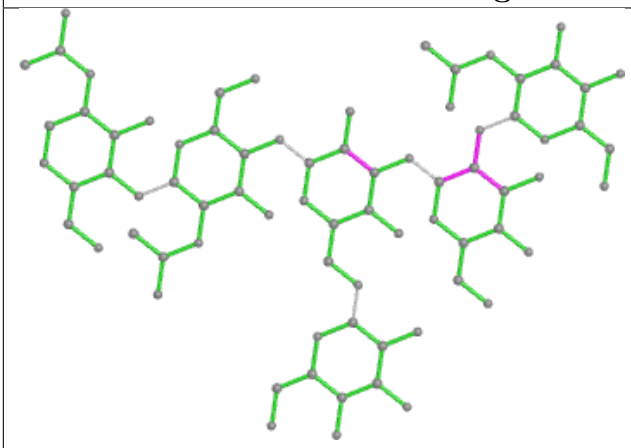
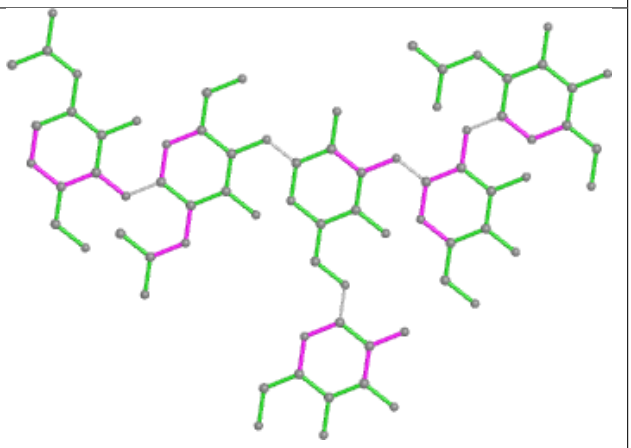
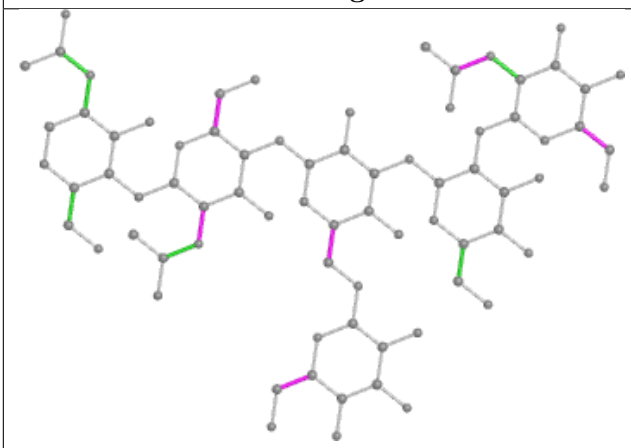
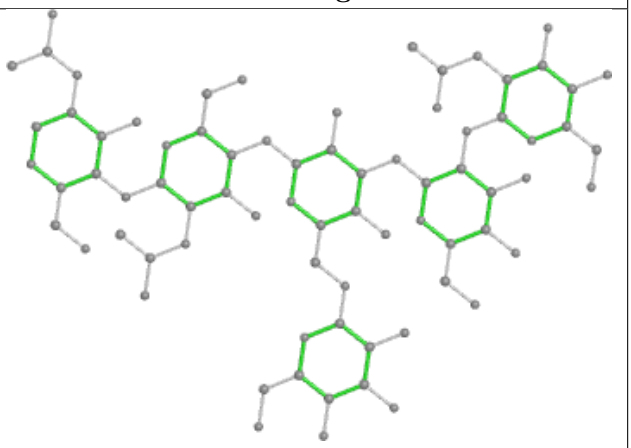
Bond angles

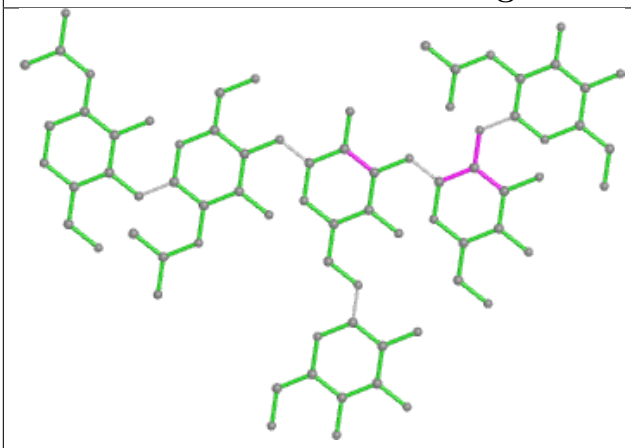
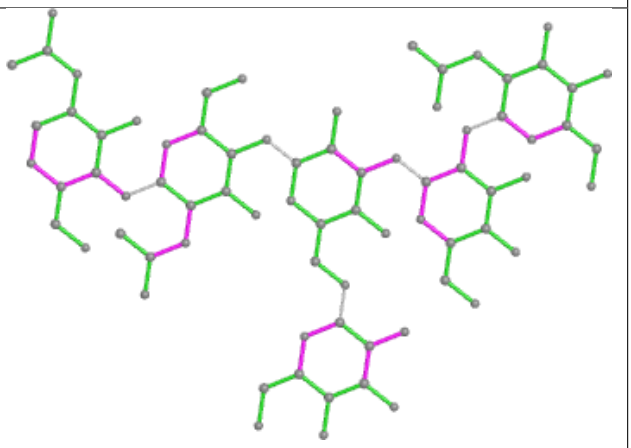
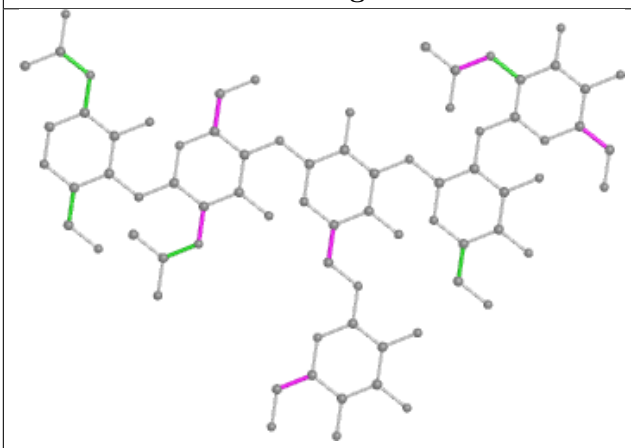
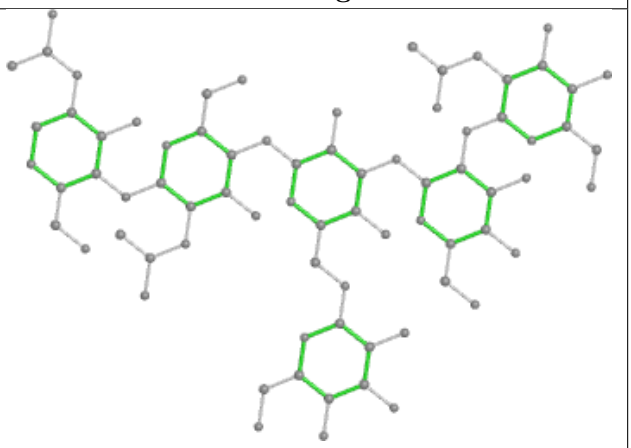


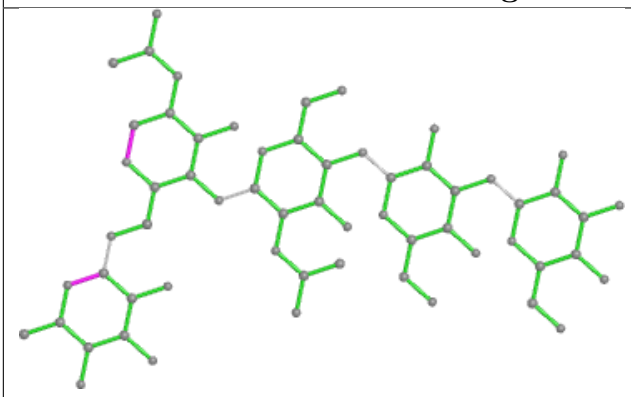
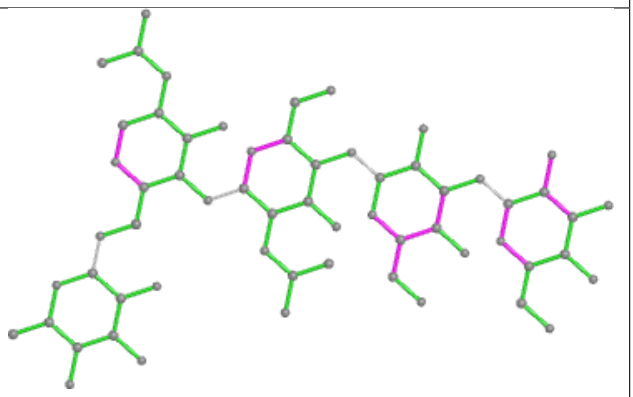
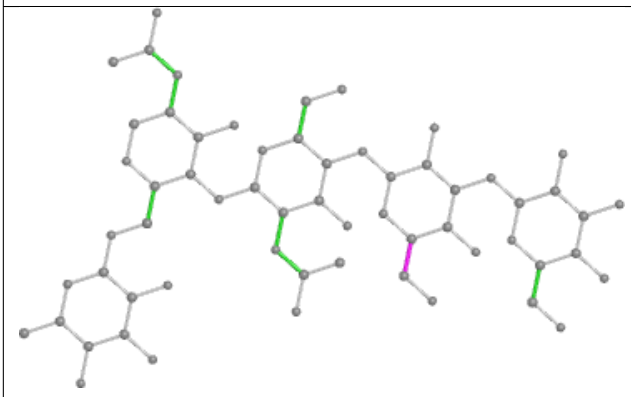
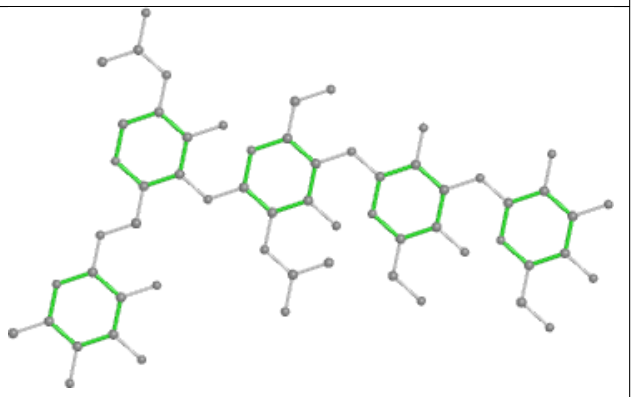
Torsions

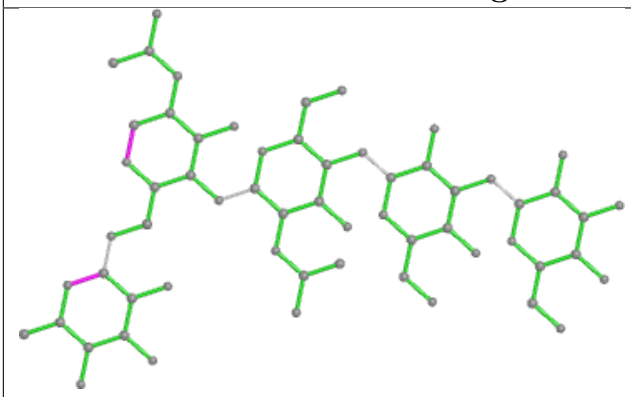
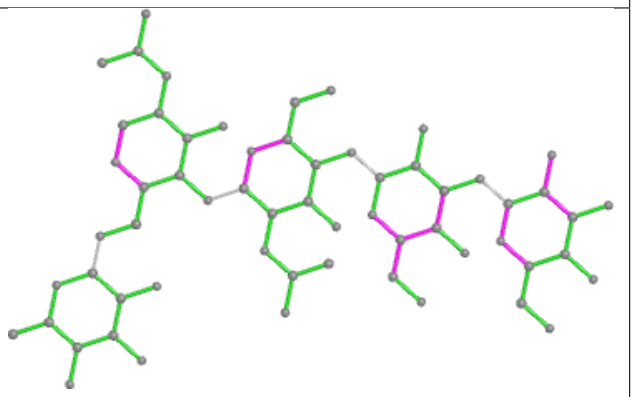
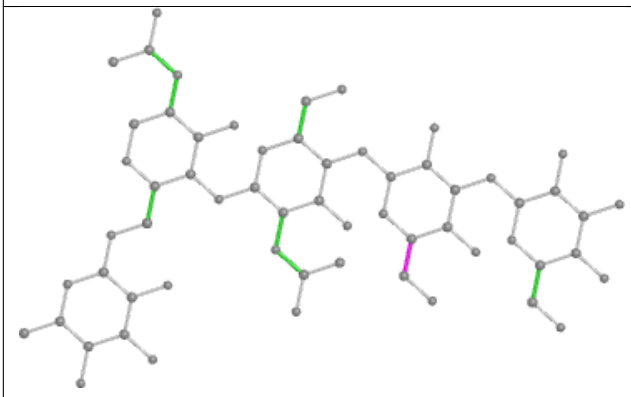
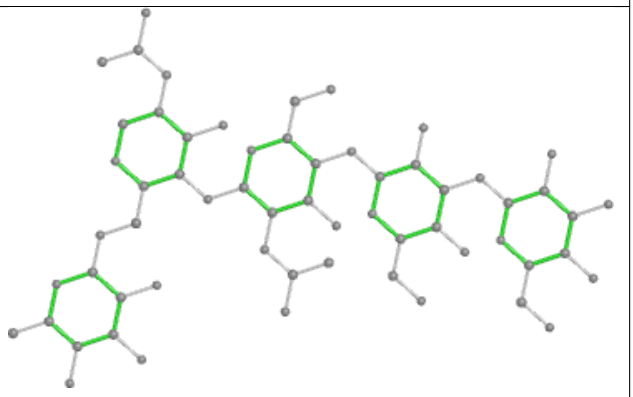


Rings

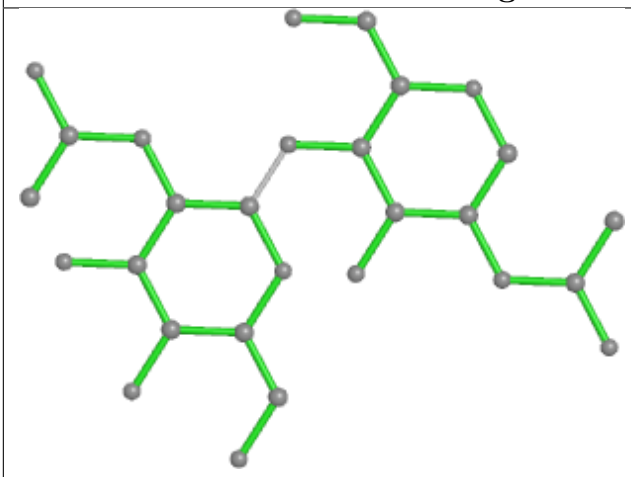
Oligosaccharide Chain H	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain L	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

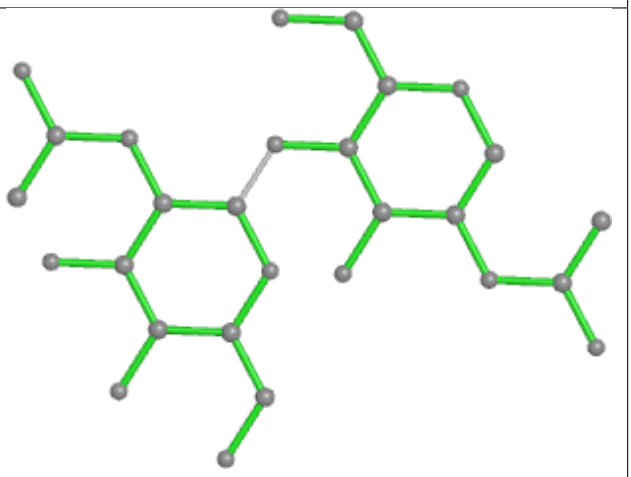
Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

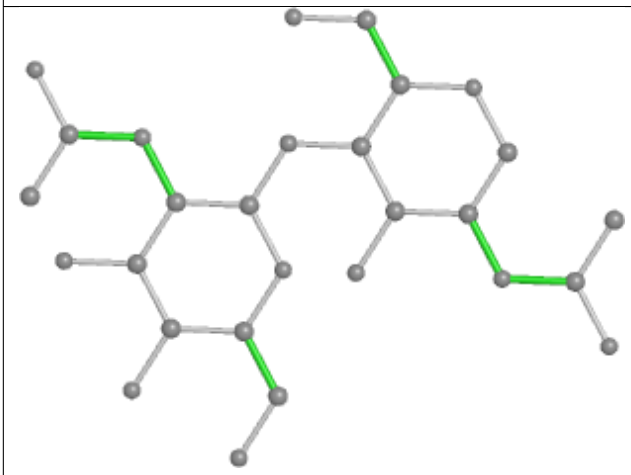
Oligosaccharide Chain J



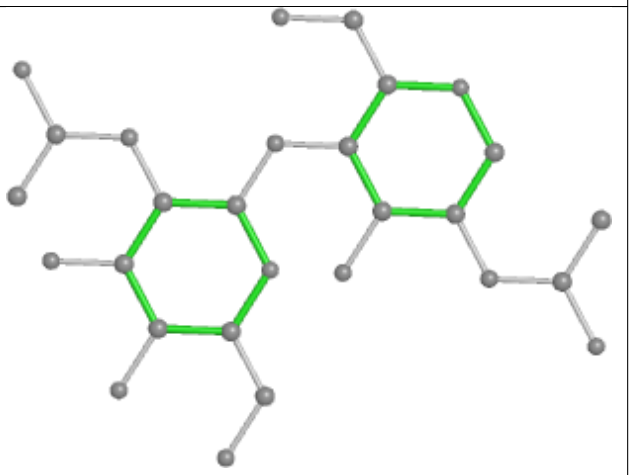
Bond lengths



Bond angles

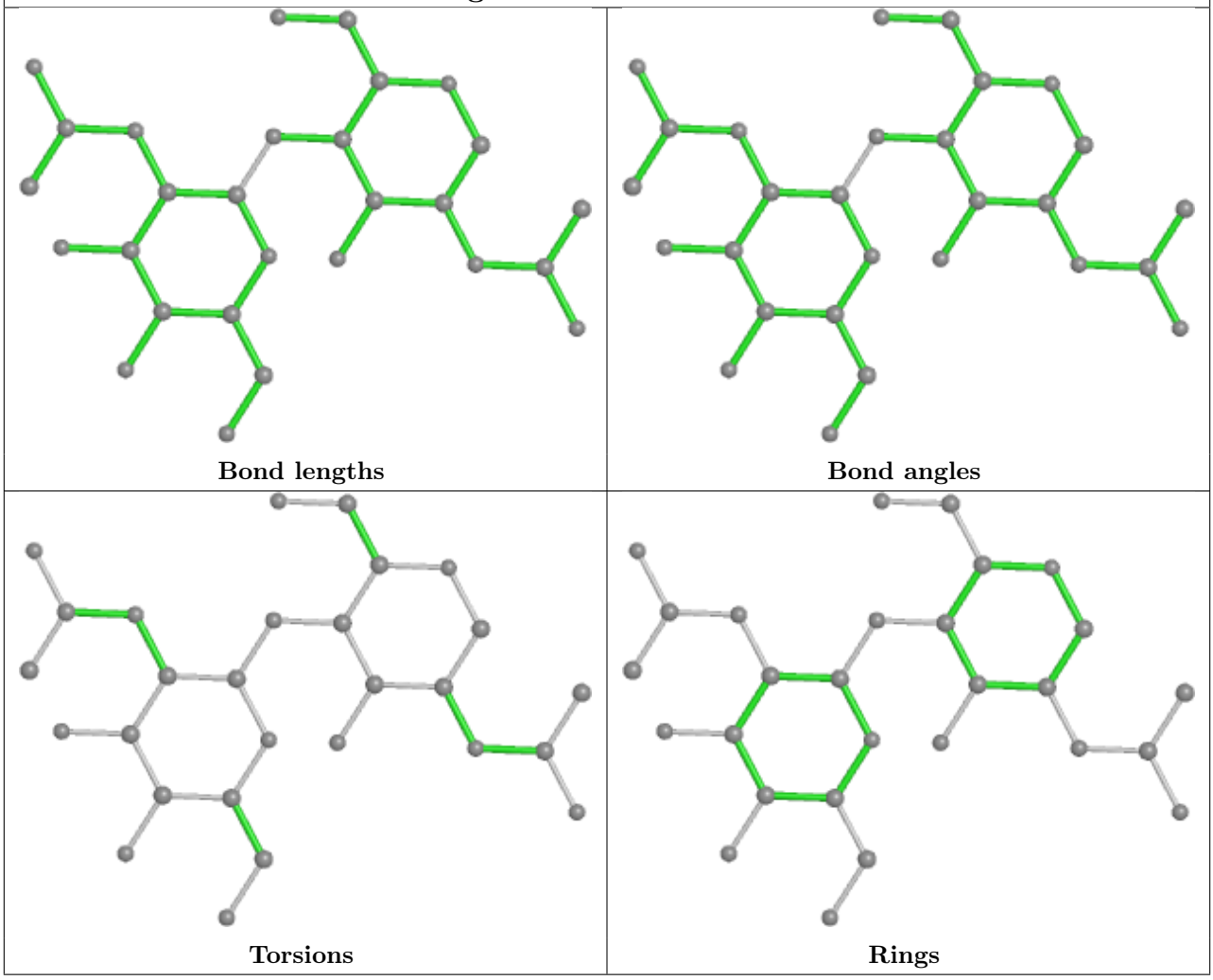


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 6 are monoatomic - leaving 34 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	$\#\|Z\| > 2$
11	CLR	C	1105	-	31,31,31	1.22	4 (12%)	48,48,48	1.56	11 (22%)
11	CLR	A	1117	-	31,31,31	1.20	3 (9%)	48,48,48	1.51	9 (18%)
12	PCW	C	1111	-	53,53,53	0.95	2 (3%)	59,61,61	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CLR	D	401	-	31,31,31	1.24	4 (12%)	48,48,48	1.55	8 (16%)
12	PCW	A	1112	-	53,53,53	0.98	2 (3%)	59,61,61	0.71	0
12	PCW	A	1111	-	53,53,53	0.95	2 (3%)	59,61,61	0.80	0
11	CLR	A	1105	-	31,31,31	1.23	4 (12%)	48,48,48	1.56	10 (20%)
12	PCW	C	1112	-	53,53,53	0.98	2 (3%)	59,61,61	0.71	0
11	CLR	C	1117	-	31,31,31	1.20	2 (6%)	48,48,48	1.51	9 (18%)
12	PCW	C	1107	-	21,21,53	0.86	0	27,29,61	1.18	3 (11%)
12	PCW	A	1114	-	53,53,53	0.99	2 (3%)	59,61,61	0.68	0
11	CLR	C	1106	-	31,31,31	1.23	5 (16%)	48,48,48	1.58	10 (20%)
12	PCW	C	1114	-	53,53,53	0.99	2 (3%)	59,61,61	0.68	0
11	CLR	B	401	-	31,31,31	1.23	4 (12%)	48,48,48	1.54	8 (16%)
12	PCW	C	1116	-	53,53,53	0.98	2 (3%)	59,61,61	0.68	0
12	PCW	C	1108	-	21,21,53	0.87	0	27,29,61	1.18	3 (11%)
12	PCW	A	1109	-	53,53,53	0.96	2 (3%)	59,61,61	0.72	0
12	PCW	E	102	-	53,53,53	0.97	2 (3%)	59,61,61	0.78	0
12	PCW	G	101	-	53,53,53	0.98	2 (3%)	59,61,61	0.75	0
12	PCW	C	1109	-	53,53,53	0.97	2 (3%)	59,61,61	0.72	0
12	PCW	A	1107	-	21,21,53	0.87	0	27,29,61	1.19	3 (11%)
12	PCW	C	1115	-	21,21,53	0.86	0	27,29,61	1.32	3 (11%)
12	PCW	C	1113	-	53,53,53	0.97	2 (3%)	59,61,61	0.73	0
12	PCW	A	1116	-	53,53,53	0.98	2 (3%)	59,61,61	0.68	0
11	CLR	A	1106	-	31,31,31	1.24	5 (16%)	48,48,48	1.58	10 (20%)
12	PCW	A	1108	-	21,21,53	0.87	0	27,29,61	1.18	3 (11%)
12	PCW	G	102	-	53,53,53	0.97	2 (3%)	59,61,61	0.78	0
10	ATP	A	1104	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
10	ATP	C	1104	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
12	PCW	A	1113	-	53,53,53	0.98	2 (3%)	59,61,61	0.73	0
12	PCW	A	1115	-	21,21,53	0.86	0	27,29,61	1.32	3 (11%)
12	PCW	A	1110	-	53,53,53	0.98	2 (3%)	59,61,61	0.76	0
12	PCW	C	1110	-	53,53,53	0.98	2 (3%)	59,61,61	0.76	0
12	PCW	E	101	-	53,53,53	0.98	2 (3%)	59,61,61	0.75	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
11	CLR	C	1105	-	-	0/10/68/68	0/4/4/4
11	CLR	A	1117	-	-	1/10/68/68	0/4/4/4
12	PCW	C	1111	-	-	13/57/57/57	-
11	CLR	D	401	-	-	0/10/68/68	0/4/4/4
12	PCW	A	1112	-	-	22/57/57/57	-
12	PCW	A	1111	-	-	13/57/57/57	-
11	CLR	A	1105	-	-	0/10/68/68	0/4/4/4
12	PCW	C	1112	-	-	22/57/57/57	-
11	CLR	C	1117	-	-	1/10/68/68	0/4/4/4
12	PCW	C	1107	-	-	6/23/23/57	-
12	PCW	A	1114	-	-	17/57/57/57	-
11	CLR	C	1106	-	-	0/10/68/68	0/4/4/4
12	PCW	C	1114	-	-	17/57/57/57	-
11	CLR	B	401	-	-	0/10/68/68	0/4/4/4
12	PCW	C	1116	-	-	22/57/57/57	-
12	PCW	C	1108	-	-	14/23/23/57	-
12	PCW	A	1109	-	-	21/57/57/57	-
12	PCW	E	102	-	-	22/57/57/57	-
12	PCW	G	101	-	-	19/57/57/57	-
12	PCW	C	1109	-	-	21/57/57/57	-
12	PCW	A	1107	-	-	6/23/23/57	-
12	PCW	C	1115	-	-	9/23/23/57	-
12	PCW	C	1113	-	-	19/57/57/57	-
12	PCW	A	1116	-	-	22/57/57/57	-
11	CLR	A	1106	-	-	0/10/68/68	0/4/4/4
12	PCW	A	1108	-	-	14/23/23/57	-
12	PCW	G	102	-	-	22/57/57/57	-
10	ATP	A	1104	-	-	5/18/38/38	0/3/3/3
10	ATP	C	1104	-	-	5/18/38/38	0/3/3/3
12	PCW	A	1113	-	-	19/57/57/57	-
12	PCW	A	1115	-	-	9/23/23/57	-
12	PCW	A	1110	-	-	18/57/57/57	-
12	PCW	C	1110	-	-	18/57/57/57	-
12	PCW	E	101	-	-	18/57/57/57	-

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1114	PCW	C40-C39	3.94	1.54	1.31
12	C	1114	PCW	C40-C39	3.93	1.54	1.31
12	A	1110	PCW	C20-C19	3.90	1.54	1.31
12	C	1110	PCW	C20-C19	3.90	1.54	1.31
12	E	101	PCW	C40-C39	3.88	1.54	1.31

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	1115	PCW	C2-O2-C31	-4.62	109.28	117.90
12	C	1115	PCW	C2-O2-C31	-4.61	109.30	117.90
12	A	1108	PCW	C2-O2-C31	-4.39	109.72	117.90
12	C	1108	PCW	C2-O2-C31	-4.35	109.78	117.90
11	C	1106	CLR	C7-C8-C9	3.85	114.38	109.71

There are no chirality outliers.

5 of 415 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1104	ATP	PB-O3A-PA-O5'
10	A	1104	ATP	C5'-O5'-PA-O1A
10	C	1104	ATP	PB-O3A-PA-O5'
10	C	1104	ATP	C5'-O5'-PA-O1A
12	A	1108	PCW	C4-O4P-P-O2P

There are no ring outliers.

30 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1105	CLR	5	0
11	A	1117	CLR	1	0
12	C	1111	PCW	7	0
11	D	401	CLR	2	0
12	A	1112	PCW	2	0
12	A	1111	PCW	7	0
11	A	1105	CLR	5	0
12	C	1112	PCW	2	0
11	C	1117	CLR	1	0
12	A	1114	PCW	13	0
11	C	1106	CLR	3	0
12	C	1114	PCW	14	0
11	B	401	CLR	2	0

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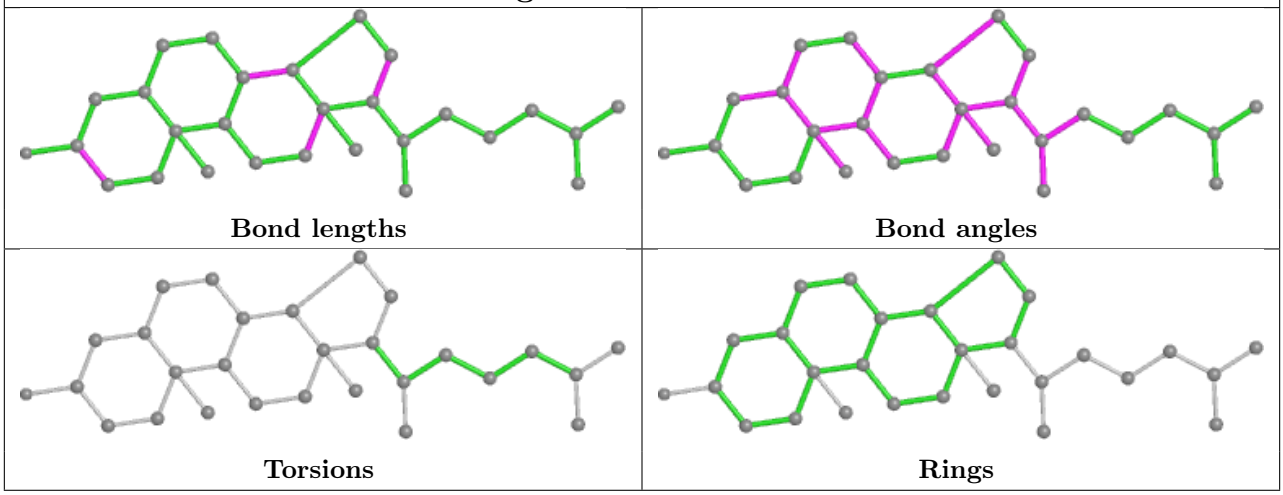
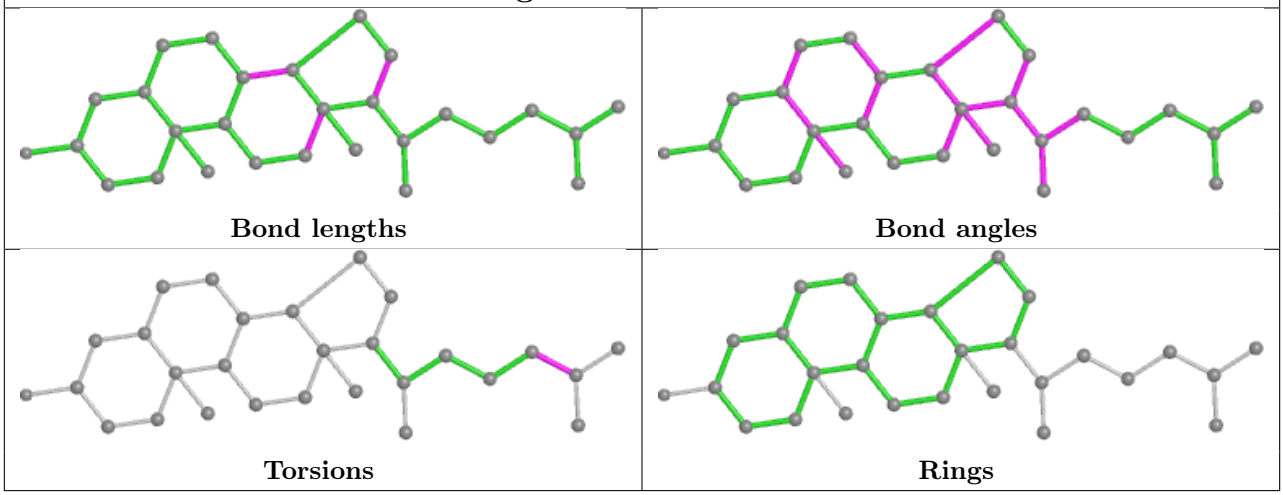
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	1116	PCW	3	0
12	A	1109	PCW	7	0
12	E	102	PCW	4	0
12	G	101	PCW	2	0
12	C	1109	PCW	7	0
12	C	1115	PCW	1	0
12	C	1113	PCW	3	0
12	A	1116	PCW	3	0
11	A	1106	CLR	3	0
12	G	102	PCW	3	0
10	A	1104	ATP	1	0
10	C	1104	ATP	1	0
12	A	1113	PCW	4	0
12	A	1115	PCW	1	0
12	A	1110	PCW	4	0
12	C	1110	PCW	4	0
12	E	101	PCW	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.

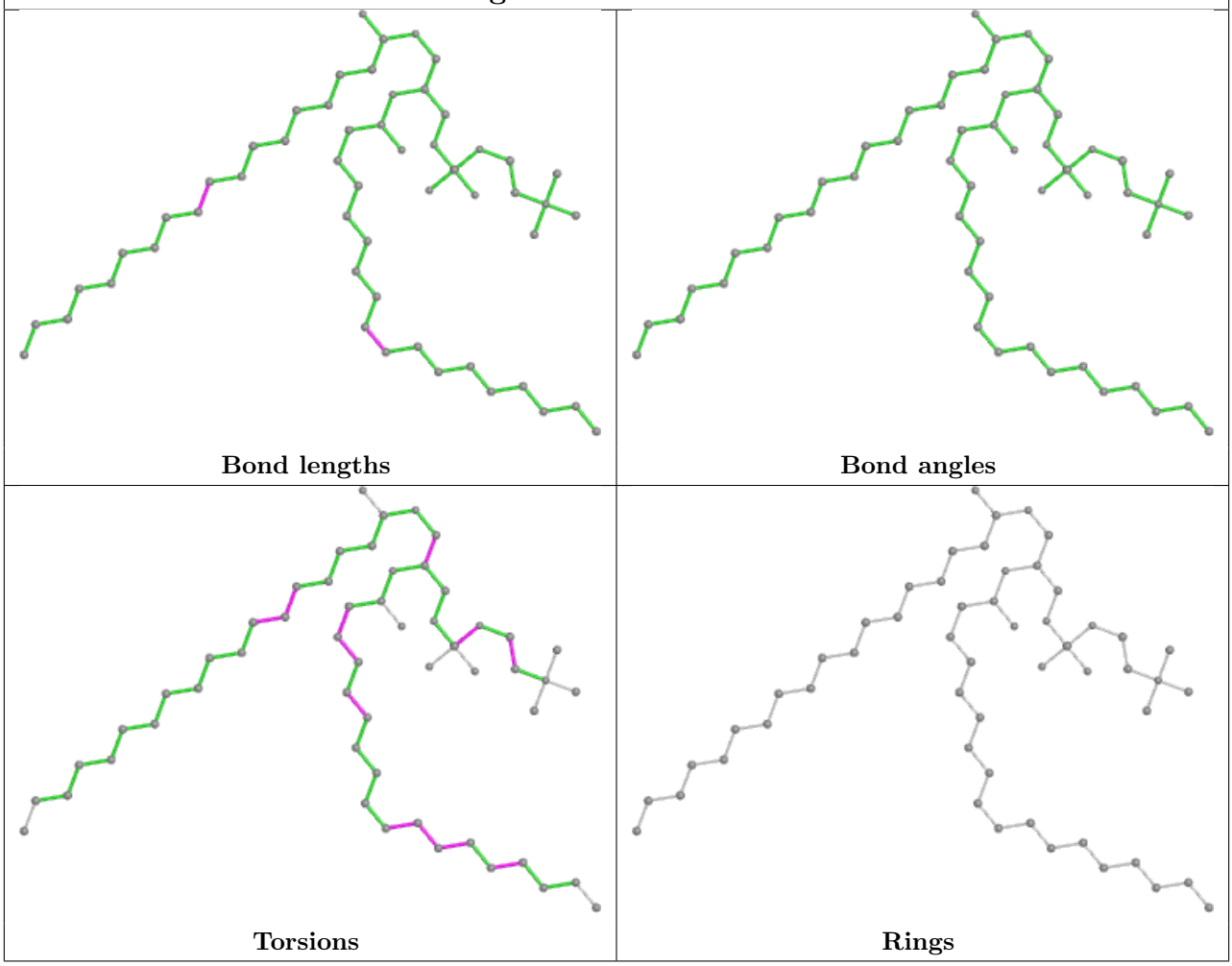
Ligand CLR C 1105



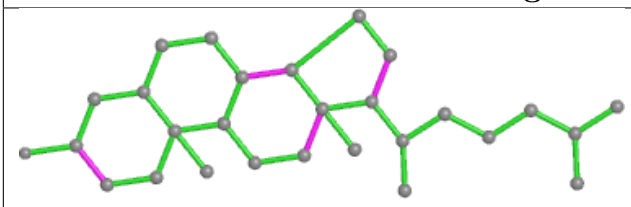
Ligand CLR A 1117



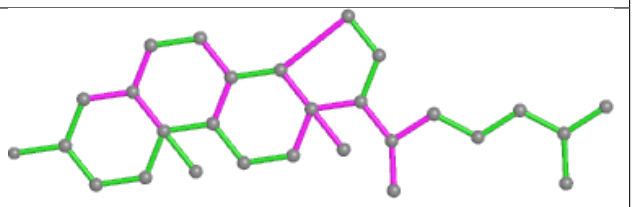
Ligand PCW C 1111



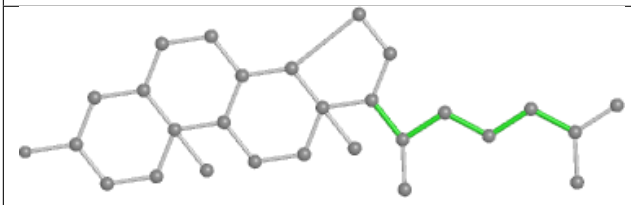
Ligand CLR D 401



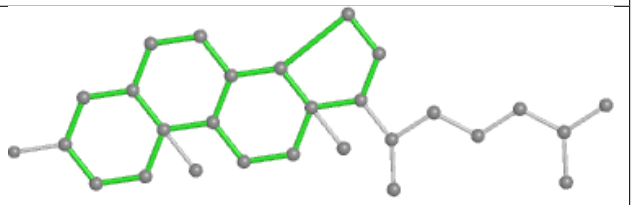
Bond lengths



Bond angles

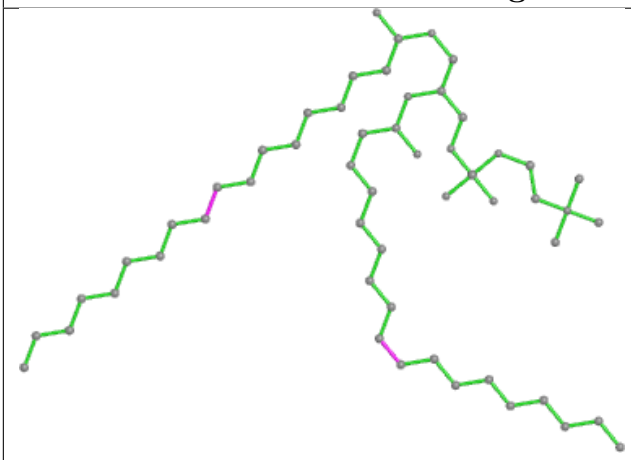


Torsions

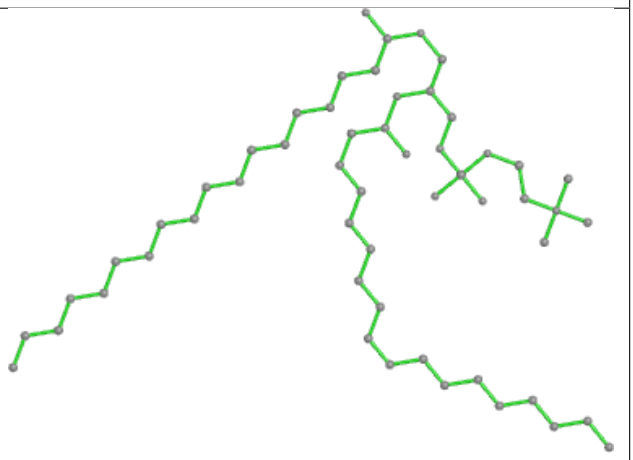


Rings

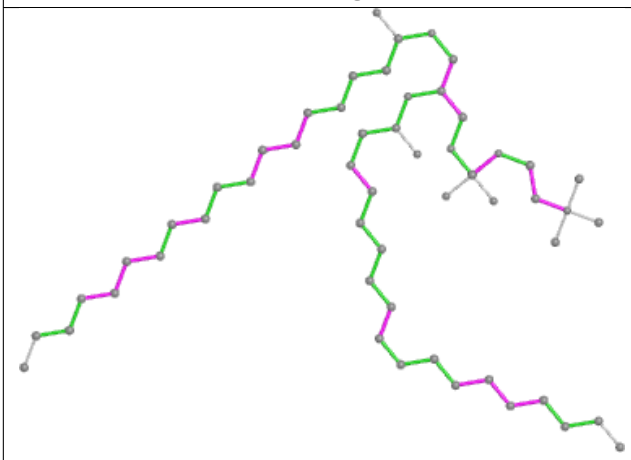
Ligand PCW A 1112



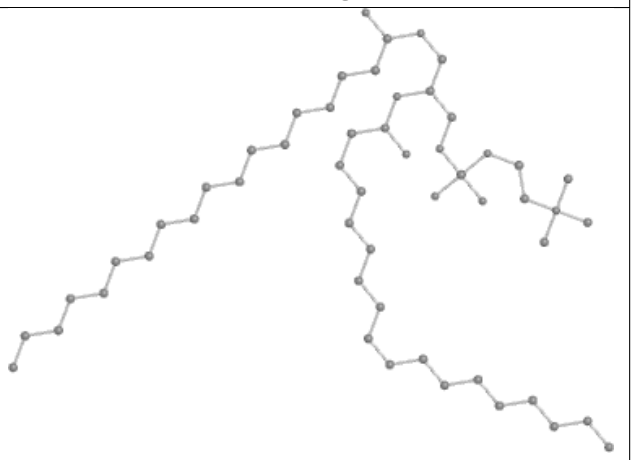
Bond lengths



Bond angles

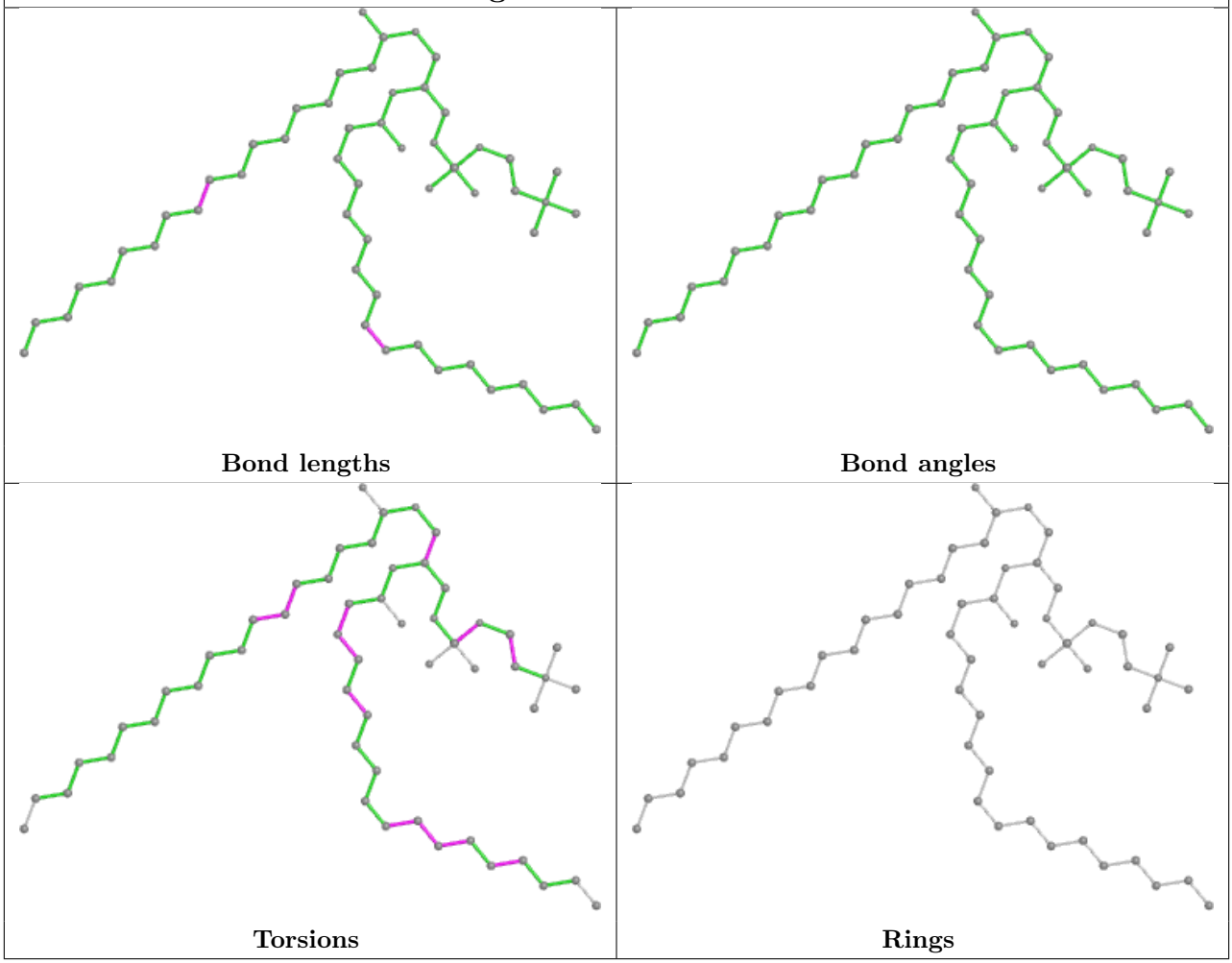


Torsions

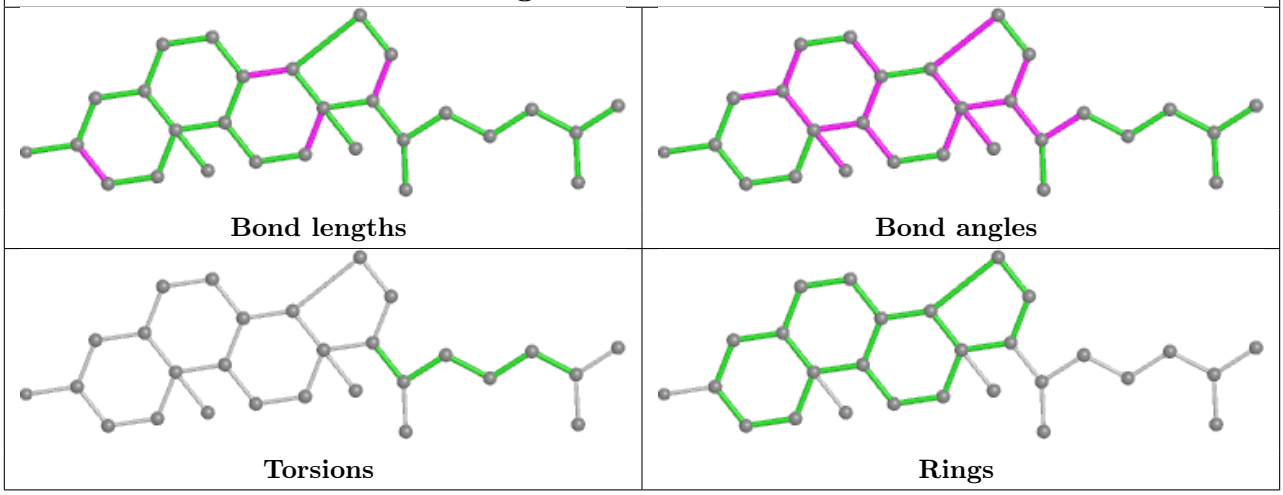


Rings

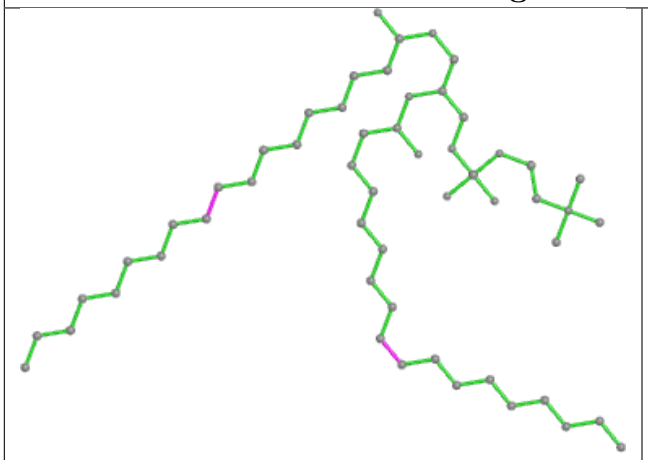
Ligand PCW A 1111



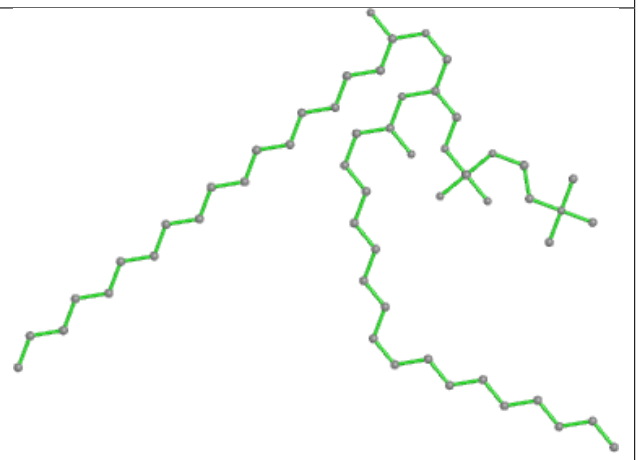
Ligand CLR A 1105



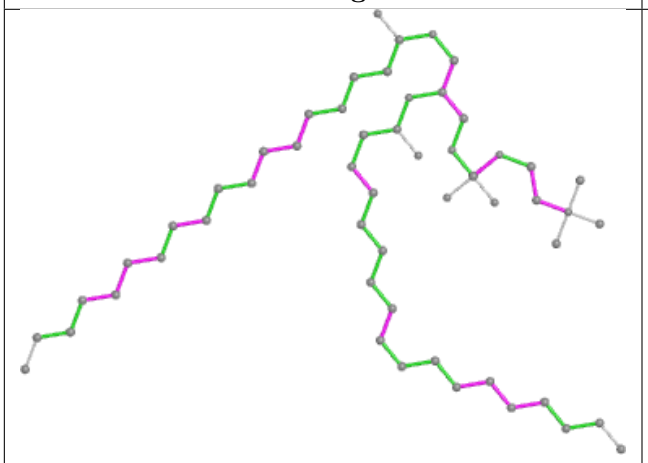
Ligand PCW C 1112



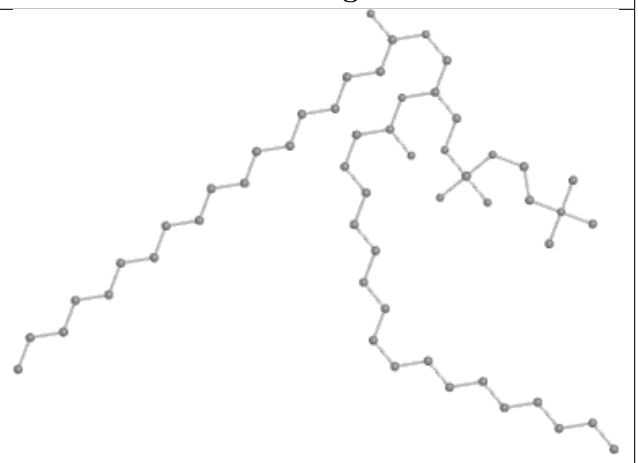
Bond lengths



Bond angles

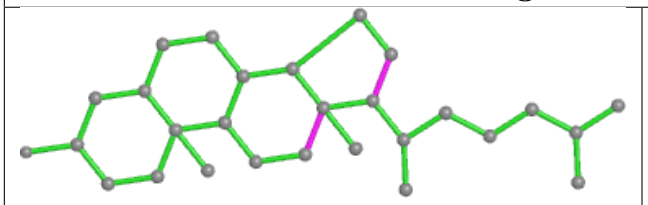


Torsions

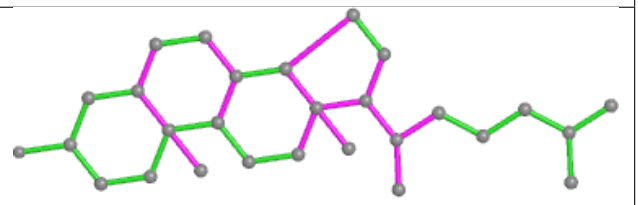


Rings

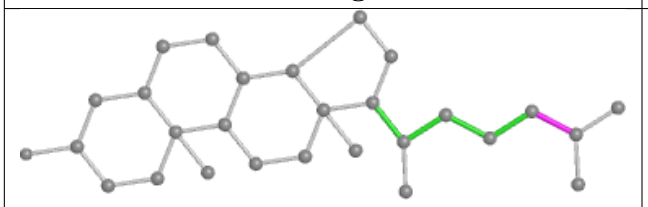
Ligand CLR C 1117



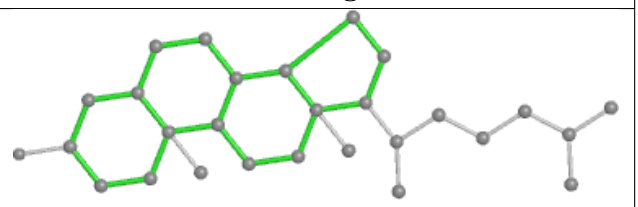
Bond lengths



Bond angles

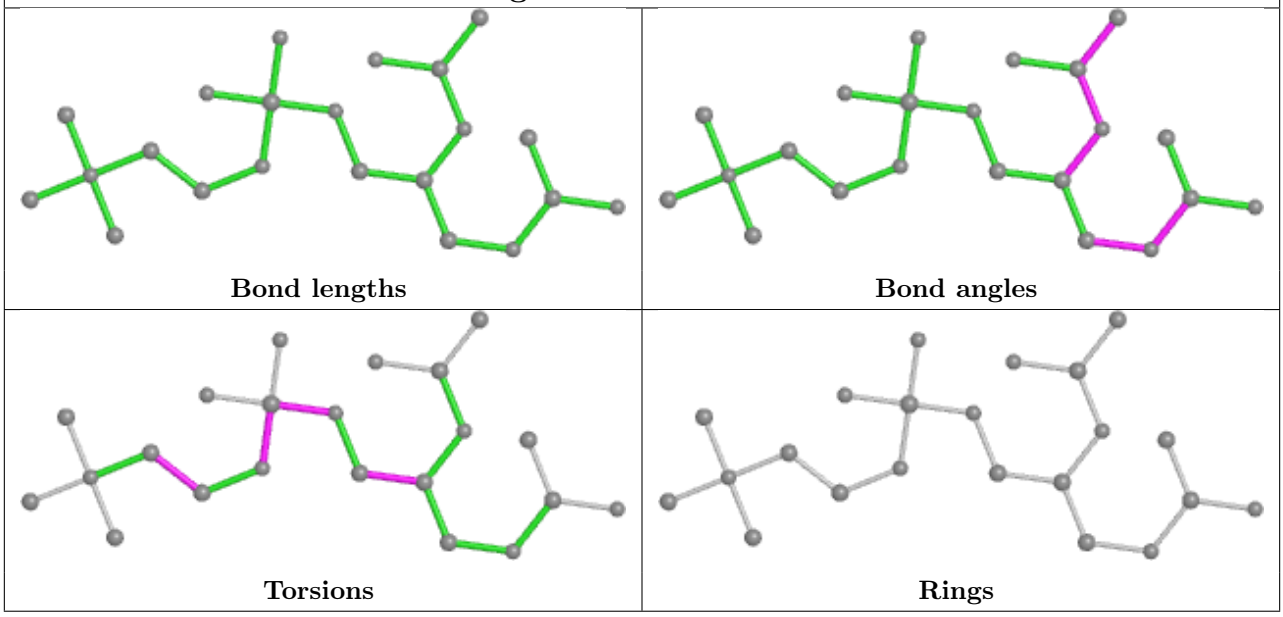


Torsions

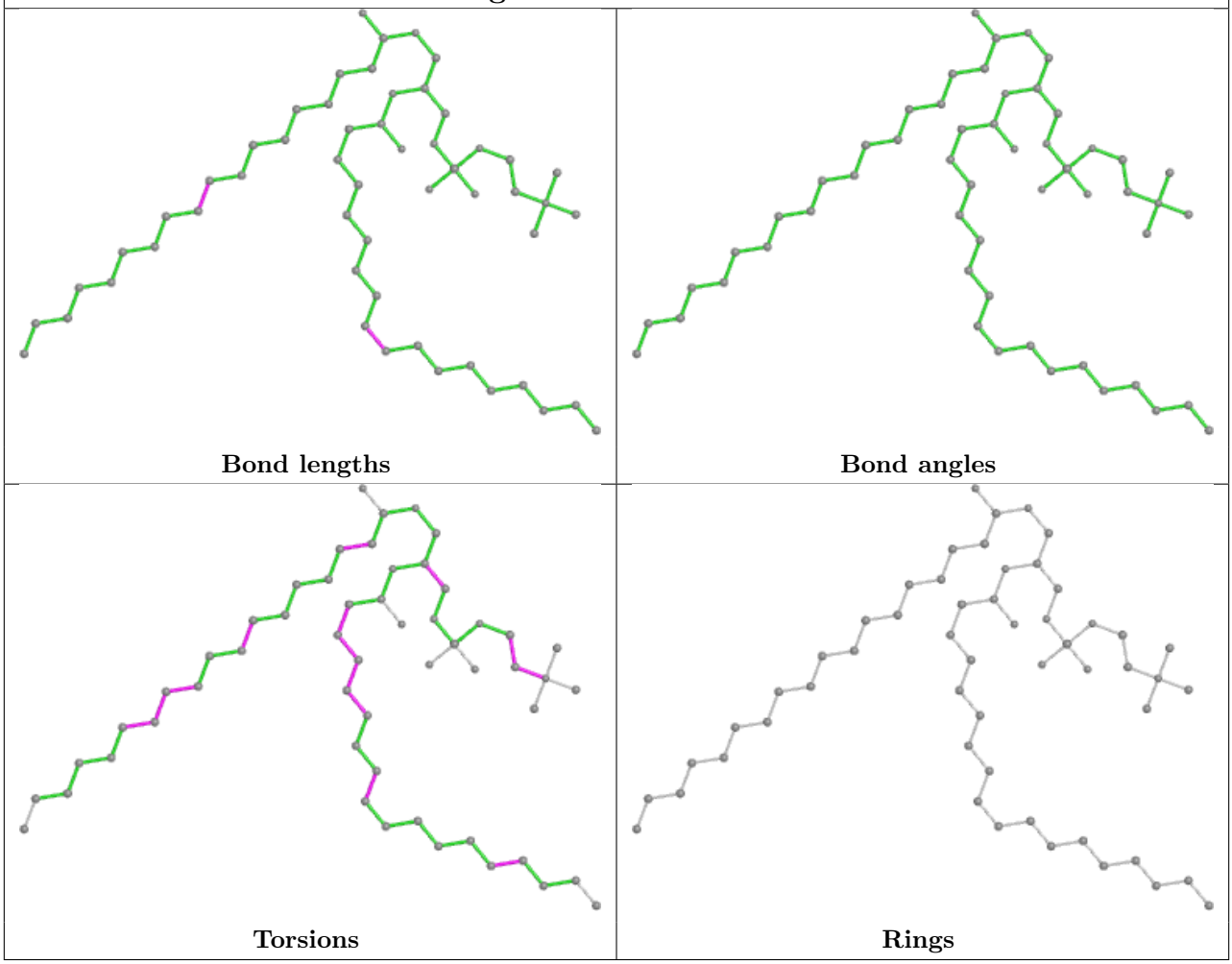


Rings

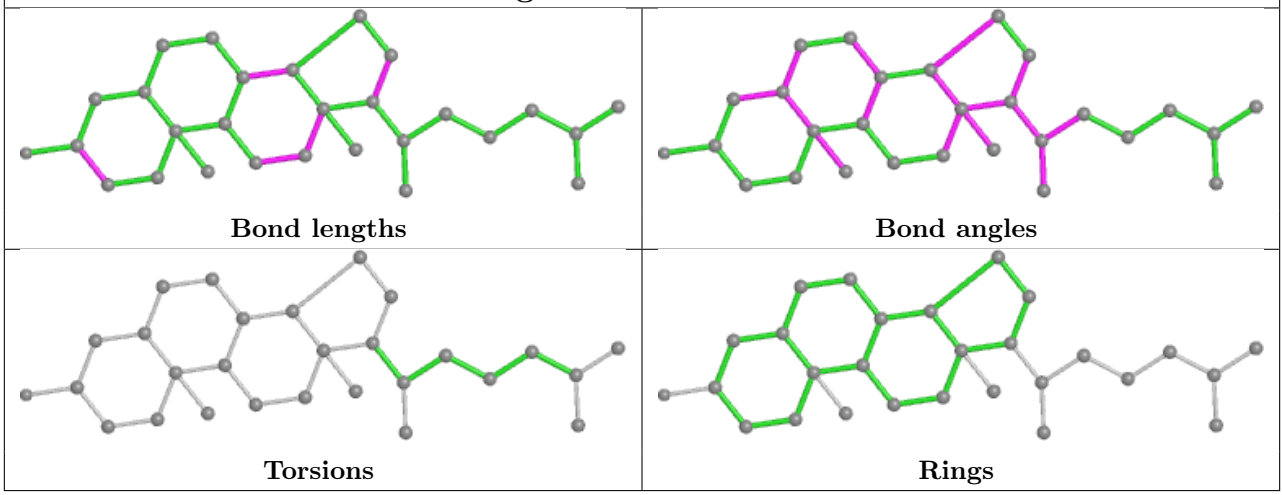
Ligand PCW C 1107



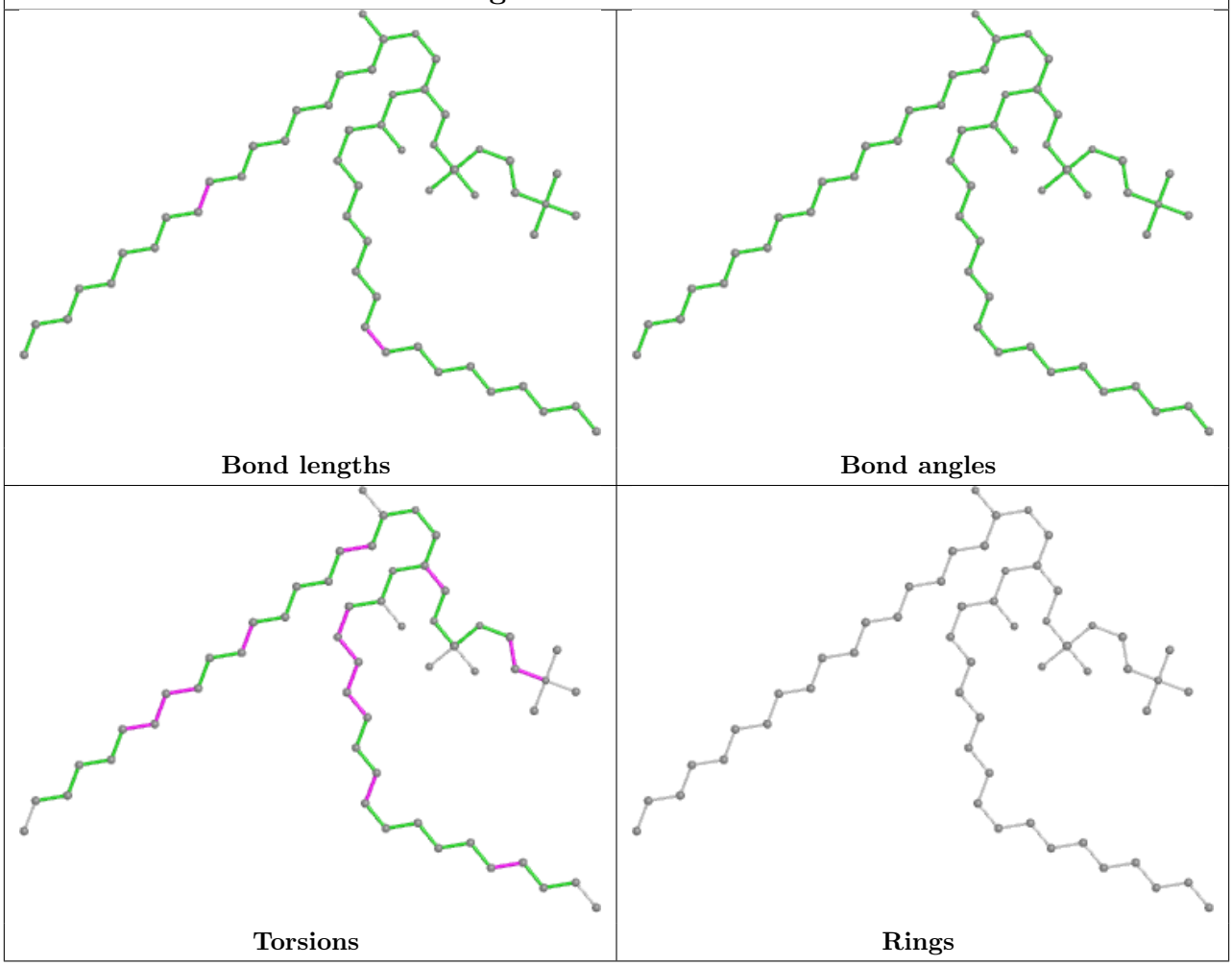
Ligand PCW A 1114



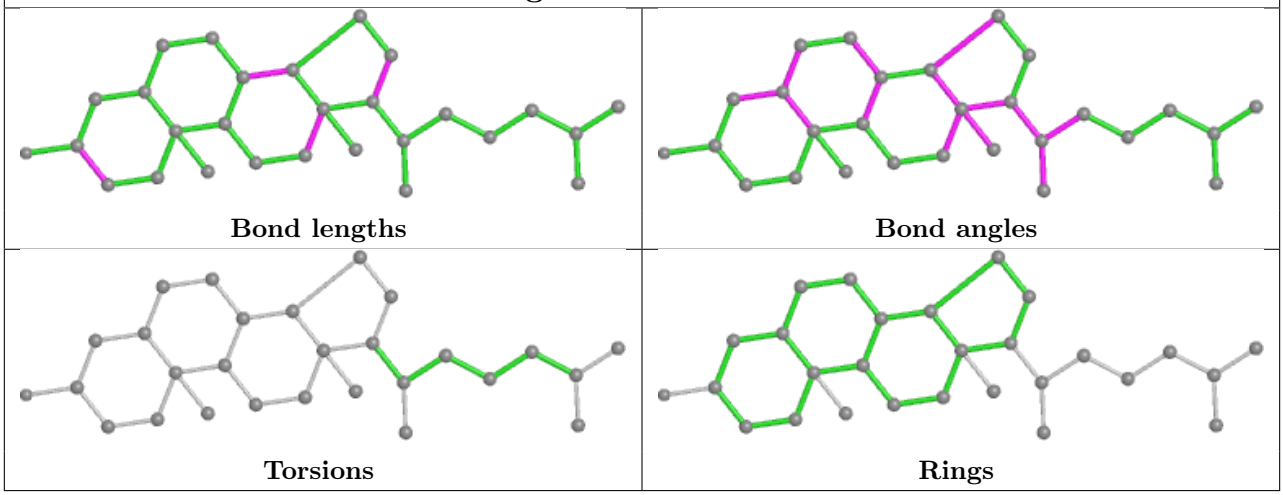
Ligand CLR C 1106



Ligand PCW C 1114



Ligand CLR B 401



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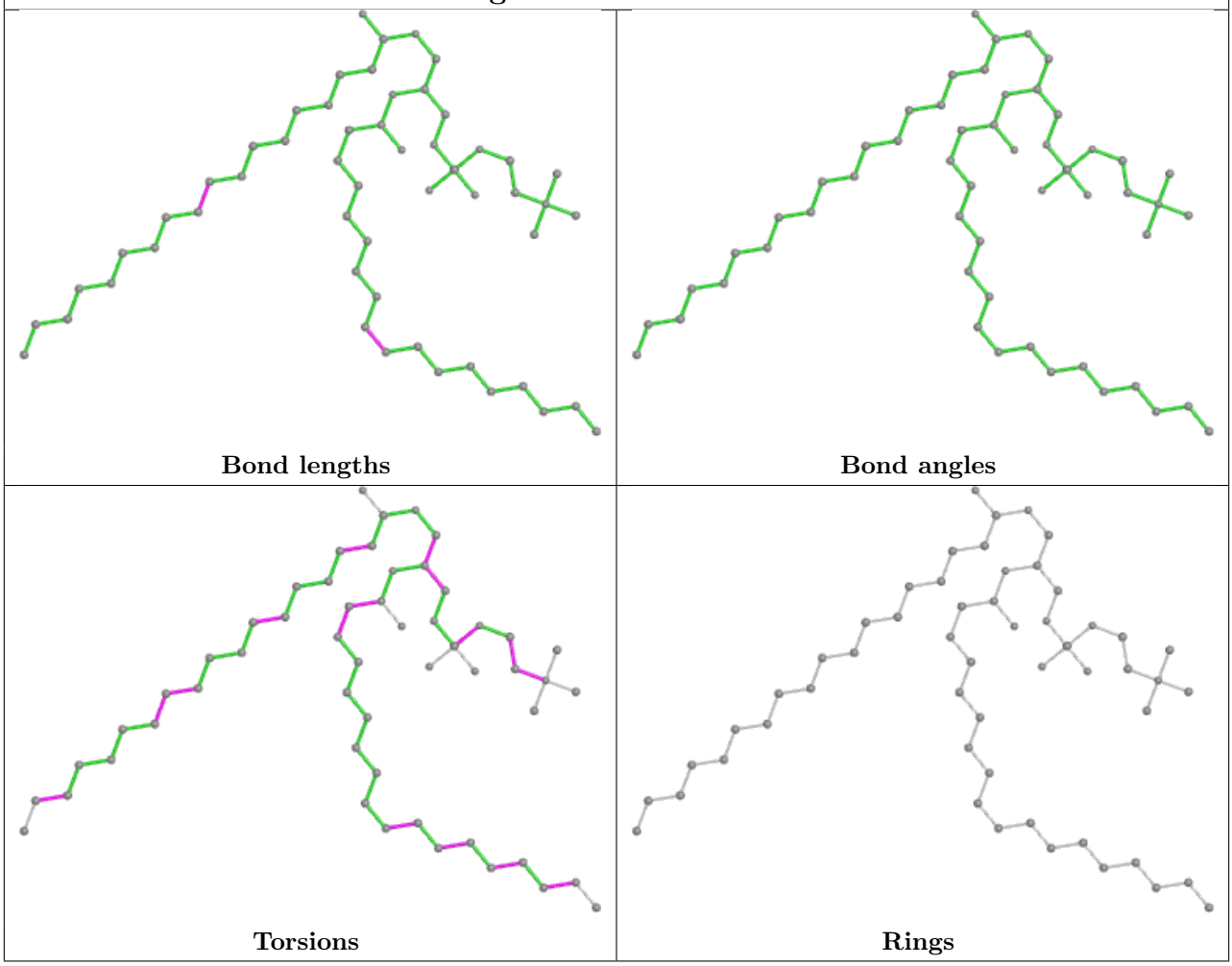

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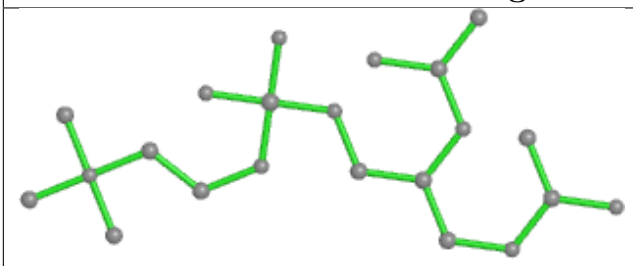
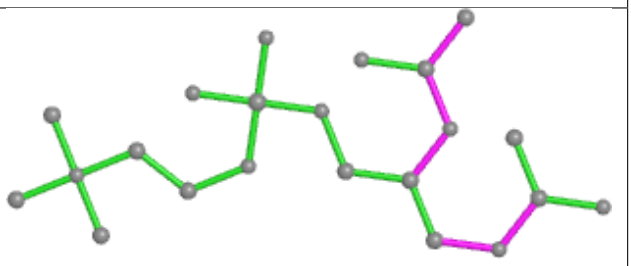
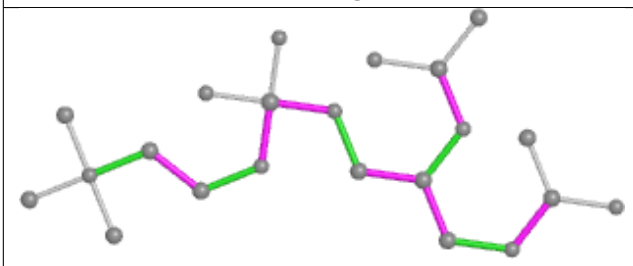


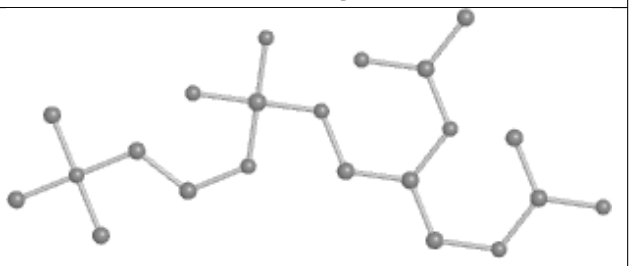
Bond lengths



Bond angles

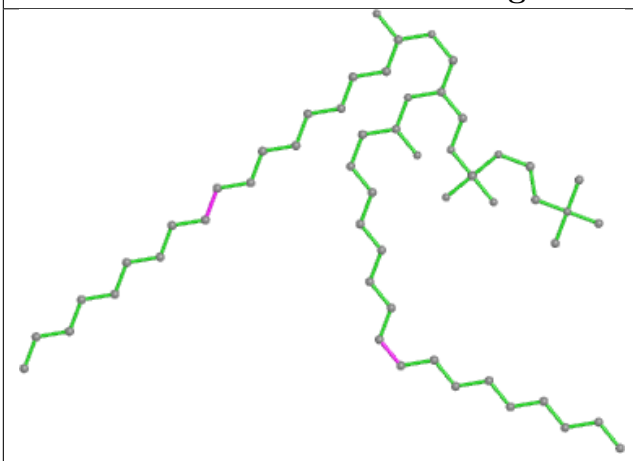


Torsions

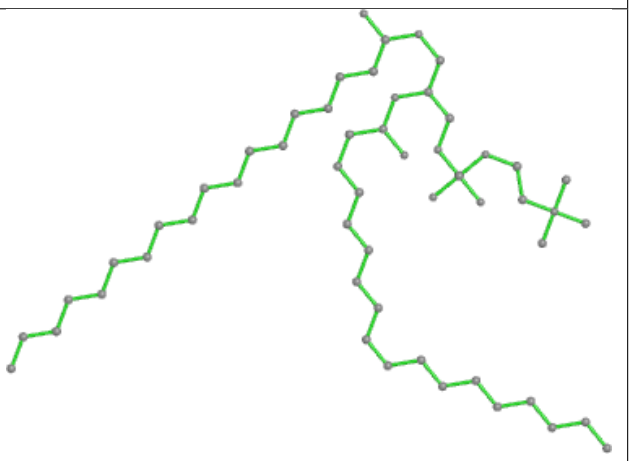


Rings

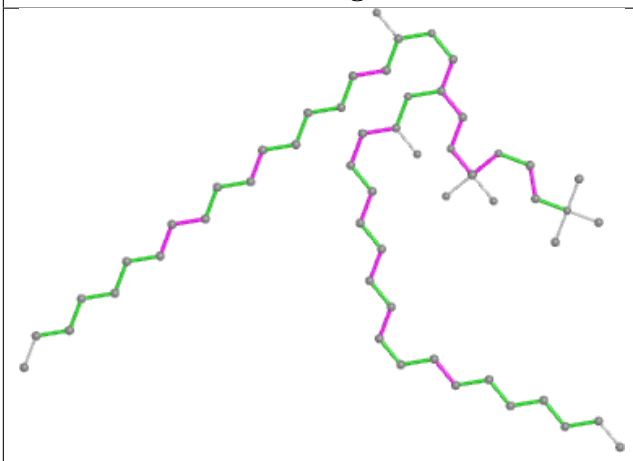
Ligand PCW A 1109



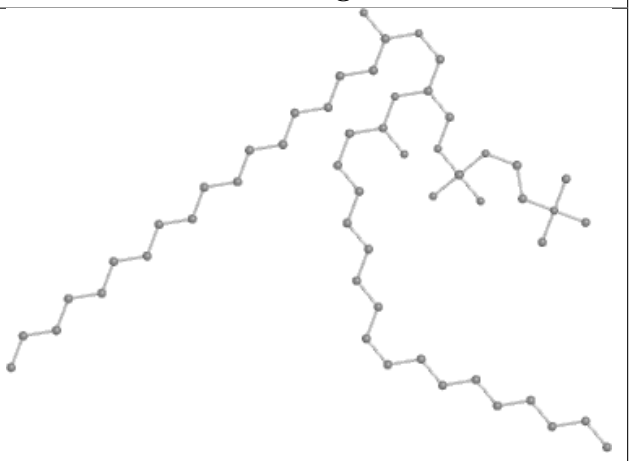
Bond lengths



Bond angles

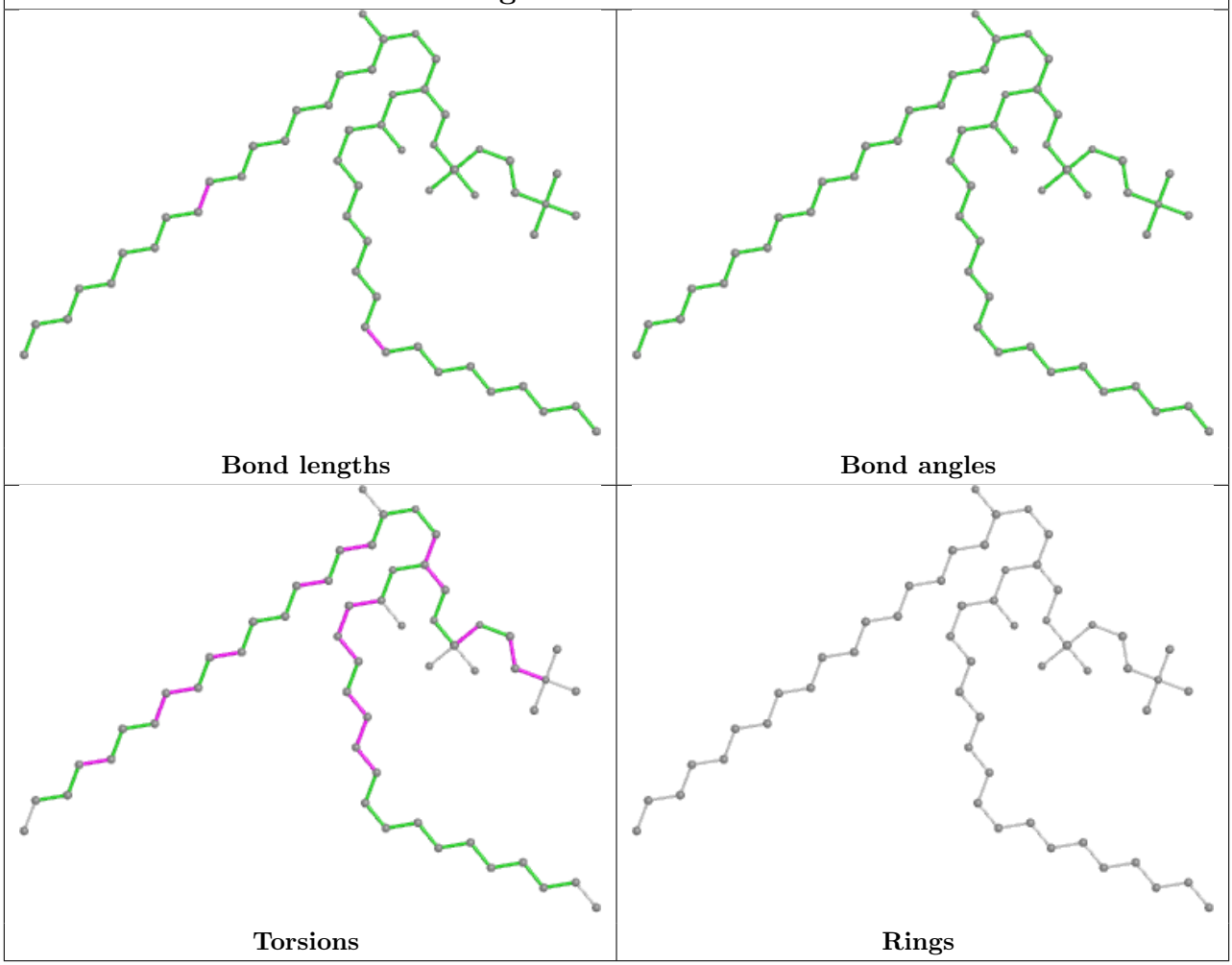


Torsions

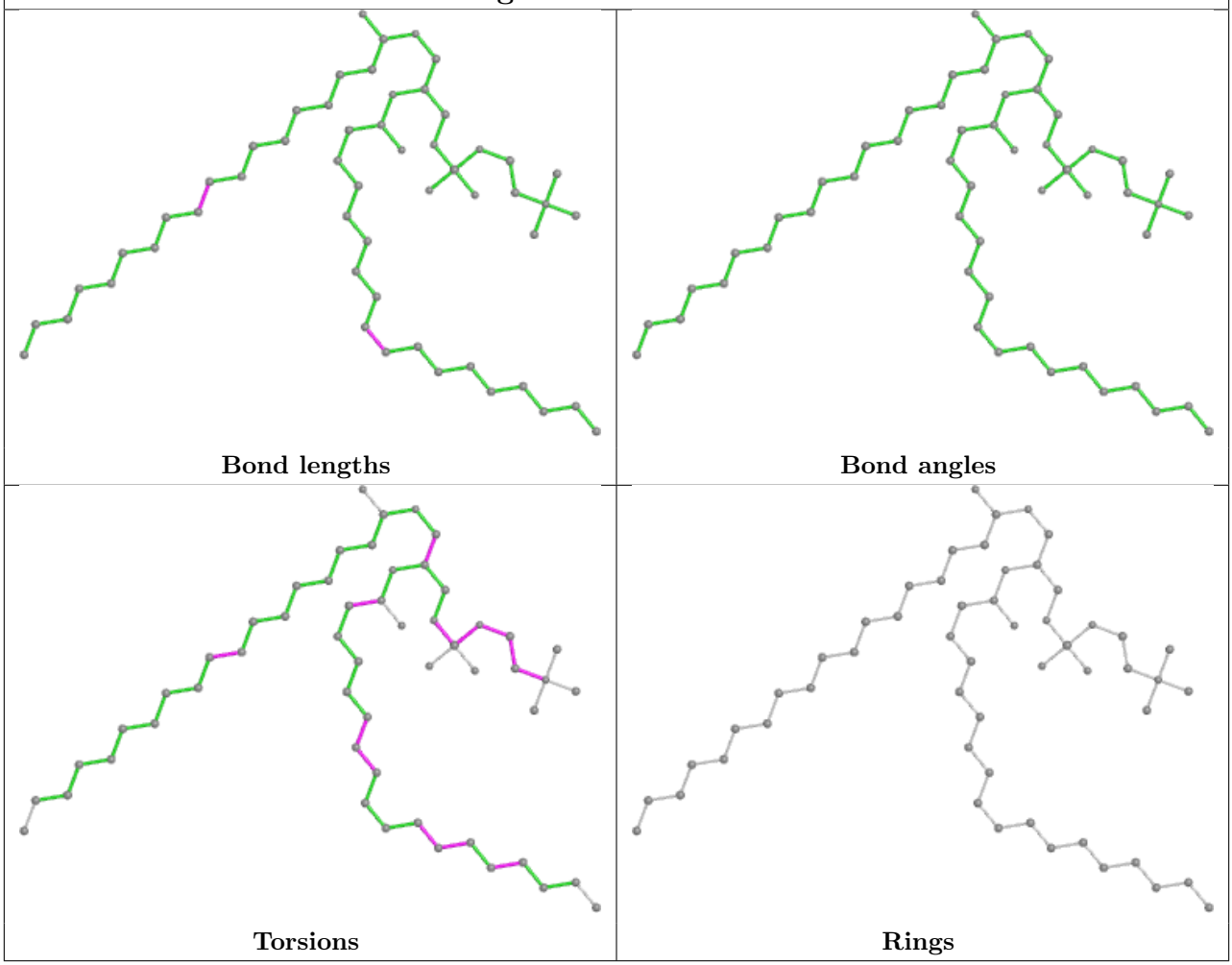


Rings

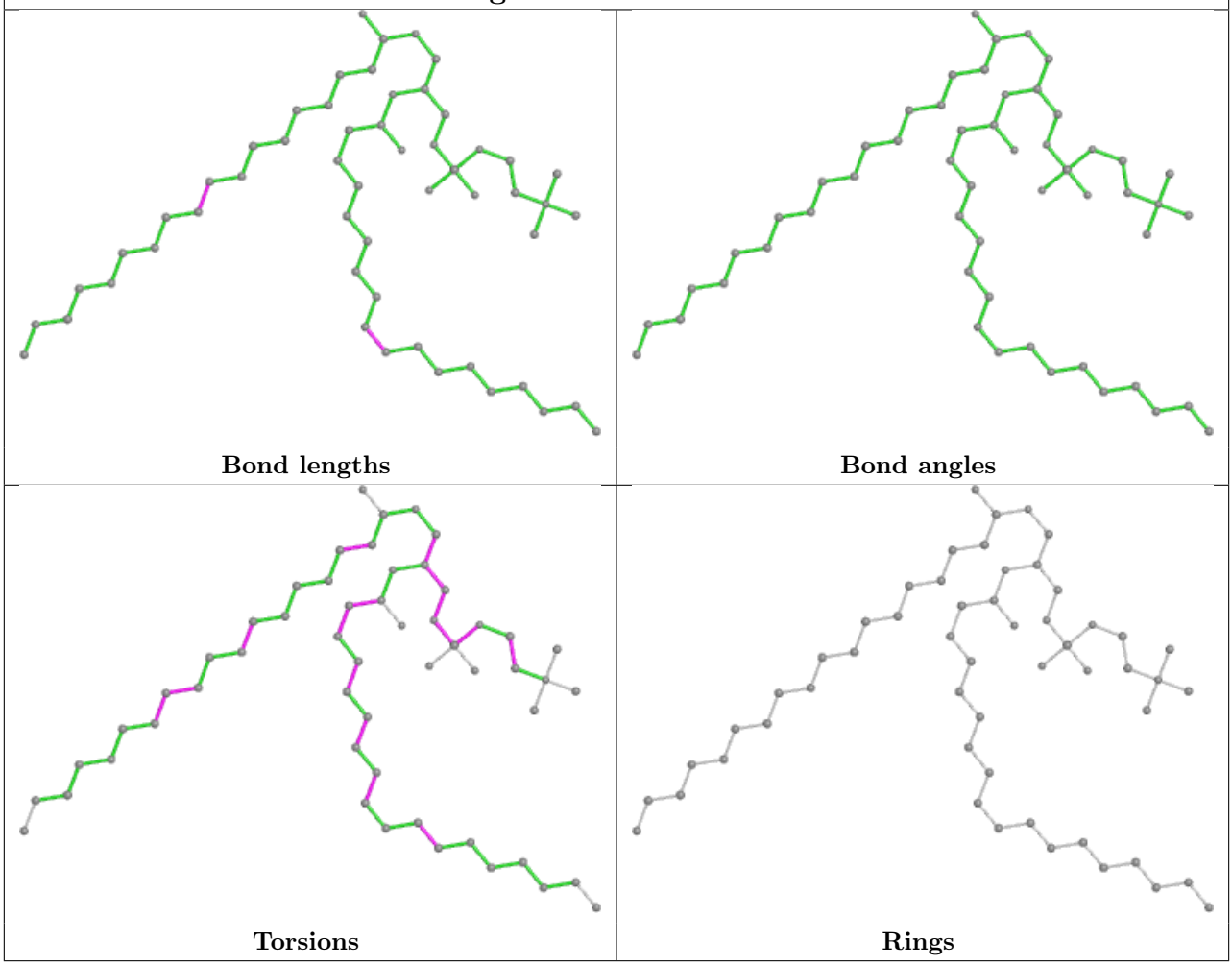
Ligand PCW E 102



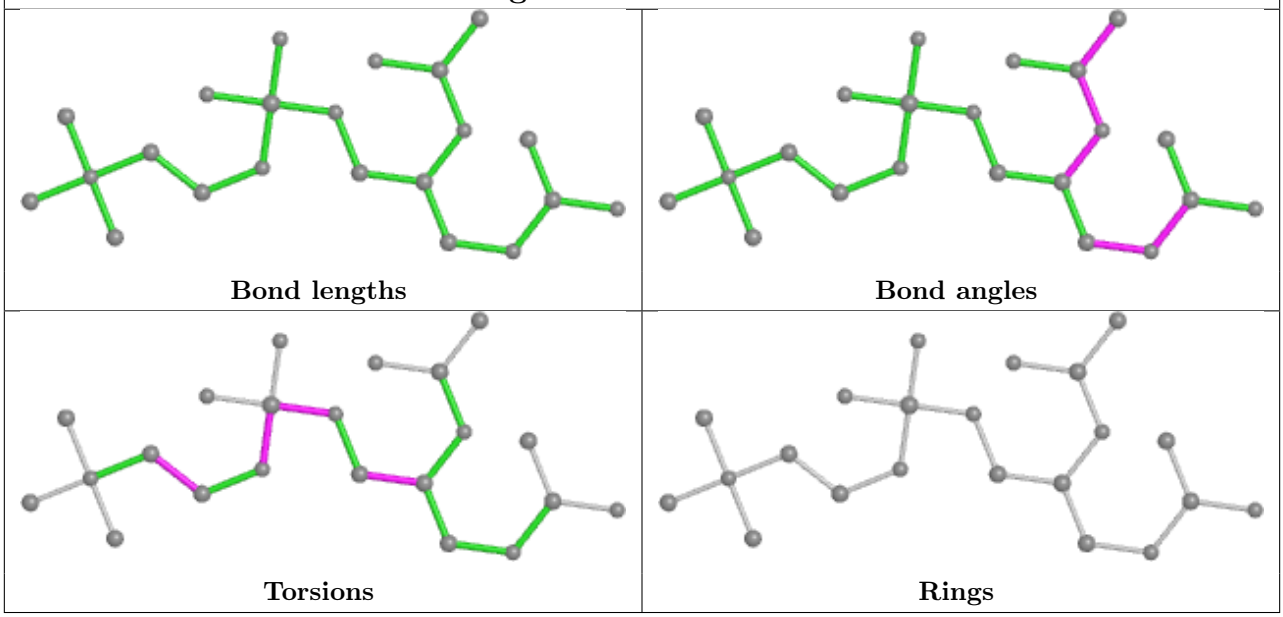
Ligand PCW G 101



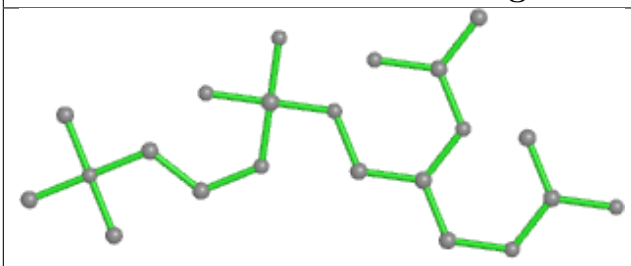
Ligand PCW C 1109



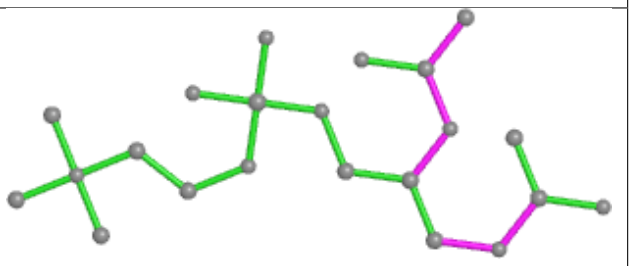
Ligand PCW A 1107



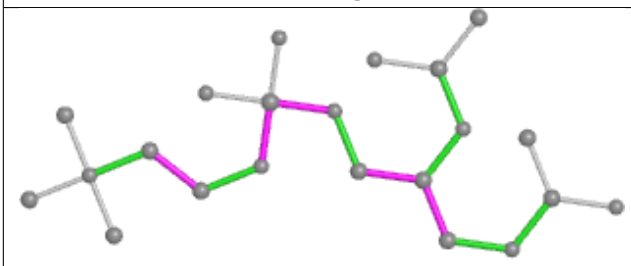
Ligand PCW C 1115



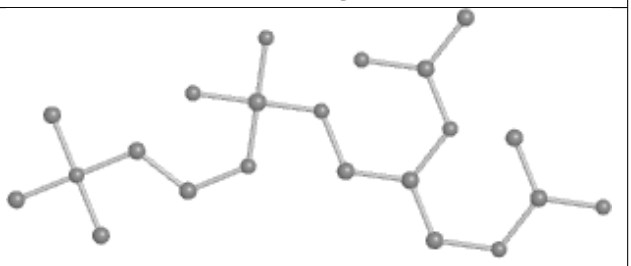
Bond lengths



Bond angles

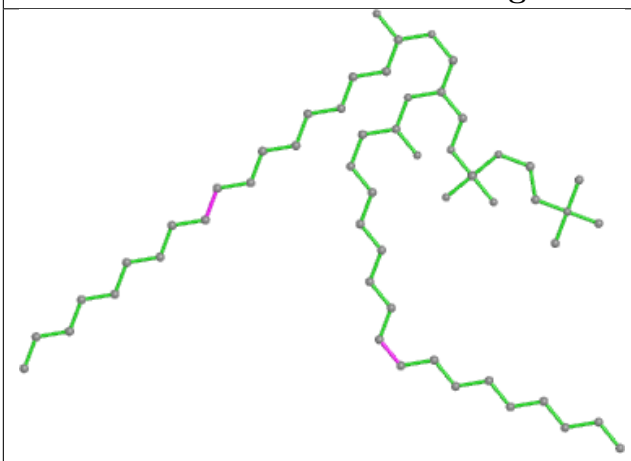


Torsions

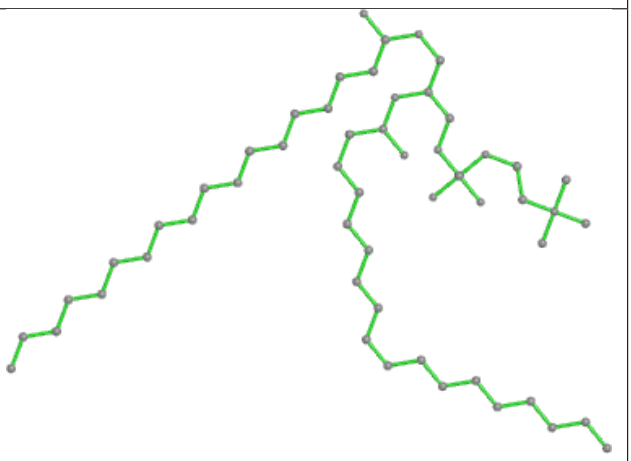


Rings

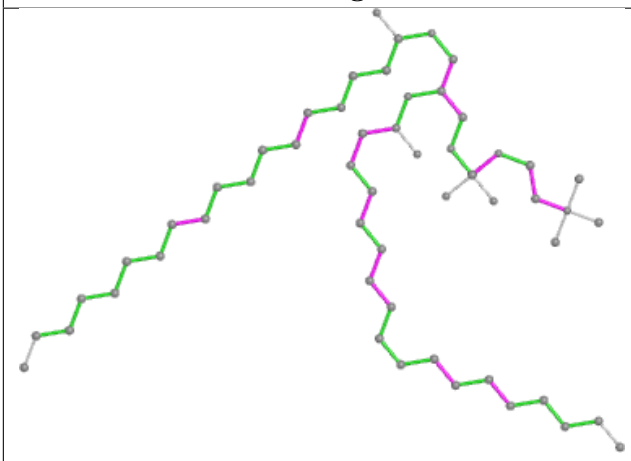
Ligand PCW C 1113



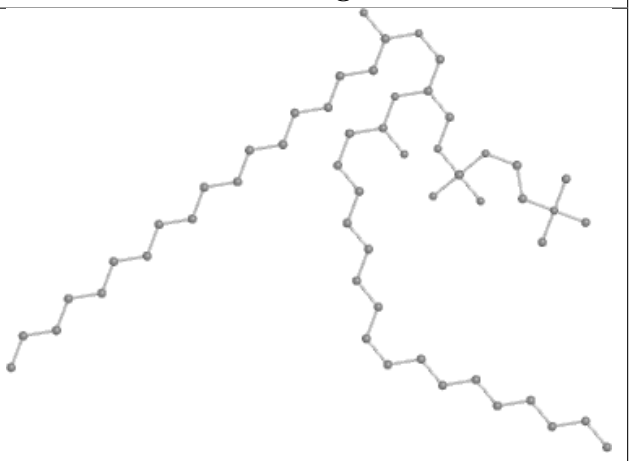
Bond lengths



Bond angles

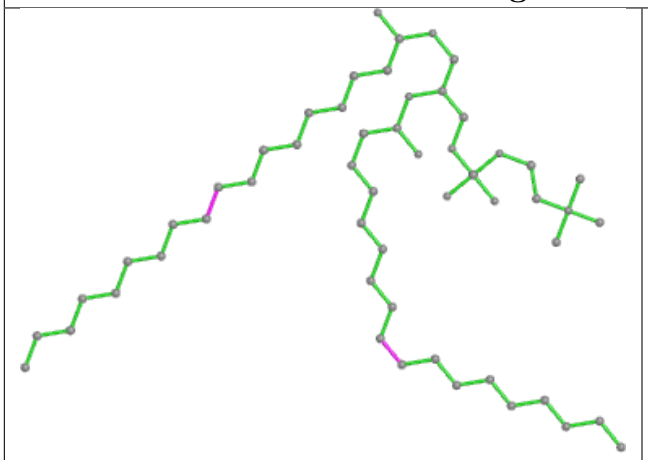


Torsions



Rings

Ligand PCW A 1116



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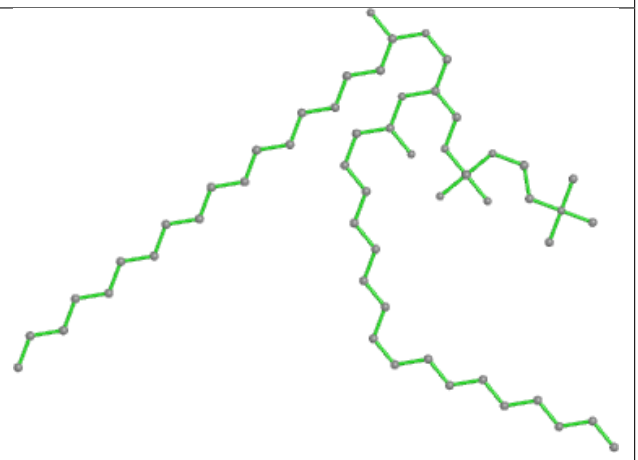
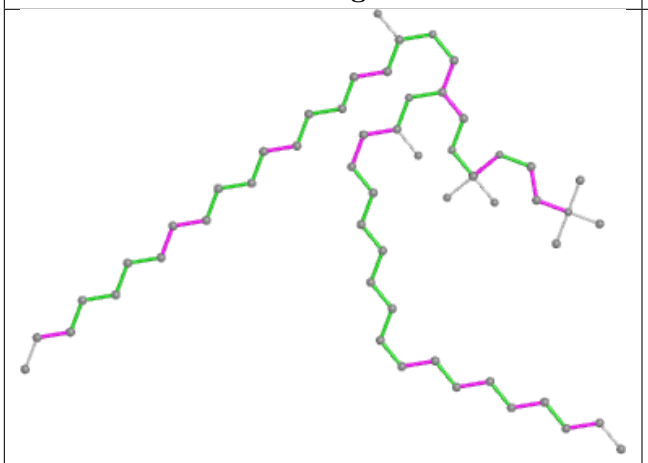
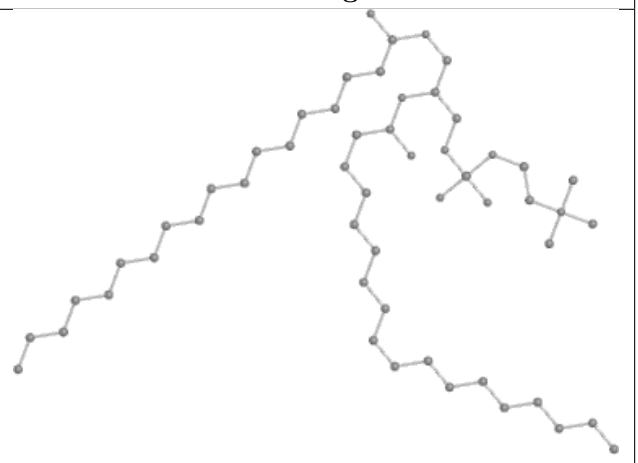


Bond angles

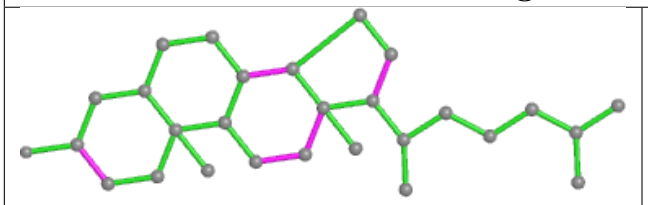


Torsions

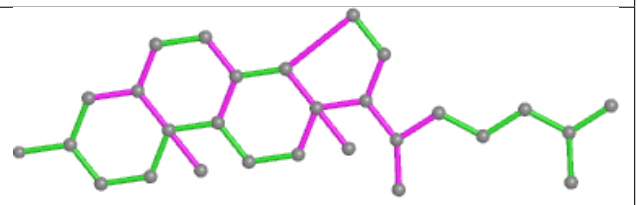


Rings

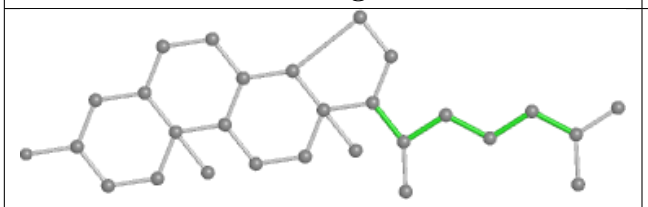
Ligand CLR A 1106



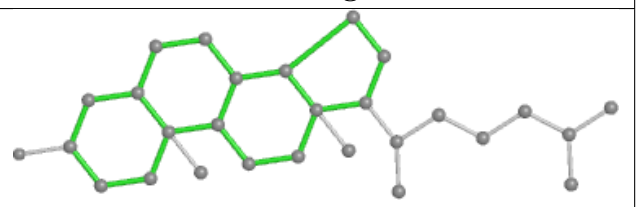
Bond lengths



Bond angles

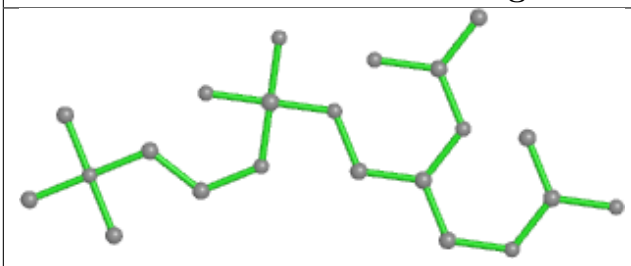


Torsions

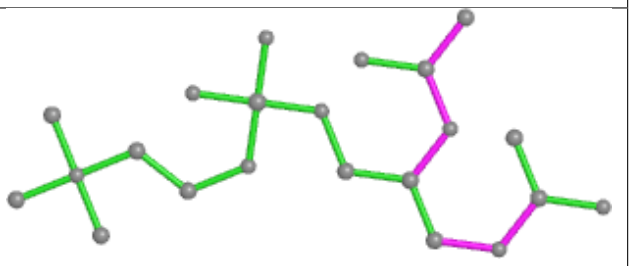


Rings

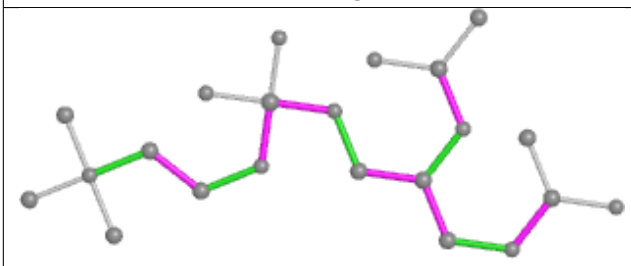
Ligand PCW A 1108



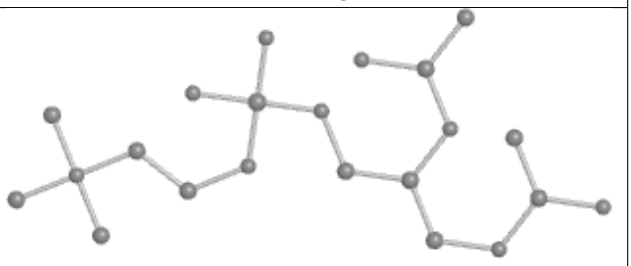
Bond lengths



Bond angles

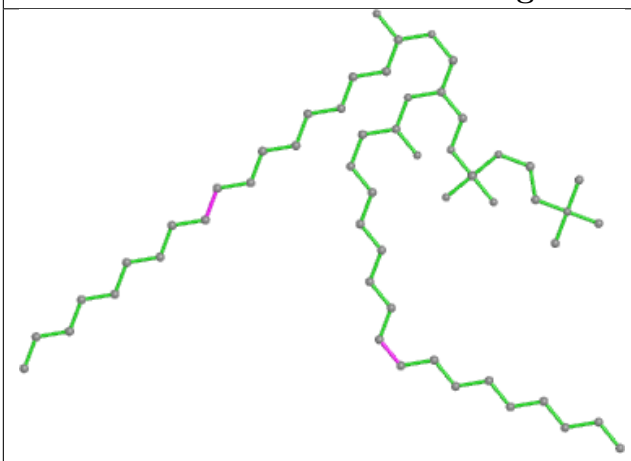


Torsions

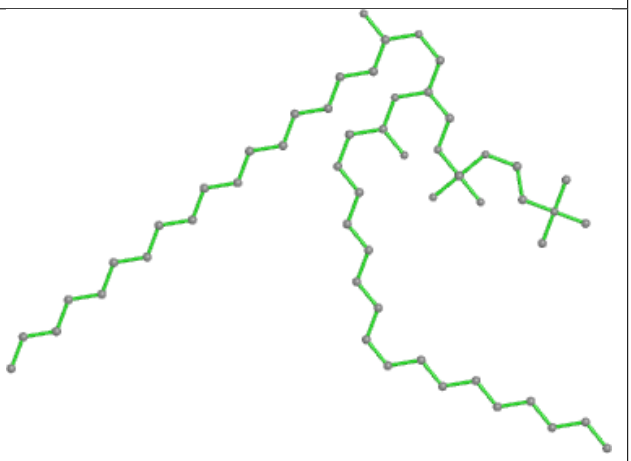


Rings

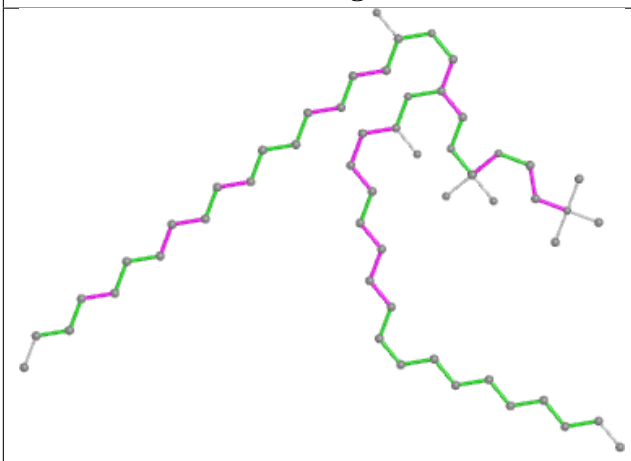
Ligand PCW G 102



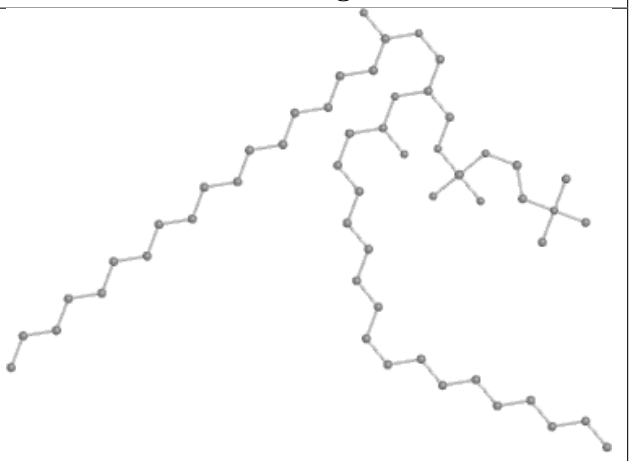
Bond lengths



Bond angles

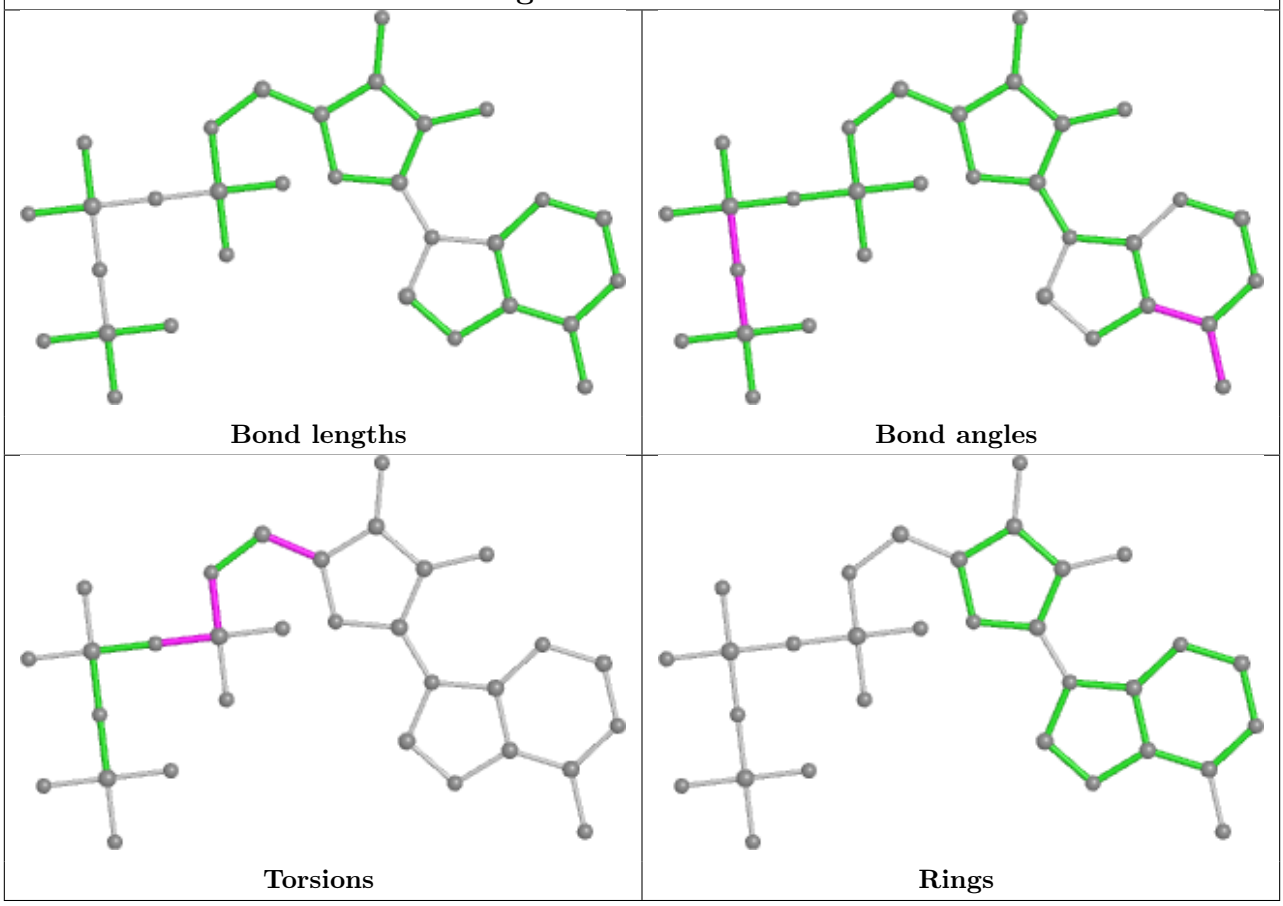


Torsions

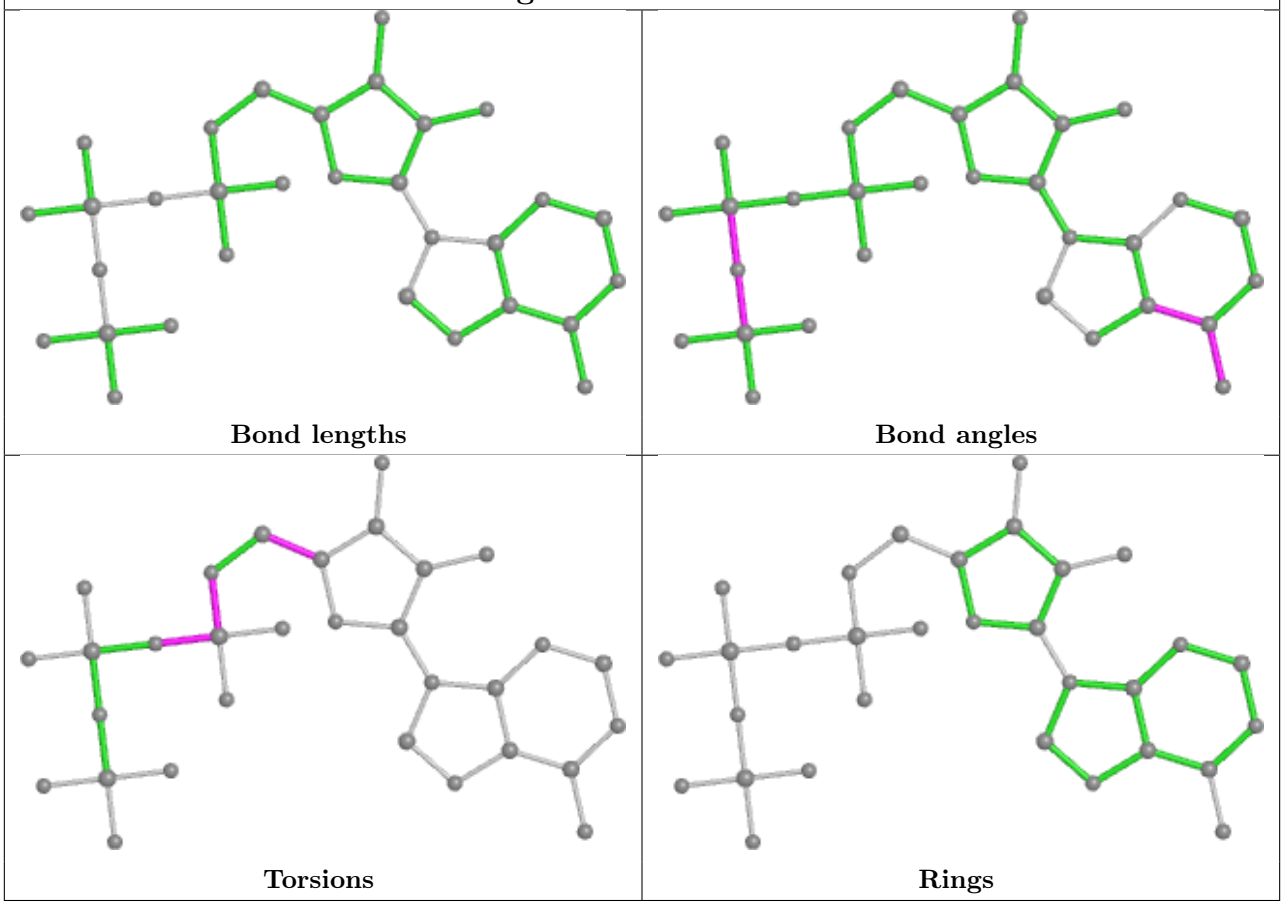


Rings

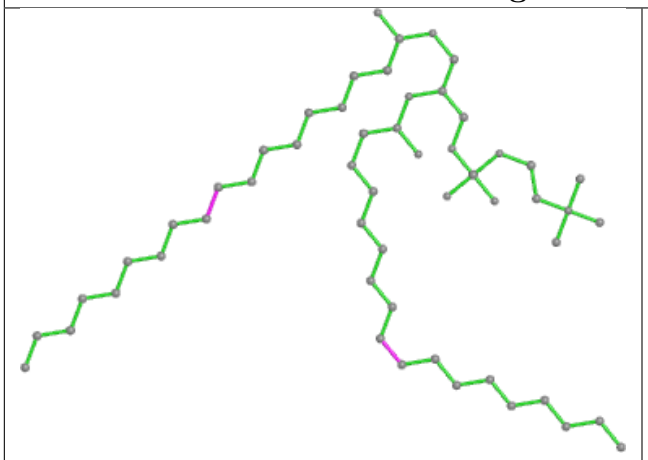
Ligand ATP A 1104



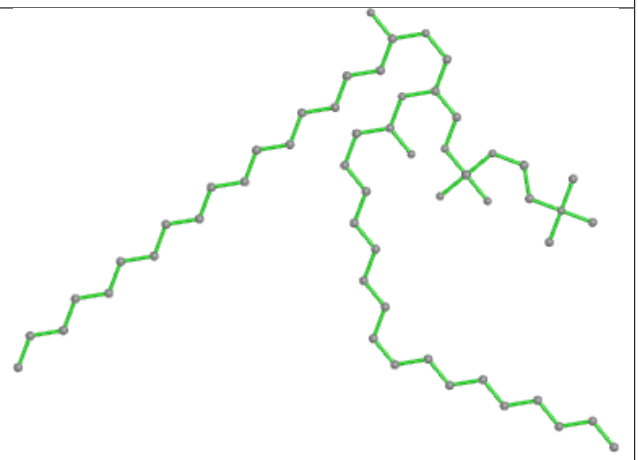
Ligand ATP C 1104



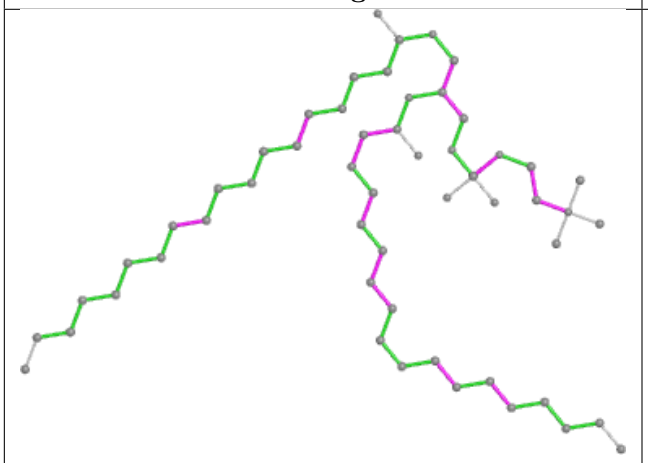
Ligand PCW A 1113



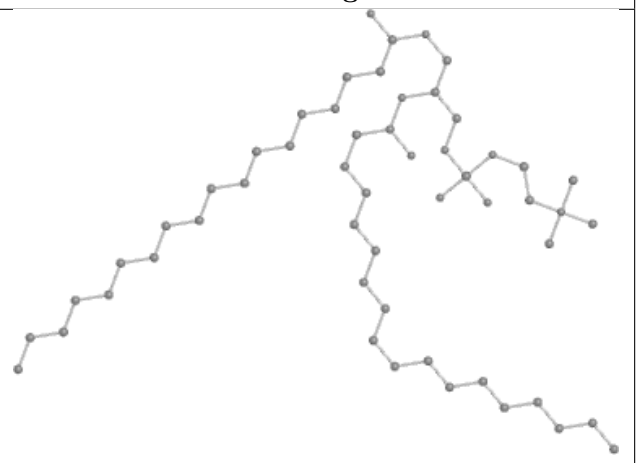
Bond lengths



Bond angles

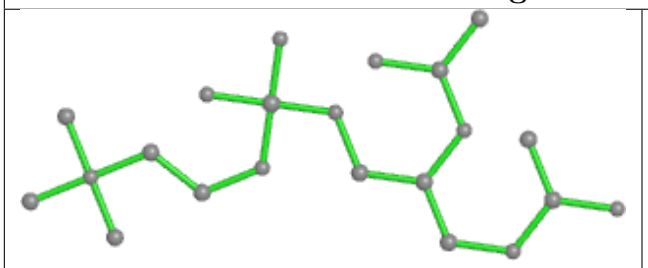


Torsions

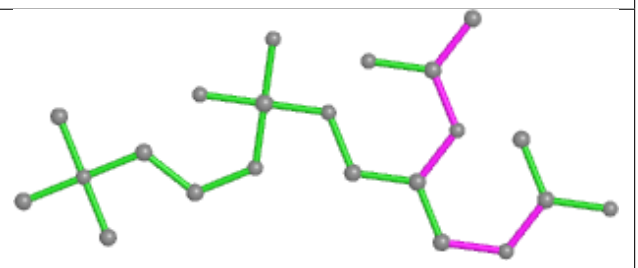


Rings

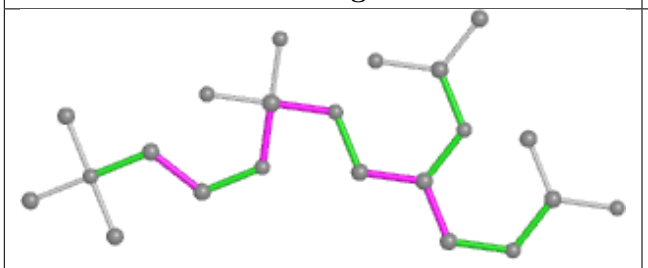
Ligand PCW A 1115



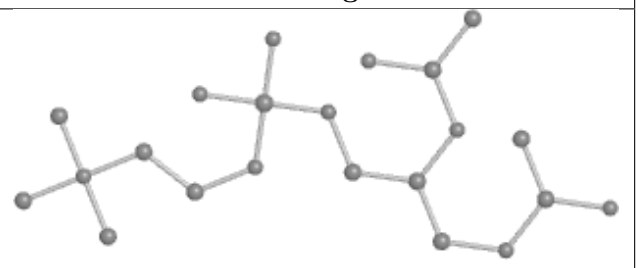
Bond lengths



Bond angles

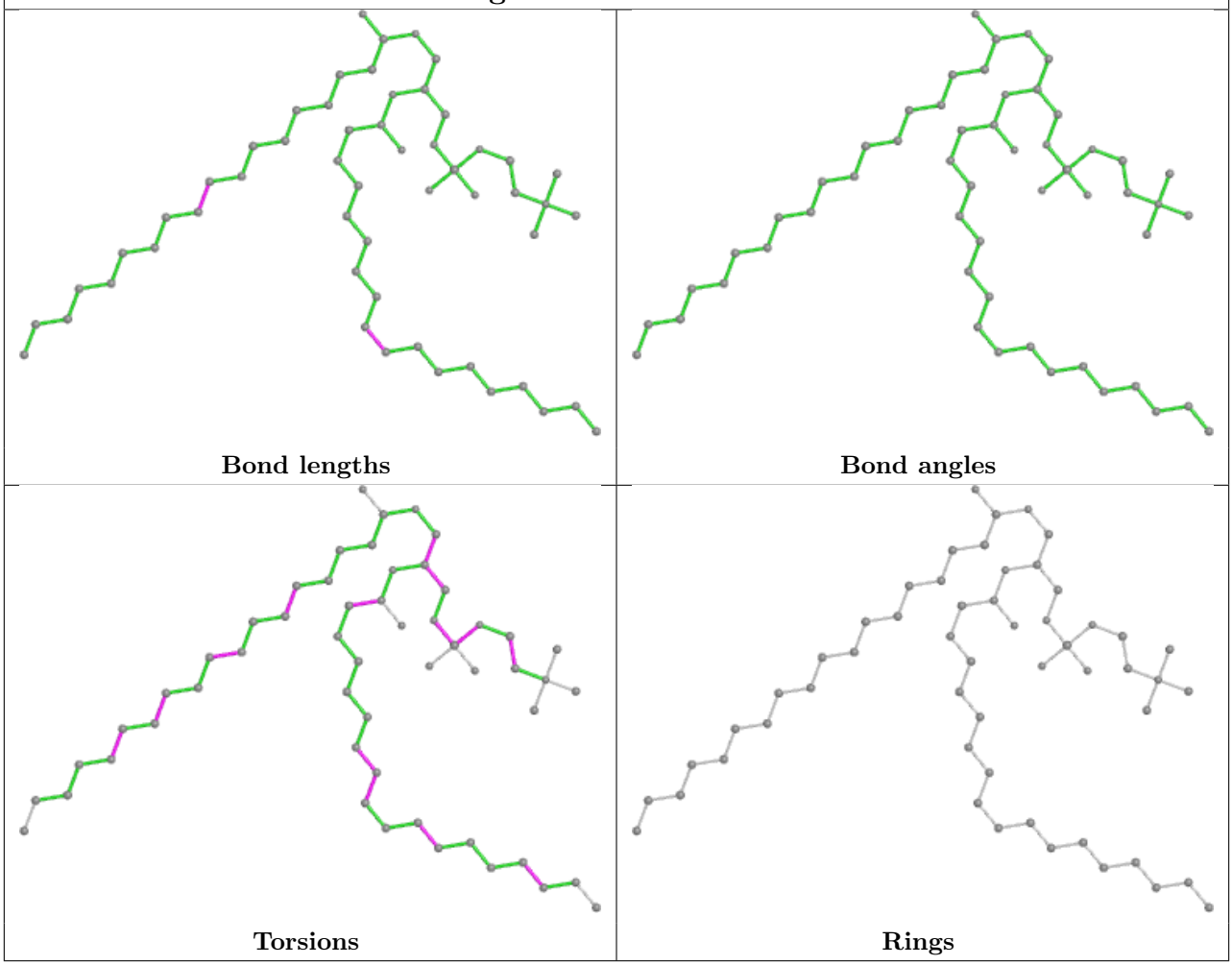


Torsions

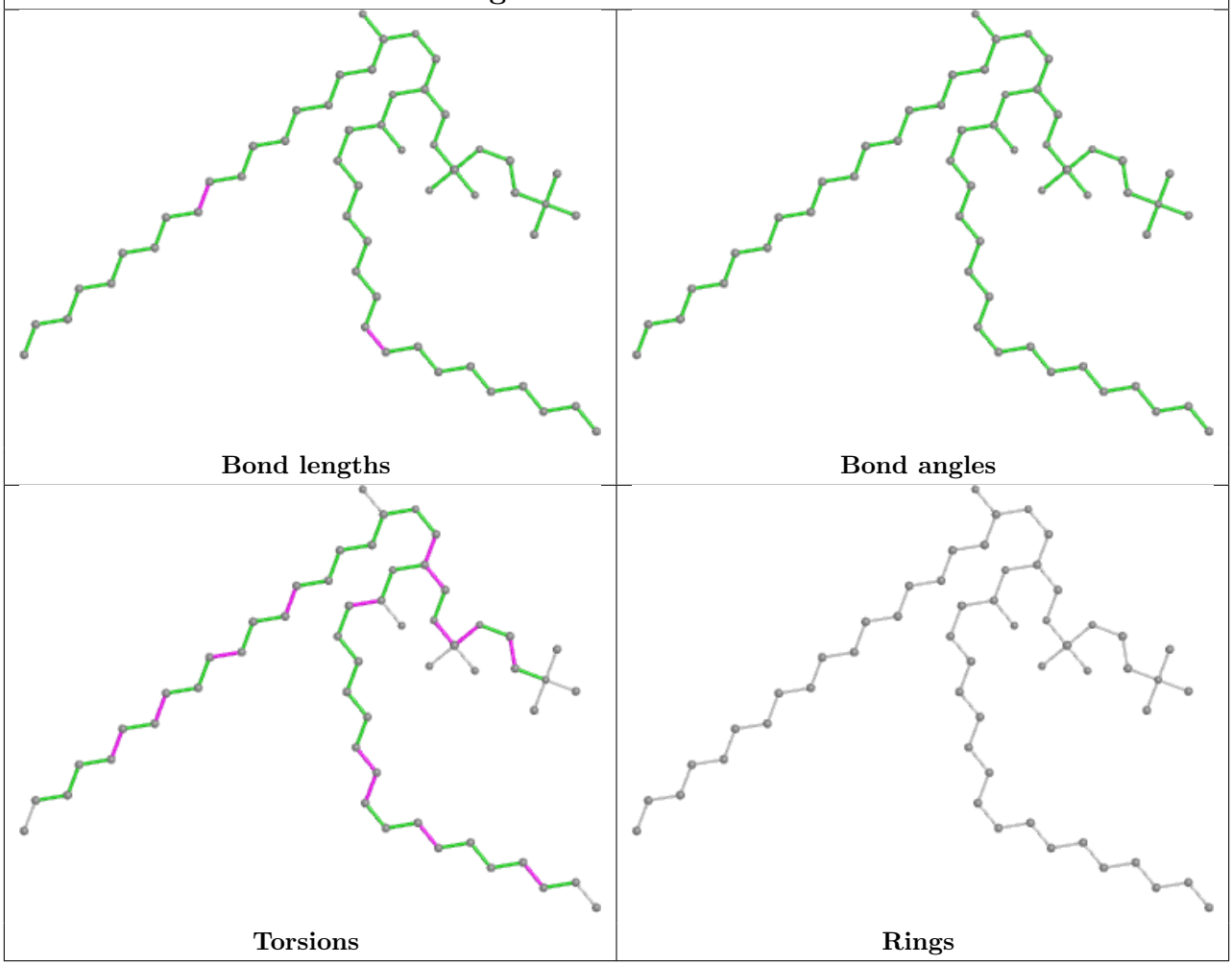


Rings

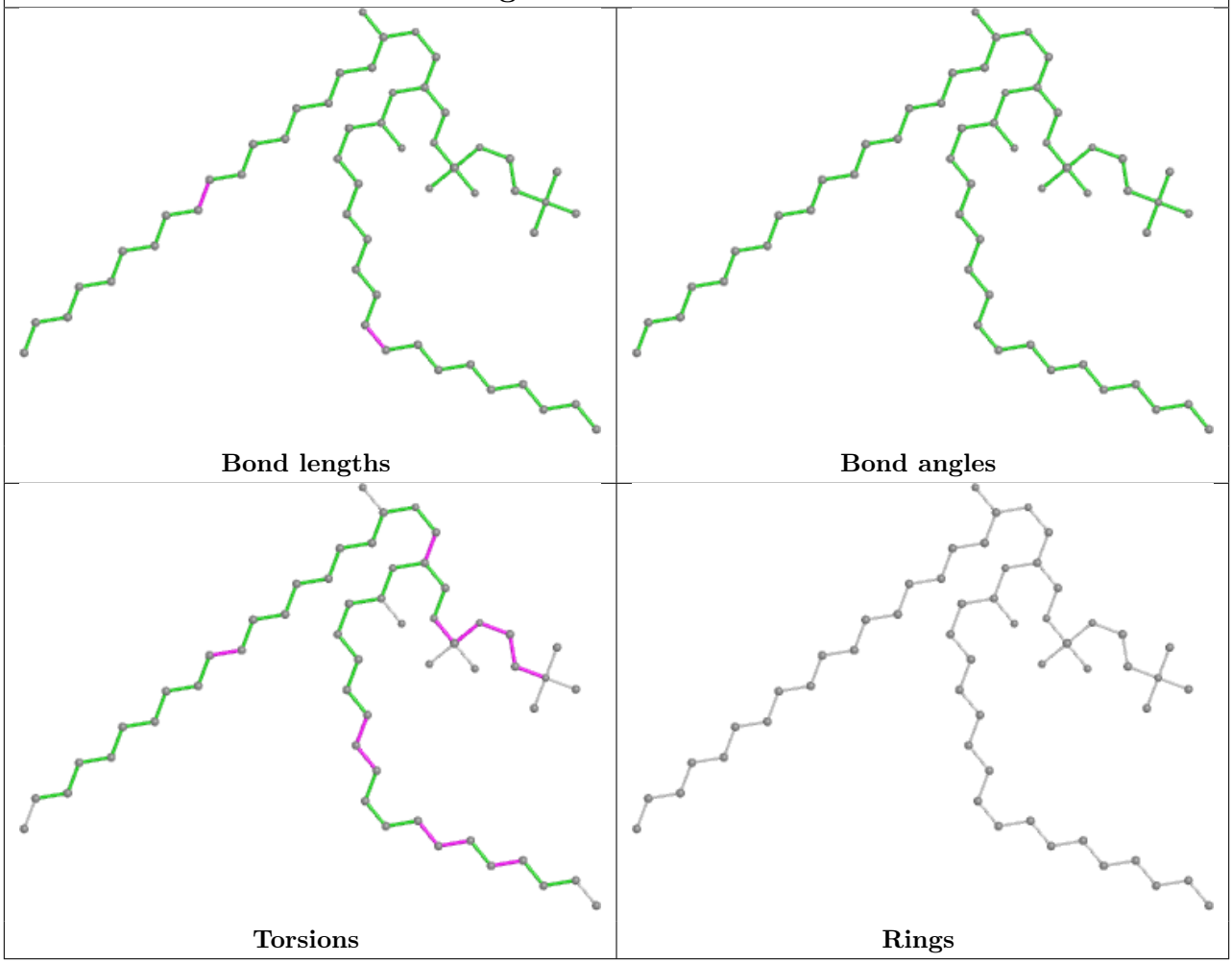
Ligand PCW A 1110



Ligand PCW C 1110



Ligand PCW E 101



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.

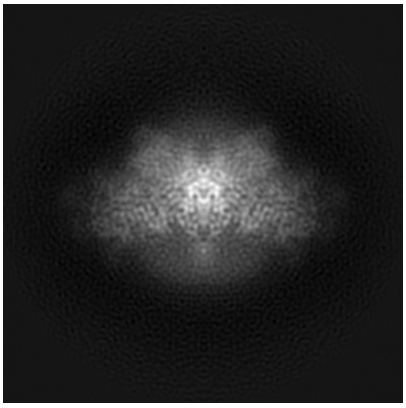
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32895. These allow visual inspection of the internal detail of the map and identification of artifacts.

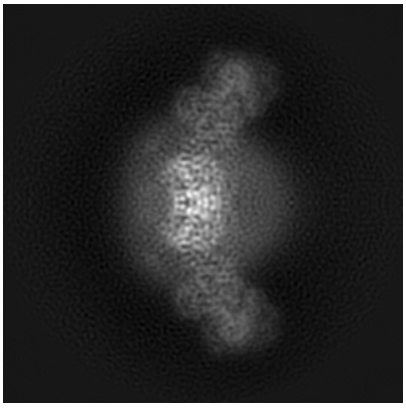
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

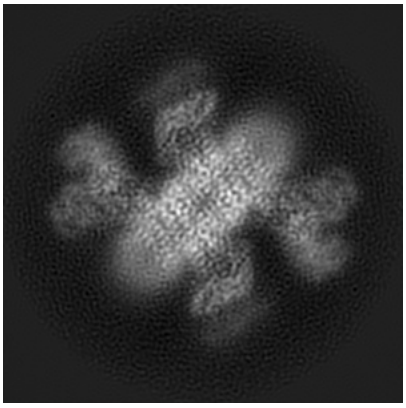
6.1.1 Primary map



X



Y

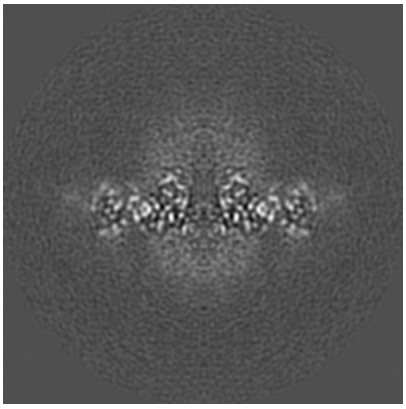


Z

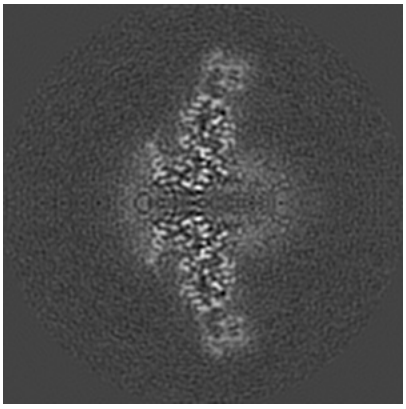
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

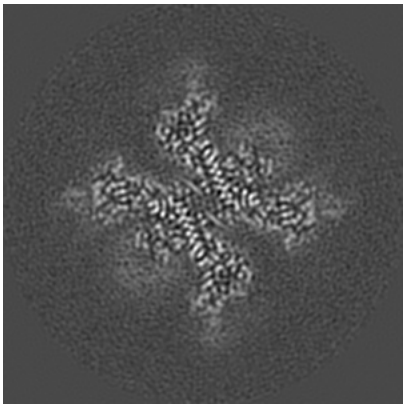
6.2.1 Primary map



X Index: 120



Y Index: 120

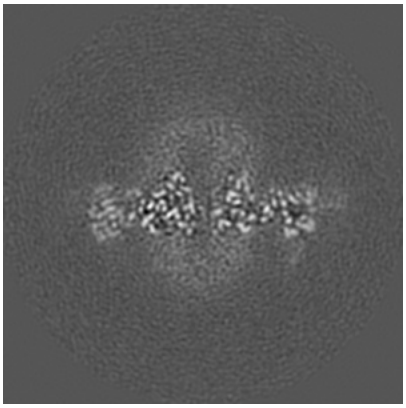


Z Index: 120

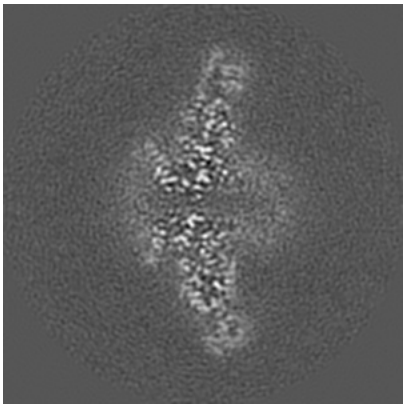
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

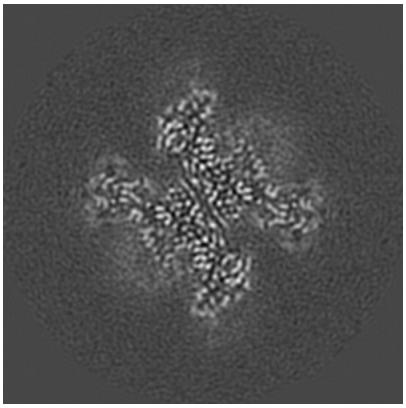
6.3.1 Primary map



X Index: 117



Y Index: 121



Z Index: 117

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

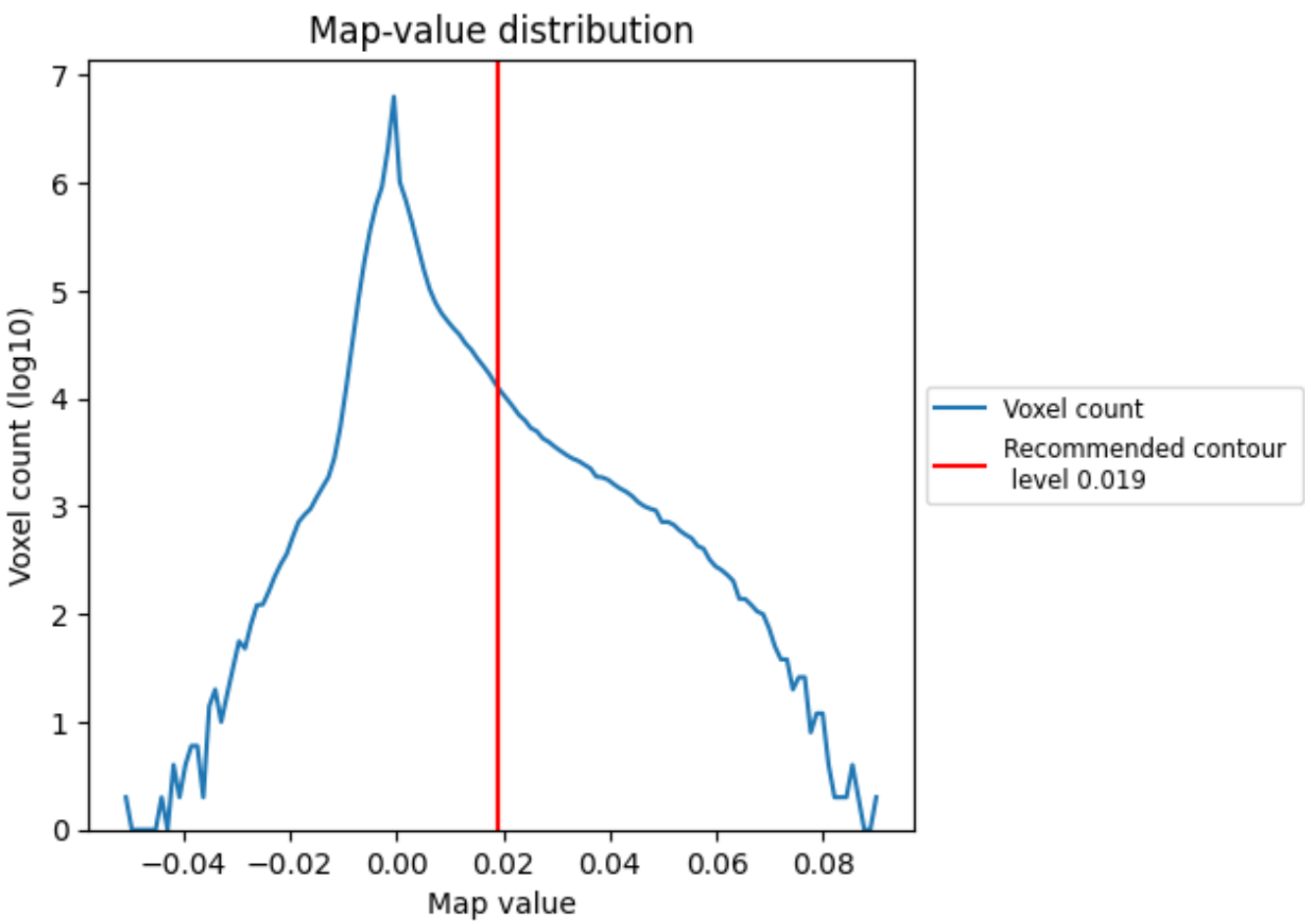
6.5 Mask visualisation (i)

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

7 Map analysis (i)

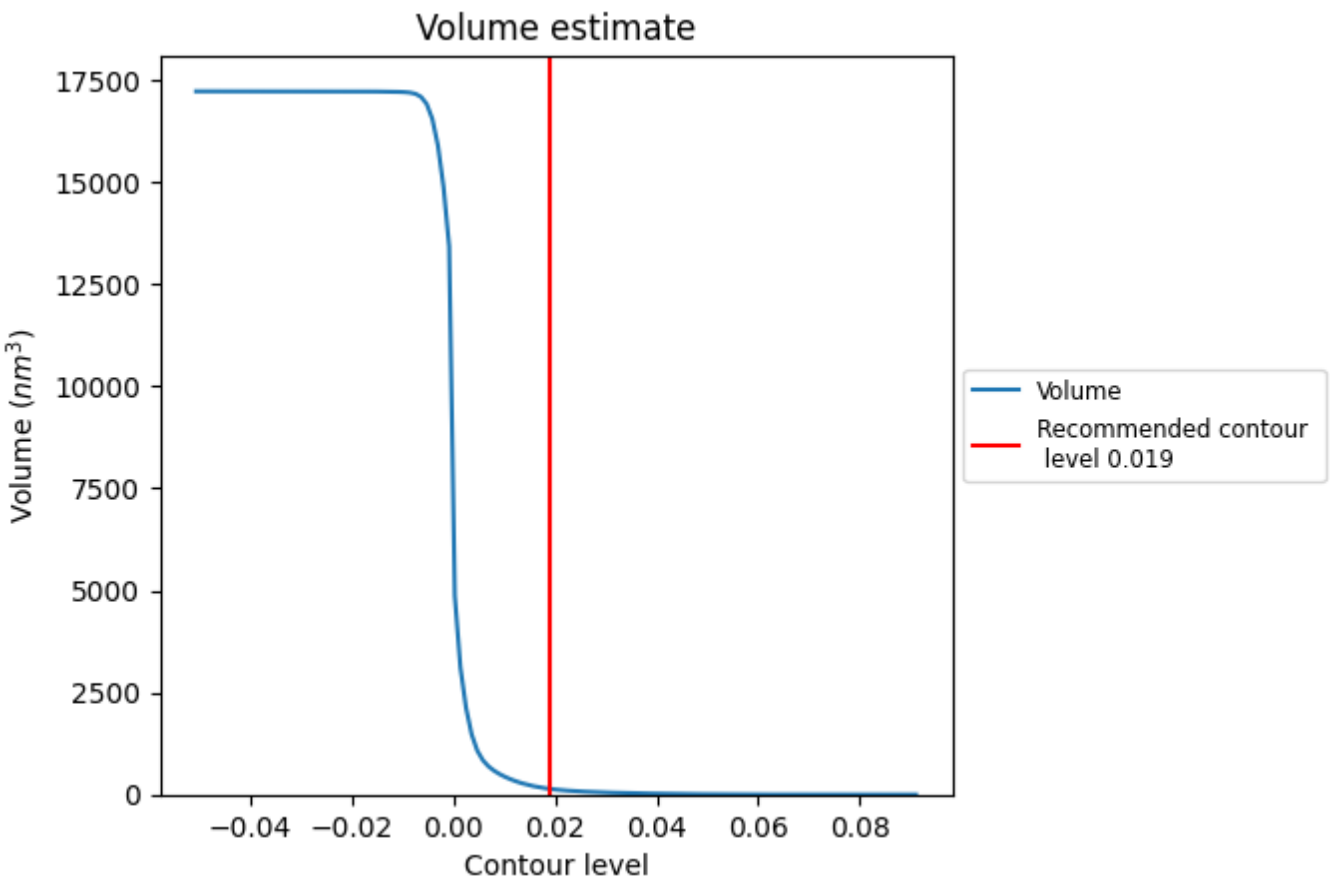
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

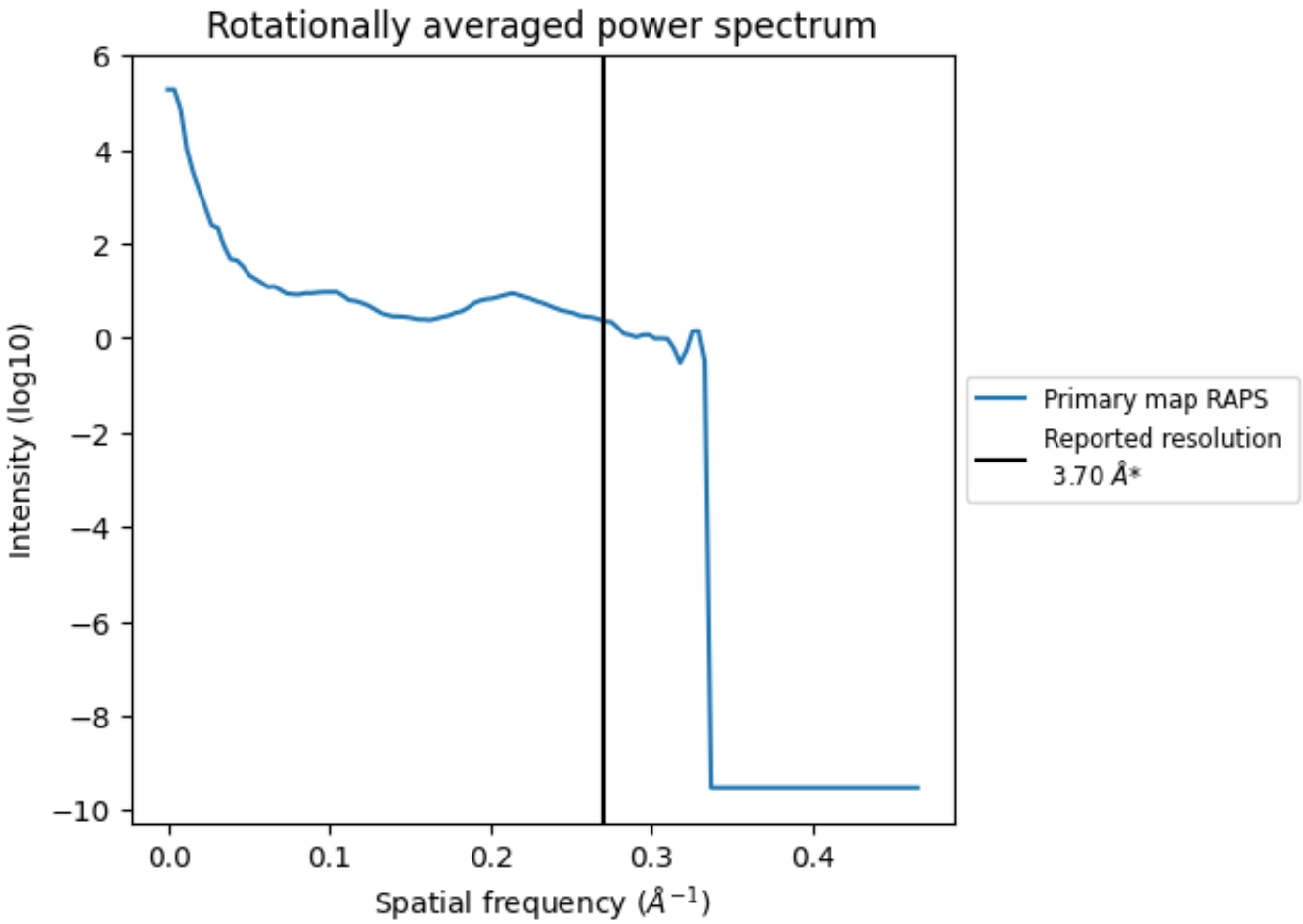
7.2 Volume estimate (i)



The volume at the recommended contour level is 138 nm^3; this corresponds to an approximate mass of 125 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)

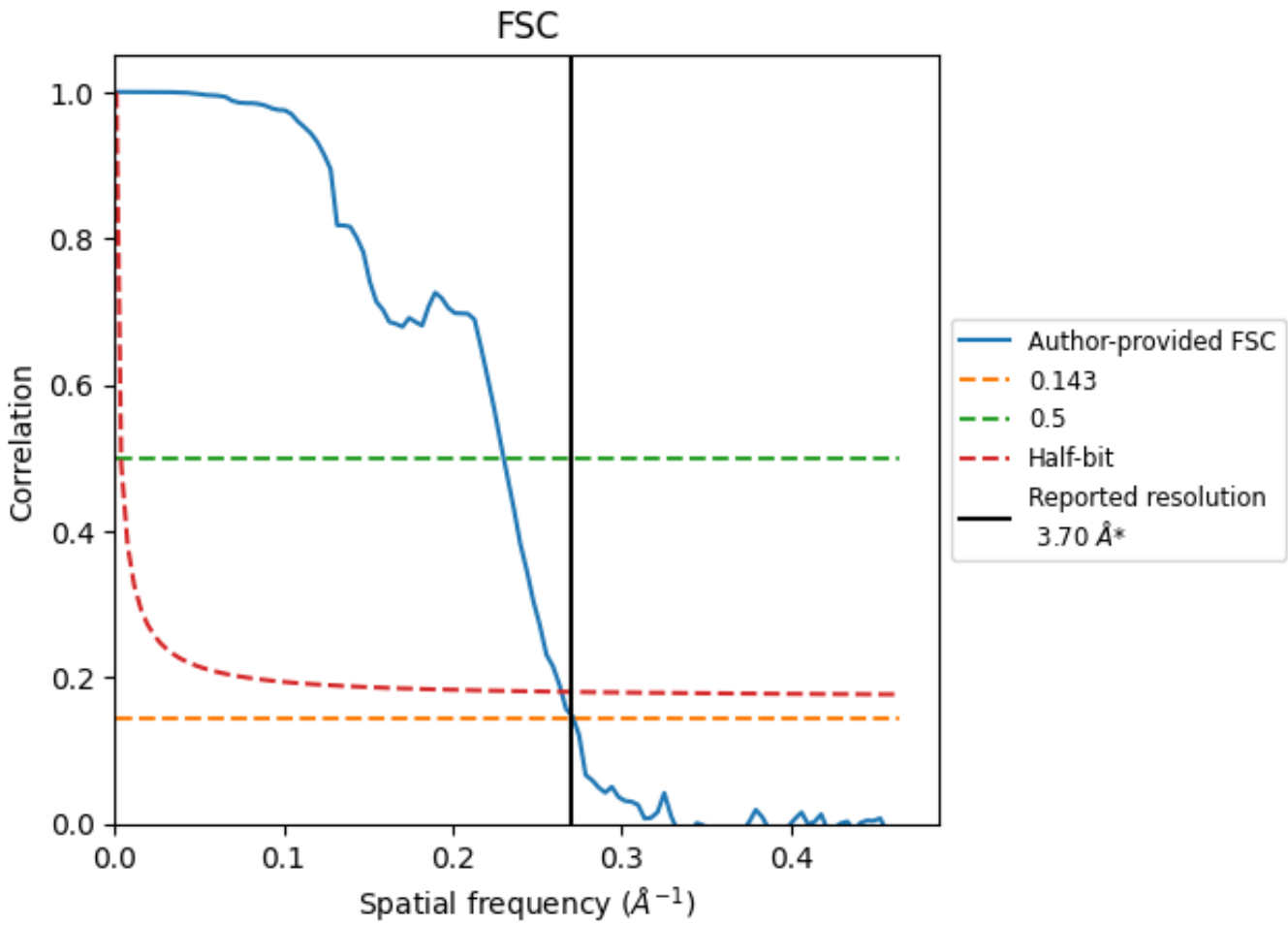


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

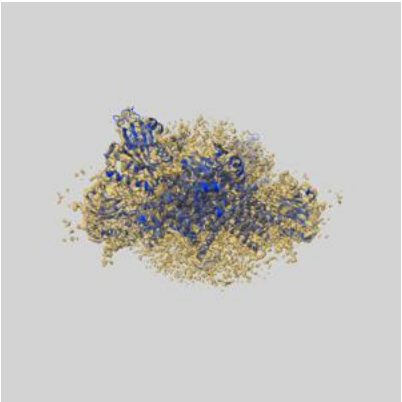
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.34	3.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

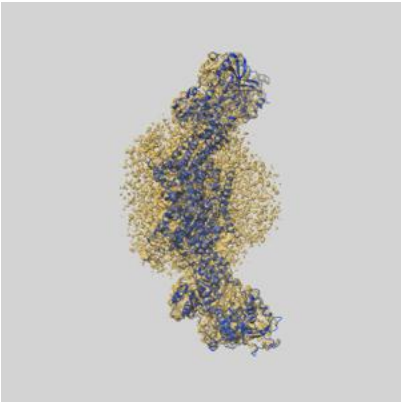
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32895 and PDB model 7WYV. Per-residue inclusion information can be found in section 3 on page 10.

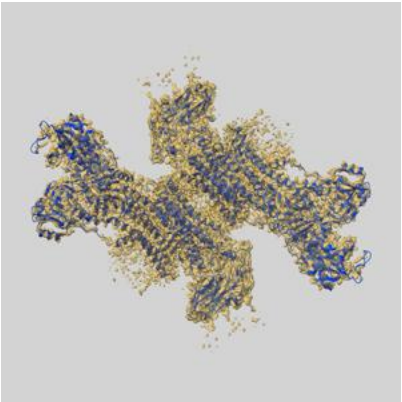
9.1 Map-model overlay (i)



X



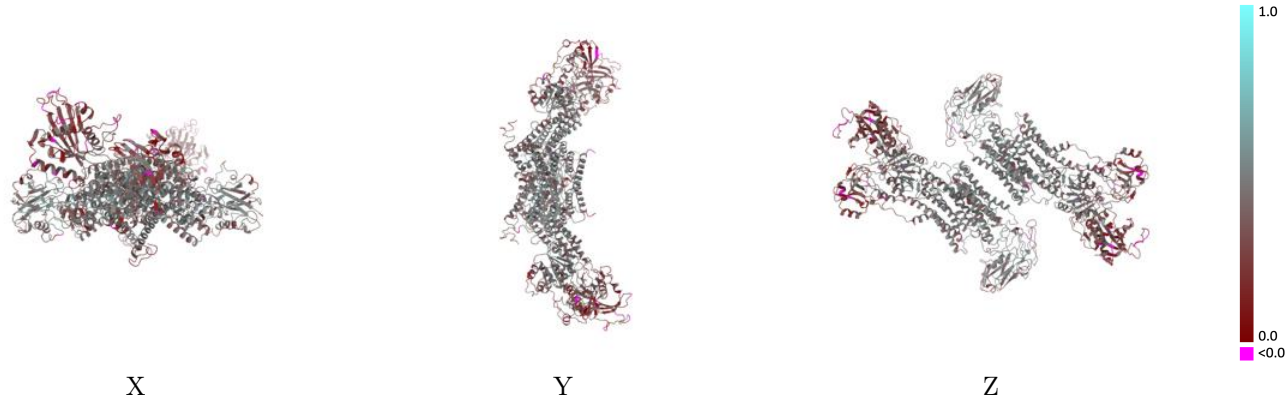
Y



Z

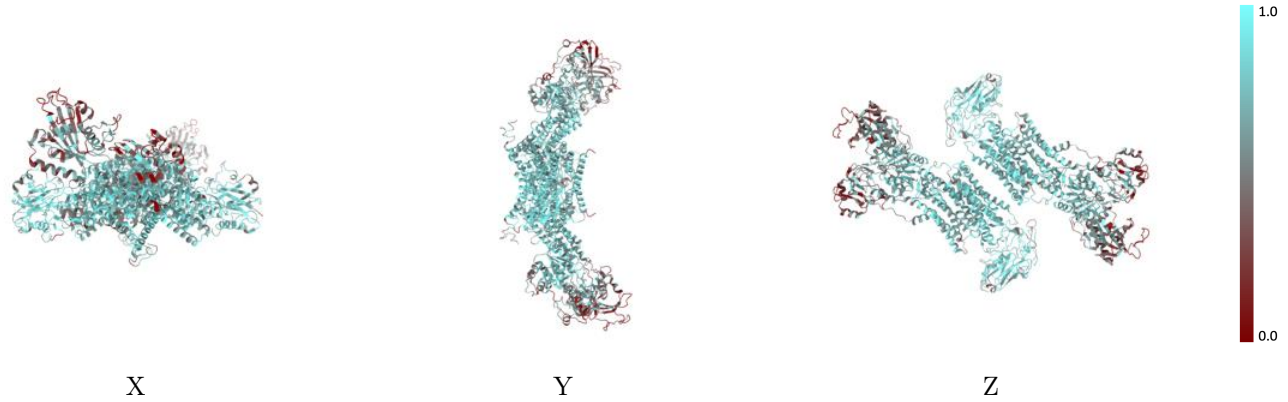
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



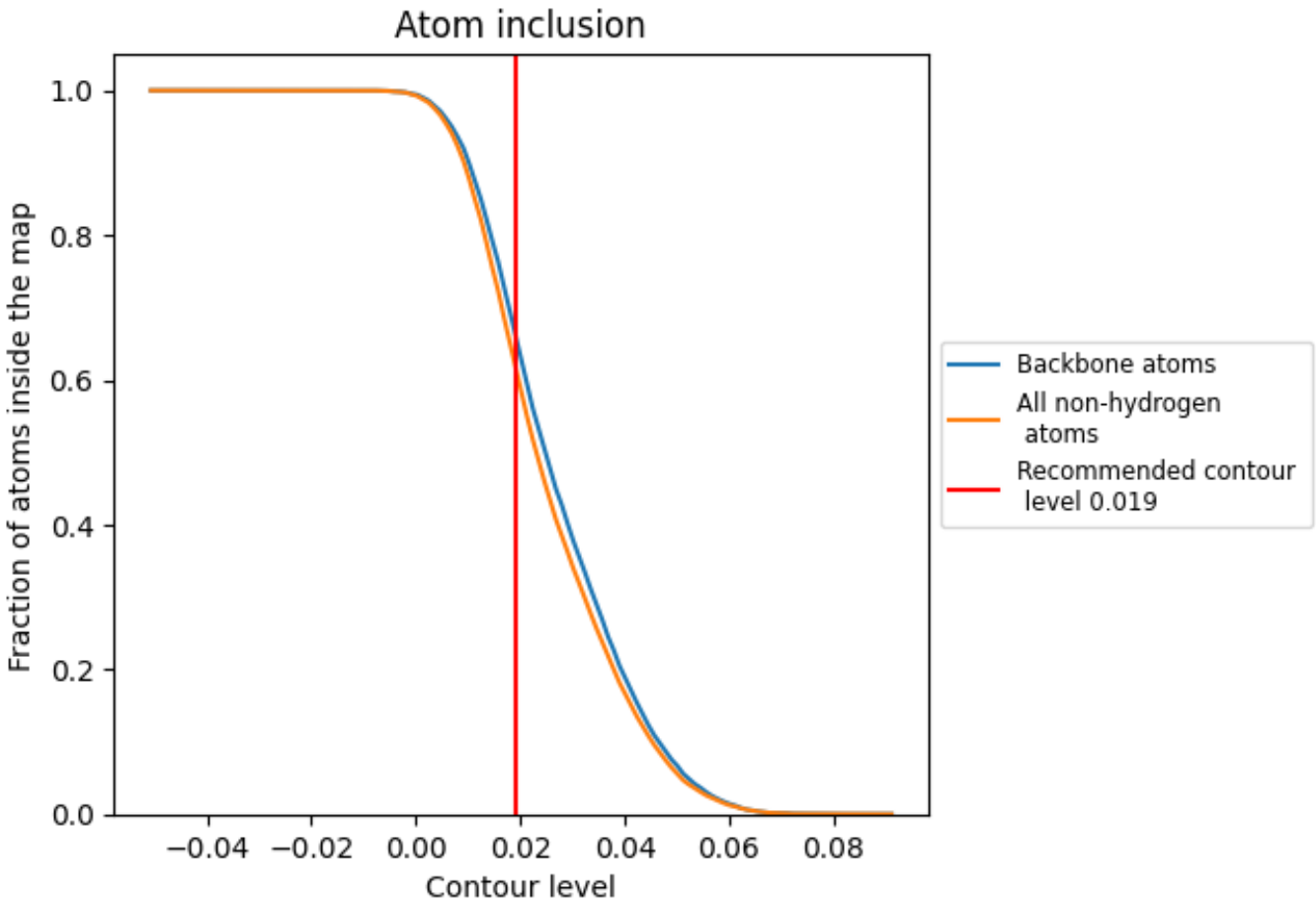
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6198	0.3850
A	0.6048	0.3790
B	0.7523	0.4320
C	0.6038	0.3780
D	0.7519	0.4330
E	0.5220	0.3420
F	0.3944	0.2600
G	0.5341	0.3470
H	0.0933	0.0990
I	0.1833	0.1710
J	0.1786	0.3360
K	0.3944	0.2570
L	0.0933	0.1090
M	0.2000	0.1660
N	0.1786	0.3270