wwPDB EM Validation Summary Report

Oct 19, 2026 – 06:29 PM JST

PDB ID	:	25YS / pdb_000025ys
EMDB ID	:	EMD-80481
Title	:	Cryo-EM structure of the Vo domain of Concanamycin A-bound V-ATPase on rat synaptic vesicles, state 3
Authors	:	Nishida, Y.; Yokoyama, K.
Deposited on	:	2026-04-23
Resolution	:	3.00 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:

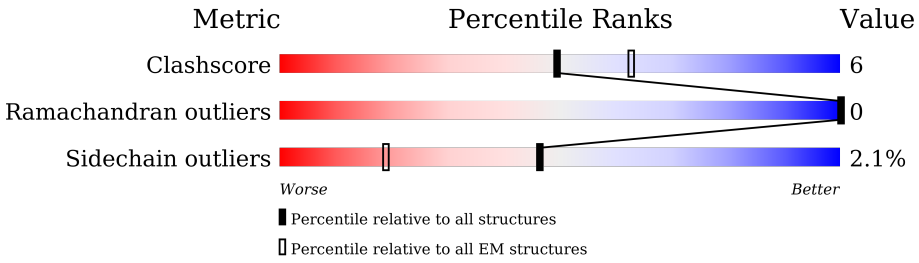
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

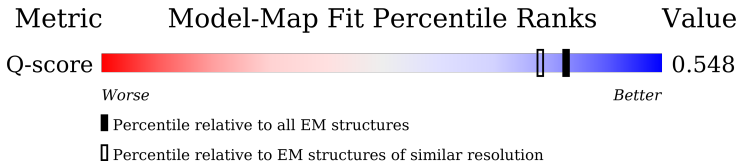
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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





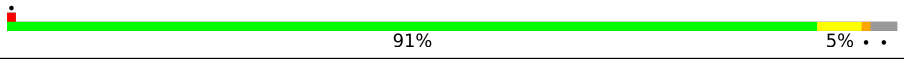
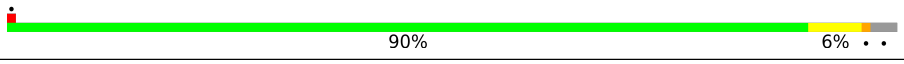
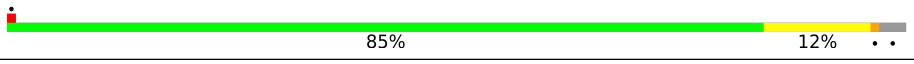
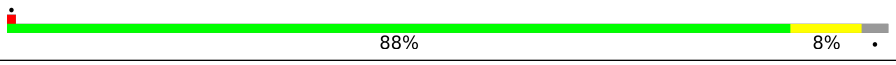
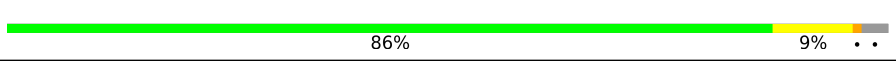
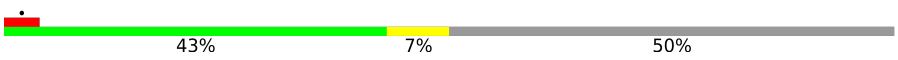
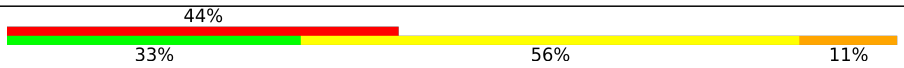
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	P	463	41% · 56%
2	b	205	87% 11% ·
3	d	351	92% 7% ·
4	e	81	77% 21% ··

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Mol	Chain	Length	Quality of chain
5	f	98	
6	h	155	
6	i	155	
6	j	155	
6	k	155	
6	l	155	
6	m	155	
6	n	155	
6	o	155	
6	r	155	
7	p	350	
8	H	226	
9	a	838	
10	Z	9	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 23318 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 V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	204	Total	C	N	O	S	0	0
			1652	1087	259	297	9		

- Molecule 2 is a protein called V-type proton ATPase 21 kDa proteolipid subunit c".

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

- Molecule 3 is a protein called V-type proton ATPase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	350	Total	C	N	O	S	0	0
			2833	1829	460	530	14		

- Molecule 4 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	80	Total	C	N	O	S	0	0
			644	443	100	98	3		

- Molecule 5 is a protein called Ribonuclease K.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	83	Total	C	N	O	S	0	0
			646	428	100	113	5		

- Molecule 6 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
6	j	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
6	k	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
6	l	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
6	m	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
6	n	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
6	o	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
6	r	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

- Molecule 7 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	p	52	Total	C	N	O	S	0	0
			432	290	63	76	3		

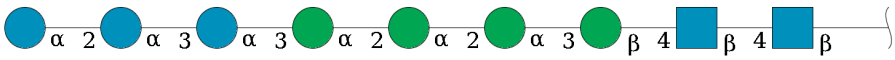
- Molecule 8 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	57	Total	C	N	O	0	0
			431	270	74	87		

- Molecule 9 is a protein called V-type proton ATPase 116 kDa subunit a 1.

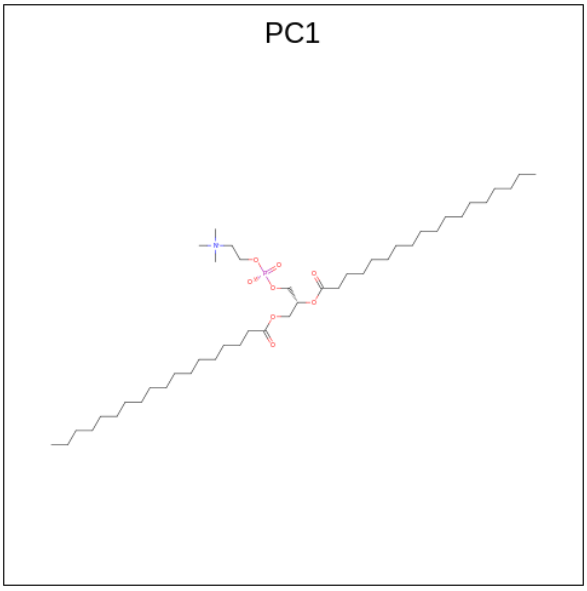
Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	415	Total	C	N	O	S	0	0
			3343	2244	525	551	23		

- Molecule 10 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



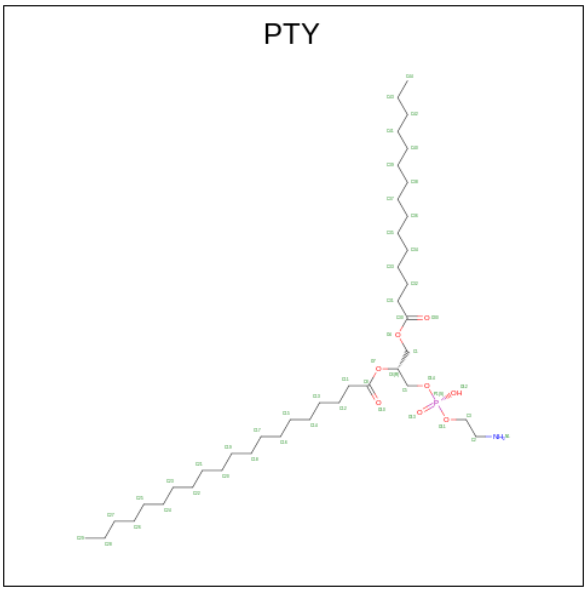
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



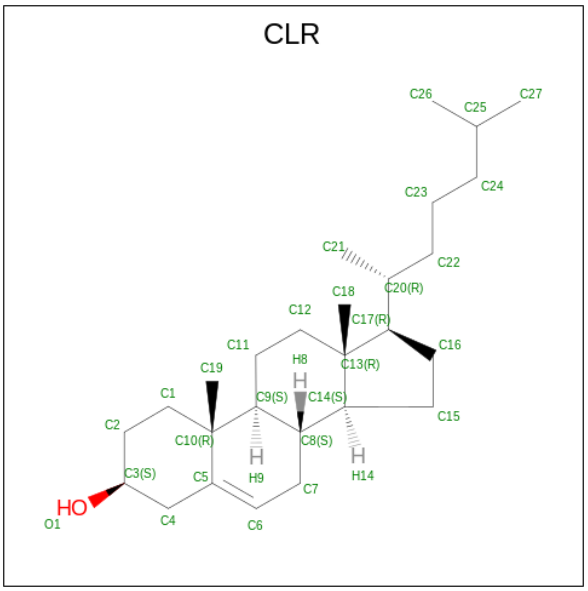
Mol	Chain	Residues	Atoms					AltConf
11	P	1	Total	C	N	O	P	0
			54	44	1	8	1	
11	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
11	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
11	k	1	Total	C	N	O	P	0
			54	44	1	8	1	
11	a	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 12 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
12	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	e	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	j	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
12	a	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 13 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



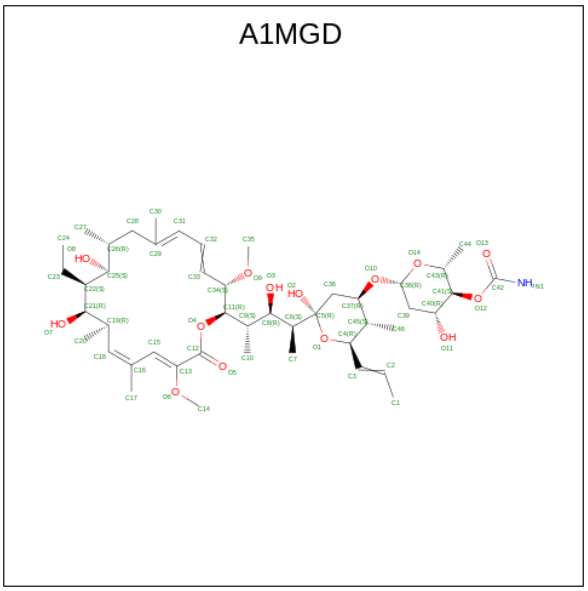
Mol	Chain	Residues	Atoms	AltConf
13	b	1	Total C O 28 27 1	0
13	h	1	Total C O 28 27 1	0
13	h	1	Total C O 28 27 1	0
13	i	1	Total C O 28 27 1	0
13	i	1	Total C O 28 27 1	0
13	i	1	Total C O 28 27 1	0
13	i	1	Total C O 28 27 1	0
13	j	1	Total C O 28 27 1	0
13	j	1	Total C O 28 27 1	0
13	j	1	Total C O 28 27 1	0
13	j	1	Total C O 28 27 1	0
13	k	1	Total C O 28 27 1	0
13	k	1	Total C O 28 27 1	0
13	k	1	Total C O 28 27 1	0

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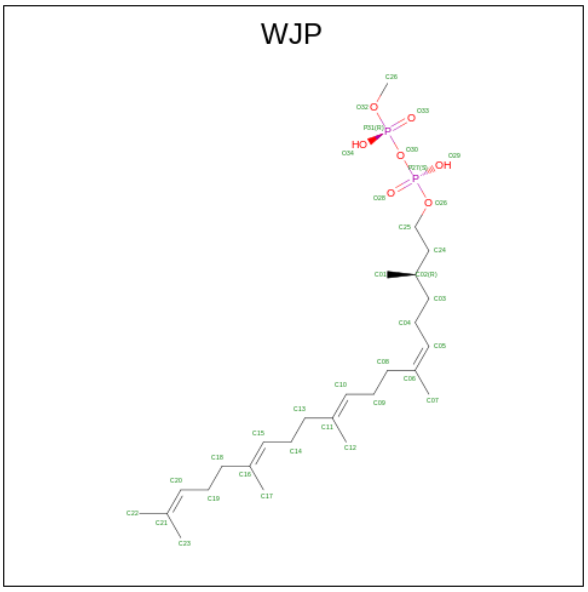
Mol	Chain	Residues	Atoms	AltConf
13	l	1	Total C O 28 27 1	0
13	l	1	Total C O 28 27 1	0
13	l	1	Total C O 28 27 1	0
13	l	1	Total C O 28 27 1	0
13	m	1	Total C O 28 27 1	0
13	m	1	Total C O 28 27 1	0
13	m	1	Total C O 28 27 1	0
13	m	1	Total C O 28 27 1	0
13	n	1	Total C O 28 27 1	0
13	n	1	Total C O 28 27 1	0
13	n	1	Total C O 28 27 1	0
13	n	1	Total C O 28 27 1	0
13	o	1	Total C O 28 27 1	0
13	o	1	Total C O 28 27 1	0
13	o	1	Total C O 28 27 1	0
13	o	1	Total C O 28 27 1	0

- Molecule 14 is concanamycin A (CCD ID: A1MGD) (formula: $C_{46}H_{75}NO_{14}$).



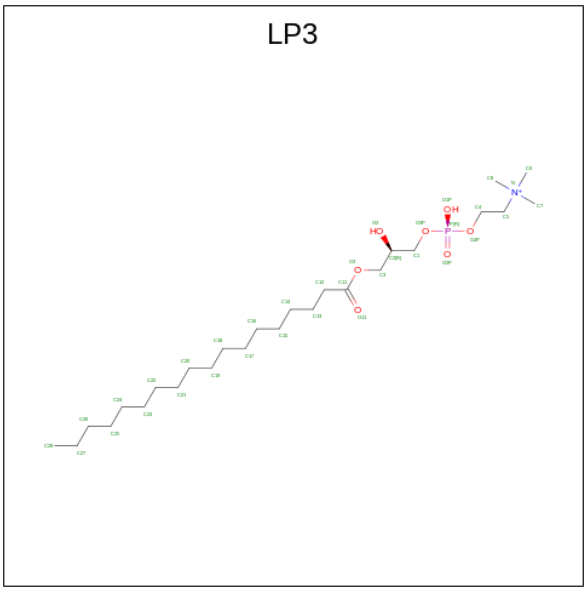
Mol	Chain	Residues	Atoms				AltConf
14	h	1	Total	C	N	O	0
			61	46	1	14	
14	i	1	Total	C	N	O	0
			61	46	1	14	
14	k	1	Total	C	N	O	0
			61	46	1	14	
14	l	1	Total	C	N	O	0
			61	46	1	14	
14	l	1	Total	C	N	O	0
			61	46	1	14	
14	n	1	Total	C	N	O	0
			61	46	1	14	
14	n	1	Total	C	N	O	0
			61	46	1	14	
14	a	1	Total	C	N	O	0
			61	46	1	14	

- Molecule 15 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (CCD ID: WJP) (formula: $C_{26}H_{48}O_7P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	a	1	34	25	7	2	0

- Molecule 16 is (7R)-4,7-DIHYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM 4-OXIDE (CCD ID: LP3) (formula: $C_{26}H_{55}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
16	a	1	35	26	1	7	1	0

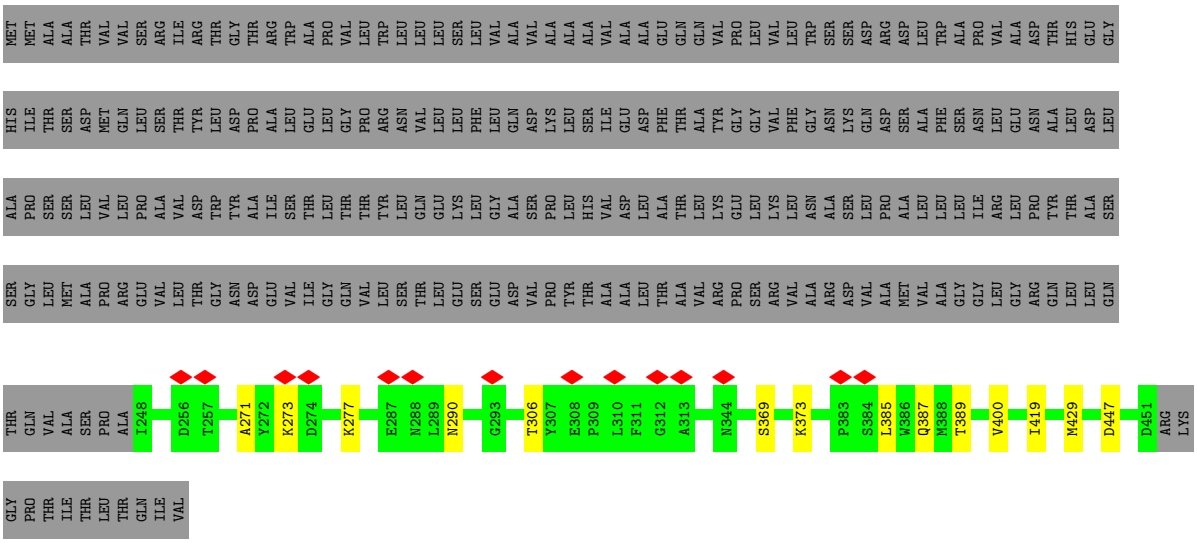
3 Residue-property plots (i)

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: V-type proton ATPase subunit S1

Chain P:

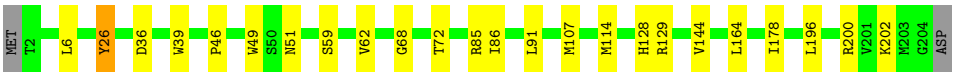




• Molecule 2: V-type proton ATPase 21 kDa proteolipid subunit c"

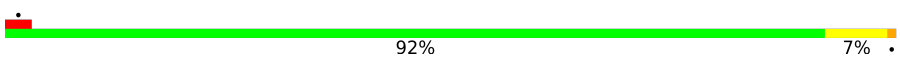
Chain b:

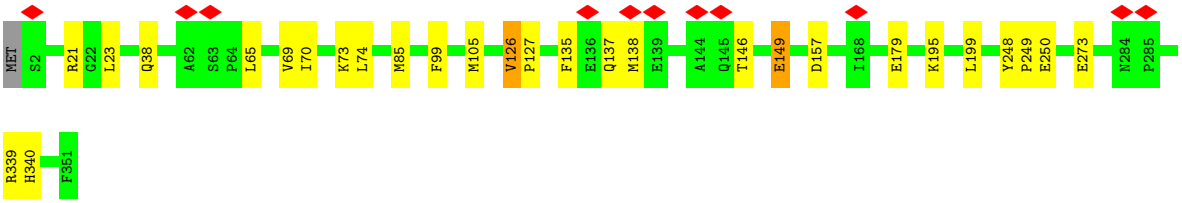




• Molecule 3: V-type proton ATPase subunit

Chain d:

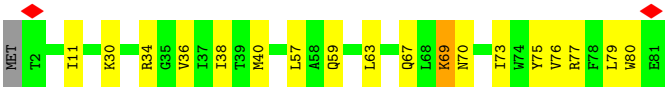




• Molecule 4: V-type proton ATPase subunit e 2

Chain e:

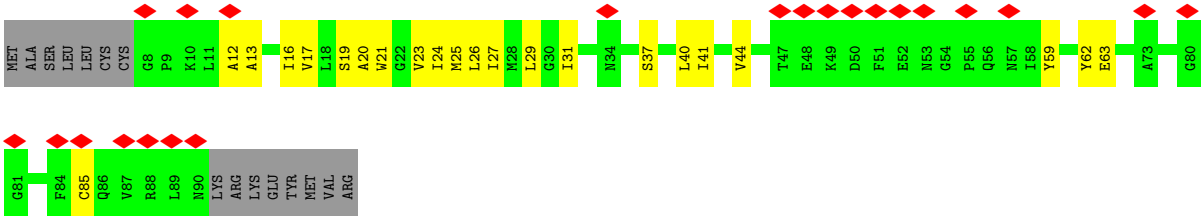




• Molecule 5: Ribonuclease K

Chain f:





• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

Chain h:

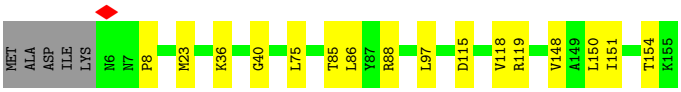




• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

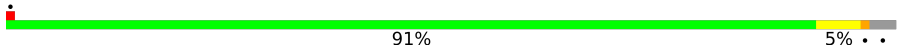
Chain i:





• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

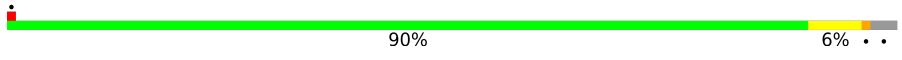
Chain j:

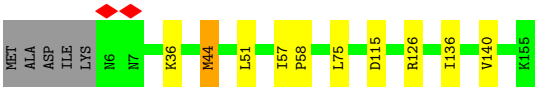




• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

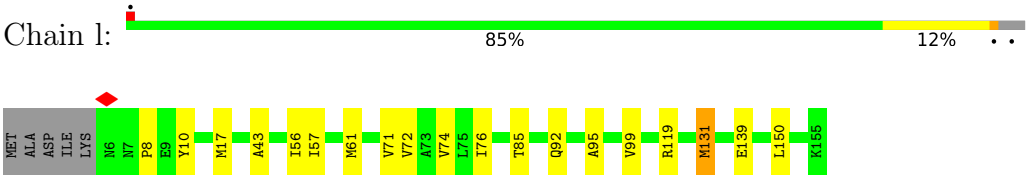
Chain k:





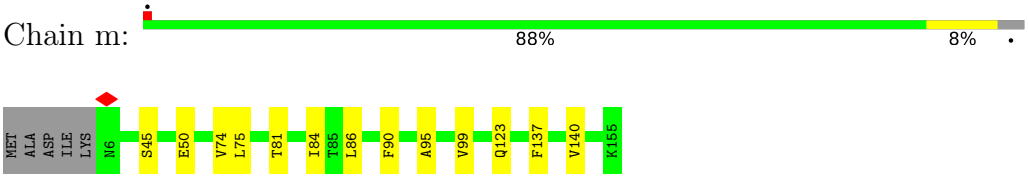
• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

Chain l:



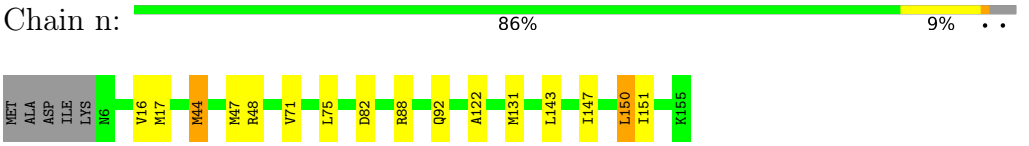
• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

Chain m:



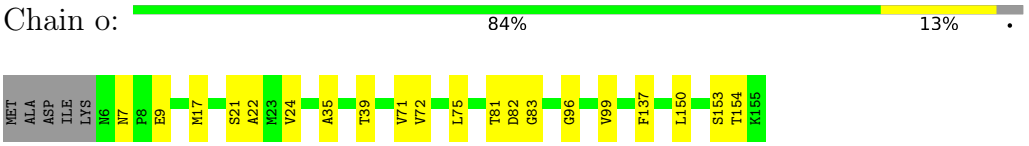
• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

Chain n:



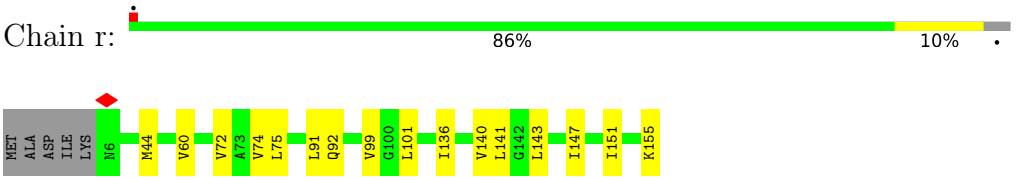
• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

Chain o:



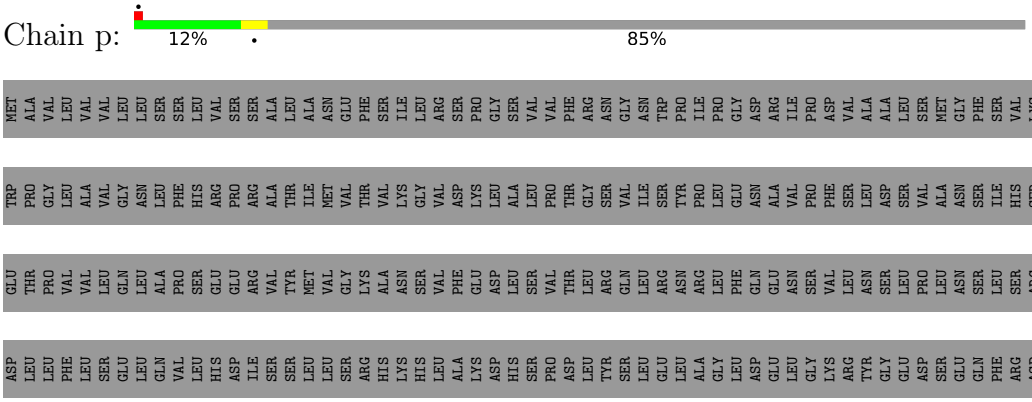
• Molecule 6: V-type proton ATPase 16 kDa proteolipid subunit c

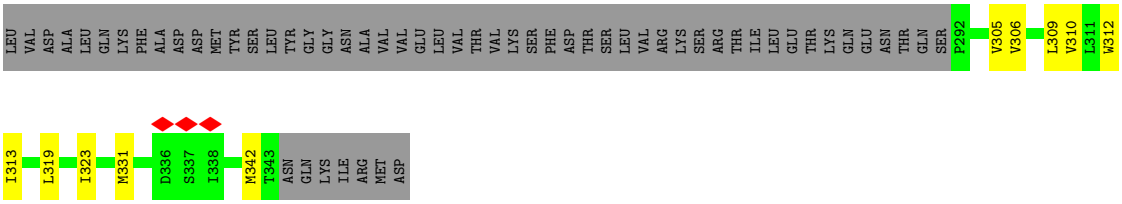
Chain r:



• Molecule 7: Renin receptor

Chain p:

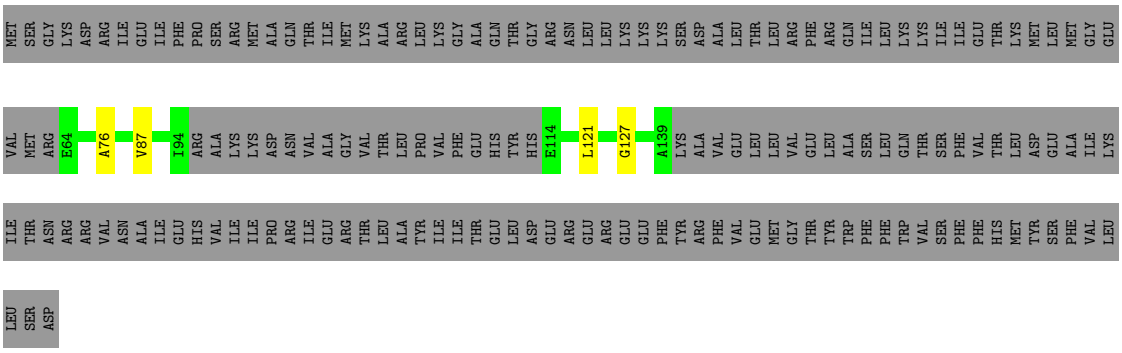




• Molecule 8: V-type proton ATPase subunit D

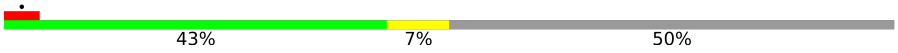
Chain H:

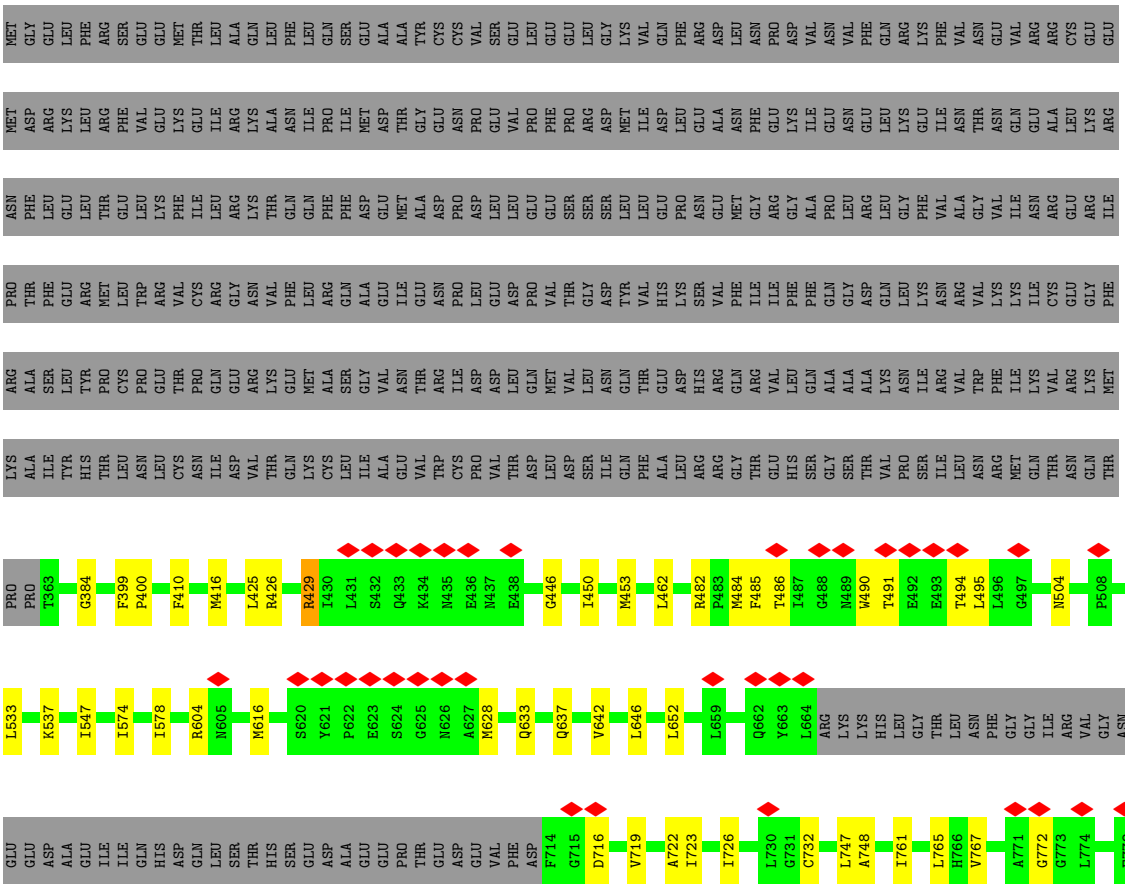


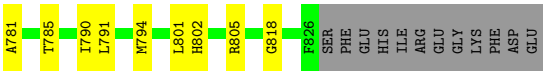


• Molecule 9: V-type proton ATPase 116 kDa subunit a 1

Chain a:



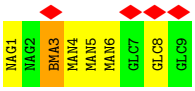




• Molecule 10: alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84902	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.189	Depositor
Minimum map value	-0.715	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.0, 425.0, 425.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0625, 1.0625, 1.0625	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, BMA, WJP, CLR, PC1, A1MGD, LP3, MAN, GLC, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	P	0.16	0/1707	0.28	0/2324
2	b	0.20	0/1537	0.33	0/2088
3	d	0.19	0/2899	0.30	0/3927
4	e	0.18	0/669	0.35	0/920
5	f	0.19	0/662	0.50	0/899
6	h	0.22	0/1083	0.37	0/1466
6	i	0.21	0/1083	0.33	0/1466
6	j	0.22	0/1083	0.34	0/1466
6	k	0.20	0/1083	0.36	0/1466
6	l	0.22	0/1083	0.32	0/1466
6	m	0.20	0/1083	0.30	0/1466
6	n	0.20	0/1083	0.32	0/1466
6	o	0.21	0/1083	0.34	0/1466
6	r	0.22	0/1083	0.33	0/1466
7	p	0.20	0/445	0.37	0/609
8	H	0.21	0/434	0.34	0/581
9	a	0.16	0/3450	0.30	0/4683
All	All	0.19	0/21550	0.33	0/29225

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1652	0	1584	10	0
2	b	1503	0	1551	15	0
3	d	2833	0	2770	20	0
4	e	644	0	659	16	0
5	f	646	0	642	15	0
6	h	1068	0	1136	10	0
6	i	1068	0	1136	11	0
6	j	1068	0	1136	7	0
6	k	1068	0	1136	5	0
6	l	1068	0	1136	15	0
6	m	1068	0	1136	9	0
6	n	1068	0	1136	13	0
6	o	1068	0	1136	13	0
6	r	1068	0	1136	12	0
7	p	432	0	428	8	0
8	H	431	0	428	2	0
9	a	3343	0	3361	43	0
10	Z	105	0	88	3	0
11	P	54	0	88	7	0
11	a	54	0	88	1	0
11	b	108	0	176	5	0
11	k	54	0	88	4	0
12	a	100	0	158	3	0
12	b	150	0	237	4	0
12	e	50	0	79	3	0
12	j	50	0	79	3	0
12	p	100	0	158	3	0
13	b	28	0	46	2	0
13	h	56	0	92	8	0
13	i	112	0	184	11	0
13	j	112	0	184	11	0
13	k	84	0	138	4	0
13	l	112	0	184	8	0
13	m	112	0	184	7	0
13	n	112	0	184	10	0
13	o	112	0	184	4	0
14	a	61	0	0	1	0
14	h	61	0	0	5	0
14	i	61	0	0	1	0
14	k	61	0	0	0	0
14	l	122	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	n	122	0	0	1	0
15	a	34	0	0	0	0
16	a	35	0	54	1	0
All	All	23318	0	24320	271	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 6.

The worst 5 of 271 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)
14:h:201:A1MGD:N1	14:h:201:A1MGD:C44	1.80	1.43
14:h:201:A1MGD:N1	14:h:201:A1MGD:C43	1.89	1.23
14:h:201:A1MGD:C44	14:h:201:A1MGD:C42	2.56	0.83
4:e:76:VAL:HG13	4:e:80:TRP:HB2	1.65	0.79
9:a:484:MET:HE1	9:a:504:ASN:HB3	1.66	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	P	202/463 (44%)	190 (94%)	12 (6%)	0	100	100
2	b	201/205 (98%)	200 (100%)	1 (0%)	0	100	100
3	d	348/351 (99%)	333 (96%)	15 (4%)	0	100	100
4	e	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
5	f	81/98 (83%)	78 (96%)	3 (4%)	0	100	100
6	h	148/155 (96%)	148 (100%)	0	0	100	100
6	i	148/155 (96%)	148 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	j	148/155 (96%)	148 (100%)	0	0	100	100
6	k	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
6	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
6	m	148/155 (96%)	148 (100%)	0	0	100	100
6	n	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
6	o	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
6	r	148/155 (96%)	148 (100%)	0	0	100	100
7	p	50/350 (14%)	47 (94%)	3 (6%)	0	100	100
8	H	53/226 (24%)	52 (98%)	1 (2%)	0	100	100
9	a	411/838 (49%)	402 (98%)	9 (2%)	0	100	100
All	All	2756/4007 (69%)	2707 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	182/395 (46%)	181 (100%)	1 (0%)	81	89
2	b	156/158 (99%)	150 (96%)	6 (4%)	29	63
3	d	305/306 (100%)	299 (98%)	6 (2%)	48	76
4	e	67/68 (98%)	65 (97%)	2 (3%)	36	69
5	f	69/83 (83%)	68 (99%)	1 (1%)	59	80
6	h	109/113 (96%)	104 (95%)	5 (5%)	24	58
6	i	109/113 (96%)	106 (97%)	3 (3%)	38	70
6	j	109/113 (96%)	107 (98%)	2 (2%)	51	77
6	k	109/113 (96%)	106 (97%)	3 (3%)	38	70
6	l	109/113 (96%)	107 (98%)	2 (2%)	51	77
6	m	109/113 (96%)	105 (96%)	4 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	n	109/113 (96%)	106 (97%)	3 (3%)	38 70
6	o	109/113 (96%)	108 (99%)	1 (1%)	70 85
6	r	109/113 (96%)	106 (97%)	3 (3%)	38 70
7	p	47/313 (15%)	47 (100%)	0	100 100
8	H	43/195 (22%)	42 (98%)	1 (2%)	44 74
9	a	360/743 (48%)	356 (99%)	4 (1%)	65 83
All	All	2210/3278 (67%)	2163 (98%)	47 (2%)	46 75

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	k	115	ASP
6	n	44	MET
6	l	85	THR
6	m	50	GLU
6	n	150	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
9	a	504	ASN
8	H	86	ASN
6	j	124	GLN
7	p	330	ASN
6	j	78	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

9 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	$\#\|Z\| > 2$
10	NAG	Z	1	10	14,14,15	0.80	0	17,19,21	0.76	0
10	NAG	Z	2	10	14,14,15	0.75	0	17,19,21	0.86	0
10	BMA	Z	3	10	11,11,12	0.86	0	15,15,17	2.08	4 (26%)
10	MAN	Z	4	10	11,11,12	0.75	0	15,15,17	1.06	1 (6%)
10	MAN	Z	5	10	11,11,12	0.82	1 (9%)	15,15,17	1.08	1 (6%)
10	MAN	Z	6	10	11,11,12	0.86	1 (9%)	15,15,17	0.96	0
10	GLC	Z	7	10	11,11,12	0.63	0	15,15,17	0.67	0
10	GLC	Z	8	10	11,11,12	0.58	0	15,15,17	1.02	1 (6%)
10	GLC	Z	9	10	11,11,12	0.58	0	15,15,17	0.86	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
10	NAG	Z	1	10	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	4	10	-	2/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	0/2/19/22	0/1/1/1
10	MAN	Z	6	10	-	1/2/19/22	0/1/1/1
10	GLC	Z	7	10	-	0/2/19/22	0/1/1/1
10	GLC	Z	8	10	-	0/2/19/22	0/1/1/1
10	GLC	Z	9	10	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	6	MAN	O5-C1	-2.18	1.40	1.43
10	Z	5	MAN	O5-C1	-2.08	1.40	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	3	BMA	C1-O5-C5	5.73	119.95	112.19
10	Z	4	MAN	C1-O5-C5	2.74	115.91	112.19
10	Z	3	BMA	C3-C4-C5	2.73	115.12	110.24
10	Z	5	MAN	C1-O5-C5	2.48	115.56	112.19
10	Z	3	BMA	C2-C3-C4	2.33	114.93	110.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	Z	4	MAN	O5-C5-C6-O6
10	Z	4	MAN	C4-C5-C6-O6
10	Z	6	MAN	O5-C5-C6-O6

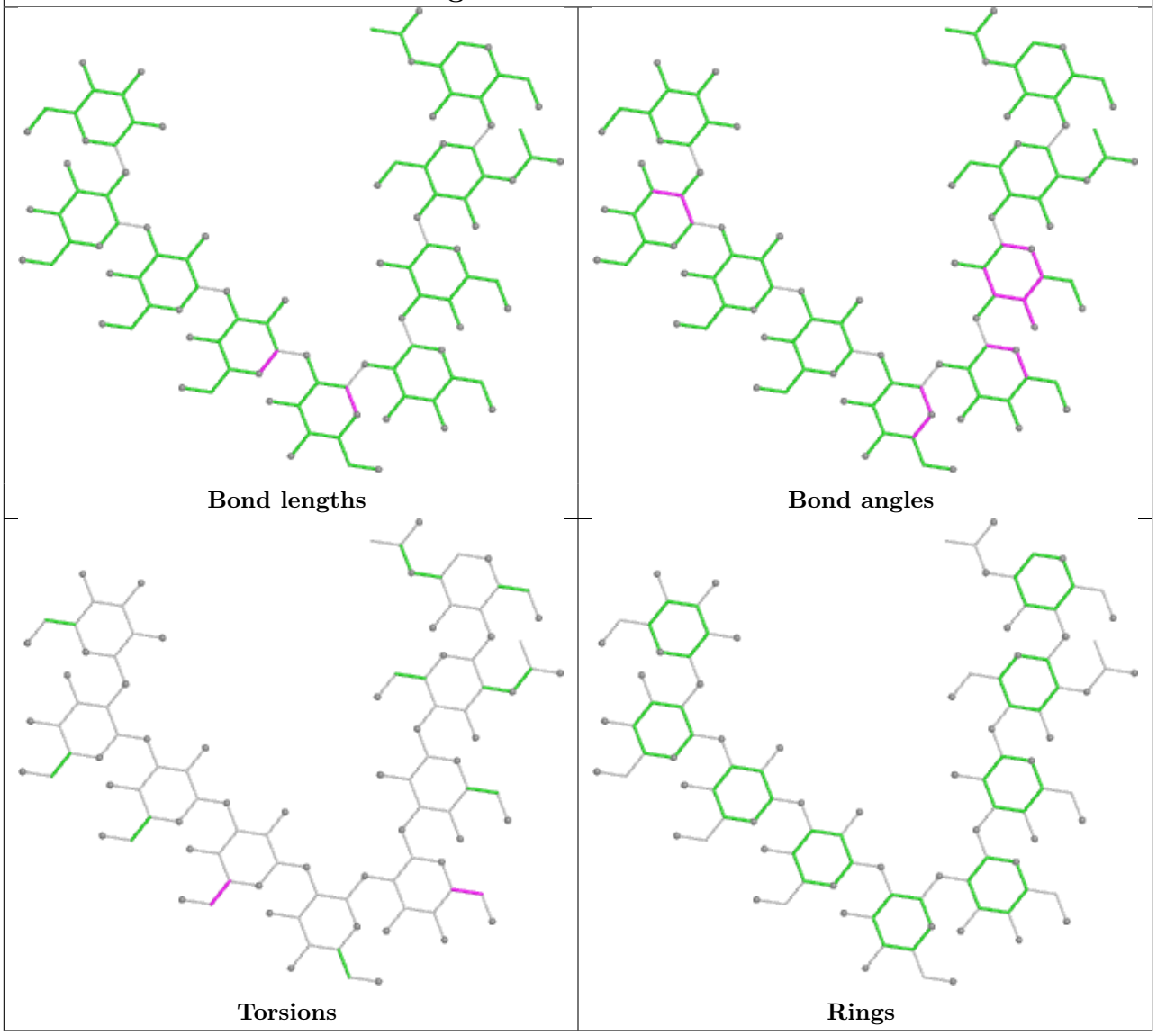
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Z	1	NAG	1	0
10	Z	3	BMA	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 oligosaccharide.

Oligosaccharide Chain Z



5.6 Ligand geometry (i)

54 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	PTY	b	306	-	49,49,49	0.46	0	52,54,54	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLR	n	205	-	31,31,31	0.35	0	48,48,48	0.58	0
13	CLR	o	203	-	31,31,31	0.37	0	48,48,48	0.52	0
11	PC1	b	302	-	53,53,53	0.49	0	59,61,61	0.55	1 (1%)
13	CLR	i	205	-	31,31,31	0.38	0	48,48,48	0.58	0
13	CLR	o	202	-	31,31,31	0.39	0	48,48,48	0.60	0
11	PC1	P	501	-	53,53,53	0.49	0	59,61,61	0.50	1 (1%)
12	PTY	e	101	-	49,49,49	0.45	0	52,54,54	0.42	0
13	CLR	n	206	-	31,31,31	0.36	0	48,48,48	0.56	0
14	A1MGD	l	201	-	60,63,63	0.72	2 (3%)	63,90,90	0.96	4 (6%)
14	A1MGD	n	202	-	60,63,63	0.69	2 (3%)	63,90,90	1.16	6 (9%)
15	WJP	a	902	-	31,33,34	0.48	0	39,43,44	0.54	1 (2%)
13	CLR	l	206	-	31,31,31	0.37	0	48,48,48	0.52	0
13	CLR	n	203	-	31,31,31	0.40	0	48,48,48	0.56	0
13	CLR	o	201	-	31,31,31	0.37	0	48,48,48	0.62	0
13	CLR	l	204	-	31,31,31	0.38	0	48,48,48	0.67	0
12	PTY	a	906	-	49,49,49	0.46	0	52,54,54	0.40	0
11	PC1	b	301	-	53,53,53	0.50	0	59,61,61	0.52	1 (1%)
13	CLR	h	203	-	31,31,31	0.38	0	48,48,48	0.49	0
13	CLR	j	203	-	31,31,31	0.36	0	48,48,48	0.50	0
13	CLR	k	203	-	31,31,31	0.38	0	48,48,48	0.67	0
14	A1MGD	i	201	-	60,63,63	0.68	2 (3%)	63,90,90	1.18	6 (9%)
14	A1MGD	l	202	-	60,63,63	0.68	2 (3%)	63,90,90	1.01	4 (6%)
13	CLR	l	205	-	31,31,31	0.37	0	48,48,48	0.48	0
12	PTY	p	401	-	49,49,49	0.47	0	52,54,54	0.41	0
12	PTY	a	905	-	49,49,49	0.46	0	52,54,54	0.40	0
13	CLR	k	202	-	31,31,31	0.36	0	48,48,48	0.57	0
13	CLR	o	204	-	31,31,31	0.38	0	48,48,48	0.50	0
16	LP3	a	903	-	34,34,34	0.52	0	39,41,41	0.52	0
11	PC1	a	904	-	53,53,53	0.48	0	59,61,61	0.49	1 (1%)
13	CLR	i	203	-	31,31,31	0.36	0	48,48,48	0.57	0
12	PTY	p	402	-	49,49,49	0.46	0	52,54,54	0.40	0
13	CLR	m	201	-	31,31,31	0.37	0	48,48,48	0.56	0
12	PTY	b	304	-	49,49,49	0.47	0	52,54,54	0.45	0
13	CLR	i	202	-	31,31,31	0.37	0	48,48,48	0.55	0
13	CLR	m	203	-	31,31,31	0.39	0	48,48,48	0.52	0
14	A1MGD	h	201	-	60,63,63	0.68	2 (3%)	63,90,90	1.22	5 (7%)
13	CLR	n	204	-	31,31,31	0.36	0	48,48,48	0.61	0
13	CLR	m	202	-	31,31,31	0.36	0	48,48,48	0.51	0
13	CLR	h	202	-	31,31,31	0.38	0	48,48,48	0.61	0
11	PC1	k	205	-	53,53,53	0.49	0	59,61,61	0.50	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	CLR	j	204	-	31,31,31	0.44	0	48,48,48	0.86	1 (2%)
12	PTY	b	303	-	49,49,49	0.49	0	52,54,54	0.45	0
12	PTY	j	201	-	49,49,49	0.46	0	52,54,54	0.43	0
14	A1MGD	k	201	-	60,63,63	0.70	2 (3%)	63,90,90	1.18	7 (11%)
13	CLR	k	204	-	31,31,31	0.38	0	48,48,48	0.54	0
13	CLR	m	204	-	31,31,31	0.38	0	48,48,48	0.68	1 (2%)
14	A1MGD	n	201	-	60,63,63	0.73	2 (3%)	63,90,90	1.22	5 (7%)
13	CLR	b	305	-	31,31,31	0.44	0	48,48,48	0.56	0
13	CLR	l	203	-	31,31,31	0.37	0	48,48,48	0.63	0
14	A1MGD	a	901	-	60,63,63	0.69	2 (3%)	63,90,90	0.96	3 (4%)
13	CLR	j	202	-	31,31,31	0.36	0	48,48,48	0.56	0
13	CLR	j	205	-	31,31,31	0.36	0	48,48,48	0.66	0
13	CLR	i	204	-	31,31,31	0.38	0	48,48,48	0.54	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
12	PTY	b	306	-	-	20/53/53/53	-
13	CLR	n	205	-	-	1/10/68/68	0/4/4/4
13	CLR	o	203	-	-	9/10/68/68	0/4/4/4
11	PC1	b	302	-	-	25/57/57/57	-
13	CLR	i	205	-	-	4/10/68/68	0/4/4/4
13	CLR	o	202	-	-	2/10/68/68	0/4/4/4
11	PC1	P	501	-	-	19/57/57/57	-
12	PTY	e	101	-	-	21/53/53/53	-
13	CLR	n	206	-	-	5/10/68/68	0/4/4/4
14	A1MGD	l	201	-	-	47/81/115/115	0/2/3/3
14	A1MGD	n	202	-	-	40/81/115/115	1/2/3/3
15	WJP	a	902	-	-	3/37/37/40	-
13	CLR	l	206	-	-	4/10/68/68	0/4/4/4
13	CLR	n	203	-	-	10/10/68/68	0/4/4/4
13	CLR	o	201	-	-	0/10/68/68	0/4/4/4
13	CLR	l	204	-	-	2/10/68/68	0/4/4/4
12	PTY	a	906	-	-	20/53/53/53	-
11	PC1	b	301	-	-	18/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLR	h	203	-	-	8/10/68/68	0/4/4/4
13	CLR	j	203	-	-	7/10/68/68	0/4/4/4
13	CLR	k	203	-	-	3/10/68/68	0/4/4/4
14	A1MGD	i	201	-	-	40/81/115/115	1/2/3/3
14	A1MGD	l	202	-	-	38/81/115/115	1/2/3/3
13	CLR	l	205	-	-	6/10/68/68	0/4/4/4
12	PTY	p	401	-	-	16/53/53/53	-
12	PTY	a	905	-	-	21/53/53/53	-
13	CLR	k	202	-	-	2/10/68/68	0/4/4/4
13	CLR	o	204	-	-	5/10/68/68	0/4/4/4
16	LP3	a	903	-	-	8/36/36/36	-
11	PC1	a	904	-	-	32/57/57/57	-
13	CLR	i	203	-	-	6/10/68/68	0/4/4/4
12	PTY	p	402	-	-	24/53/53/53	-
13	CLR	m	201	-	-	8/10/68/68	0/4/4/4
12	PTY	b	304	-	-	19/53/53/53	-
13	CLR	i	202	-	-	2/10/68/68	0/4/4/4
13	CLR	m	203	-	-	6/10/68/68	0/4/4/4
14	A1MGD	h	201	-	-	49/81/115/115	0/2/3/3
13	CLR	n	204	-	-	2/10/68/68	0/4/4/4
13	CLR	m	202	-	-	6/10/68/68	0/4/4/4
13	CLR	h	202	-	-	4/10/68/68	0/4/4/4
11	PC1	k	205	-	-	25/57/57/57	-
13	CLR	j	204	-	-	8/10/68/68	0/4/4/4
12	PTY	b	303	-	-	26/53/53/53	-
12	PTY	j	201	-	-	23/53/53/53	-
14	A1MGD	k	201	-	-	45/81/115/115	0/2/3/3
13	CLR	k	204	-	-	5/10/68/68	0/4/4/4
13	CLR	m	204	-	-	6/10/68/68	0/4/4/4
14	A1MGD	n	201	-	-	36/81/115/115	0/2/3/3
13	CLR	b	305	-	-	1/10/68/68	0/4/4/4
13	CLR	l	203	-	-	1/10/68/68	0/4/4/4
14	A1MGD	a	901	-	-	32/81/115/115	0/2/3/3
13	CLR	j	202	-	-	10/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLR	j	205	-	-	4/10/68/68	0/4/4/4
13	CLR	i	204	-	-	5/10/68/68	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	k	201	A1MGD	C15-C16	-3.69	1.38	1.45
14	n	202	A1MGD	C15-C16	-3.61	1.38	1.45
14	a	901	A1MGD	C15-C16	-3.58	1.38	1.45
14	h	201	A1MGD	C15-C16	-3.54	1.38	1.45
14	l	202	A1MGD	C15-C16	-3.50	1.38	1.45

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	h	201	A1MGD	C19-C21-C22	5.87	126.88	114.95
14	k	201	A1MGD	C19-C21-C22	5.24	125.59	114.95
14	n	202	A1MGD	C19-C21-C22	5.12	125.36	114.95
14	l	202	A1MGD	C19-C21-C22	5.05	125.20	114.95
14	i	201	A1MGD	C19-C21-C22	4.92	124.95	114.95

There are no chirality outliers.

5 of 789 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	P	501	PC1	C11-O13-P-O12
11	P	501	PC1	C11-O13-P-O14
11	P	501	PC1	C11-O13-P-O11
11	P	501	PC1	C22-C21-O21-C2
11	b	301	PC1	C11-O13-P-O12

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	n	202	A1MGD	C38-C39-C40-C41-C43-O14
14	l	202	A1MGD	C38-C39-C40-C41-C43-O14
14	i	201	A1MGD	C38-C39-C40-C41-C43-O14

47 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	b	306	PTY	2	0
13	n	205	CLR	2	0
13	o	203	CLR	2	0
11	b	302	PC1	2	0
13	i	205	CLR	3	0
11	P	501	PC1	7	0
12	e	101	PTY	3	0
13	n	206	CLR	3	0
14	n	202	A1MGD	1	0
13	l	206	CLR	3	0
13	n	203	CLR	5	0
13	l	204	CLR	3	0
12	a	906	PTY	1	0
11	b	301	PC1	3	0
13	h	203	CLR	5	0
13	j	203	CLR	3	0
13	k	203	CLR	1	0
14	i	201	A1MGD	1	0
14	l	202	A1MGD	5	0
13	l	205	CLR	3	0
12	p	401	PTY	2	0
12	a	905	PTY	2	0
13	k	202	CLR	1	0
13	o	204	CLR	2	0
16	a	903	LP3	1	0
11	a	904	PC1	1	0
13	i	203	CLR	3	0
12	p	402	PTY	1	0
13	m	201	CLR	4	0
12	b	304	PTY	1	0
13	i	202	CLR	5	0
13	m	203	CLR	2	0
14	h	201	A1MGD	5	0
13	n	204	CLR	1	0
13	m	202	CLR	1	0
13	h	202	CLR	5	0
11	k	205	PC1	4	0
13	j	204	CLR	4	0
12	b	303	PTY	1	0
12	j	201	PTY	3	0
13	k	204	CLR	3	0
13	b	305	CLR	2	0
13	l	203	CLR	1	0

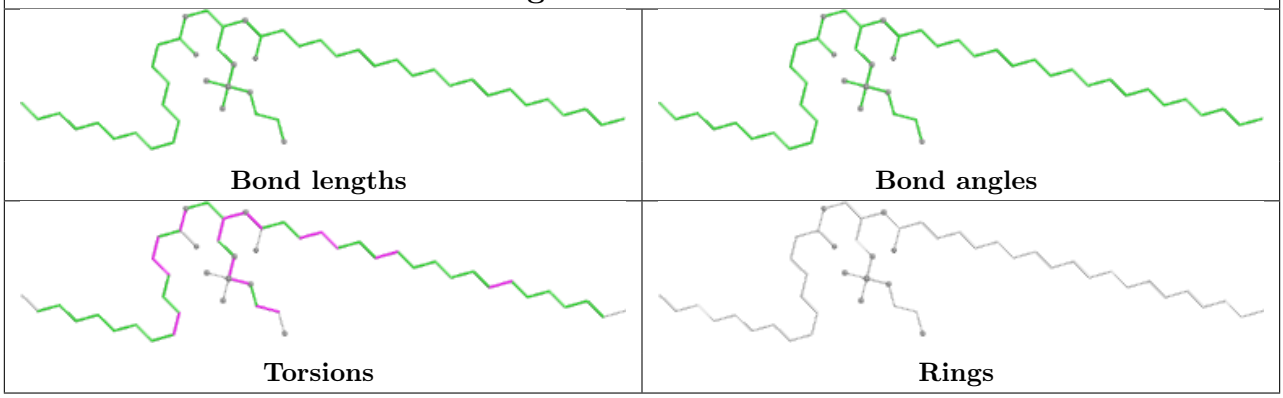
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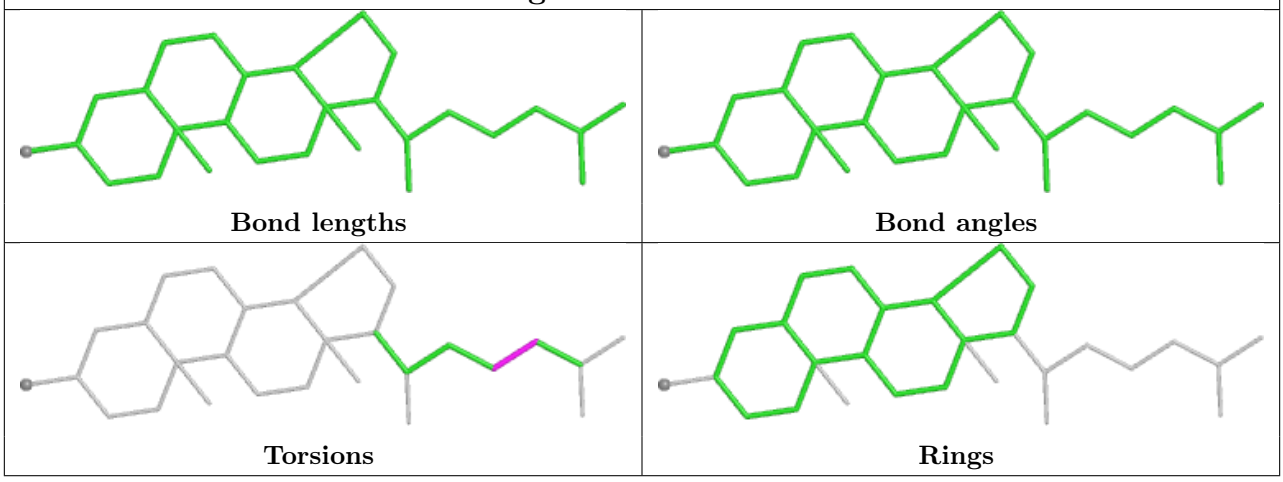
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	901	A1MGD	1	0
13	j	202	CLR	4	0
13	j	205	CLR	2	0
13	i	204	CLR	2	0

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.

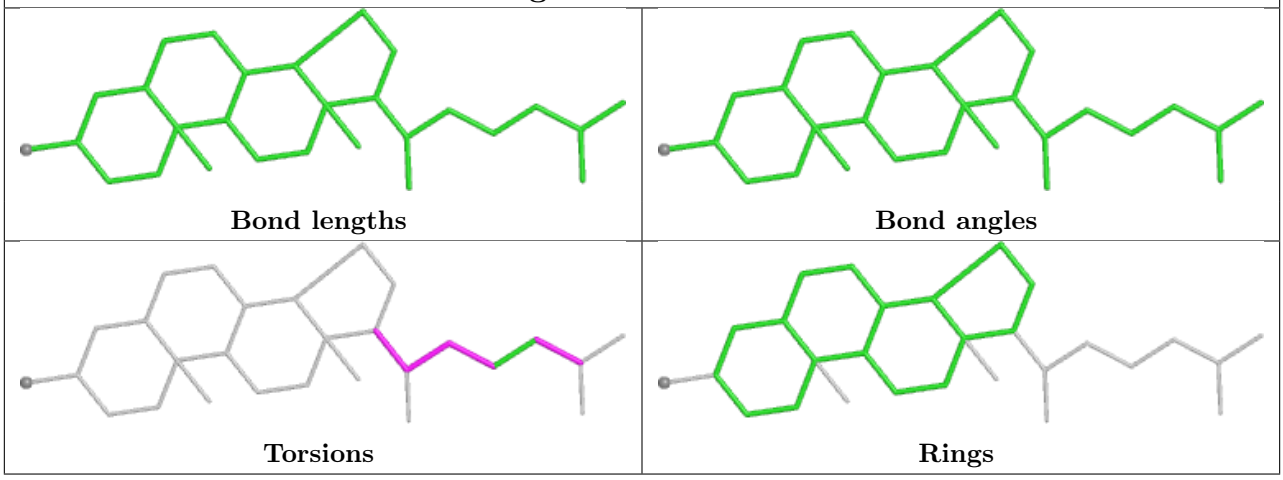
Ligand PTY b 306



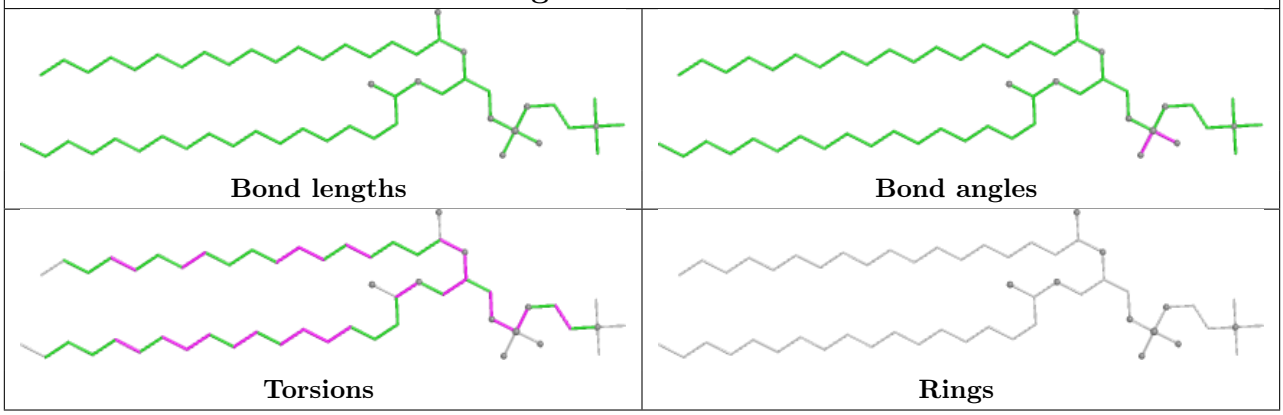
Ligand CLR n 205



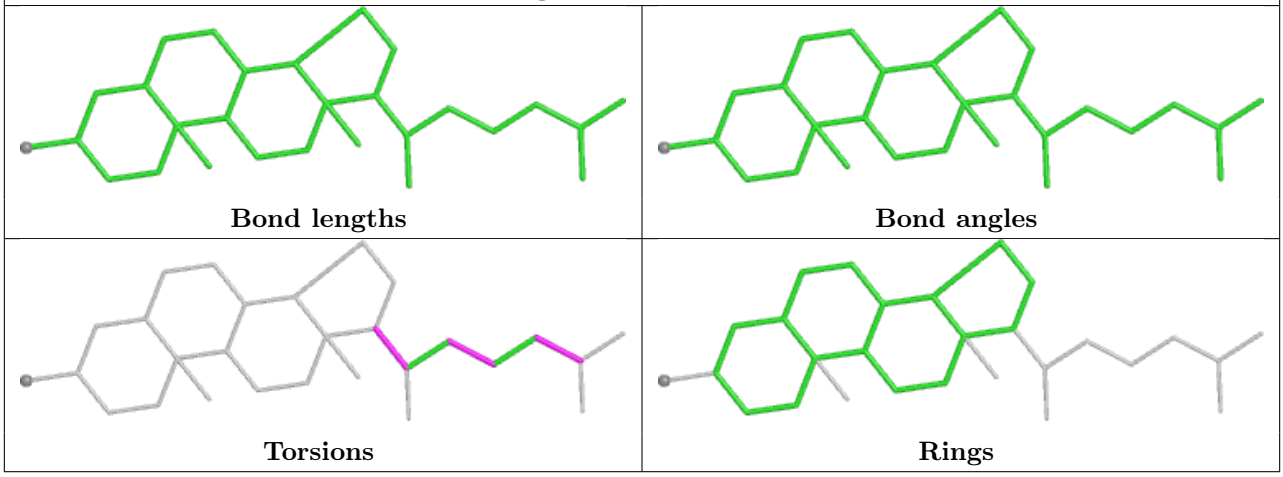
Ligand CLR o 203



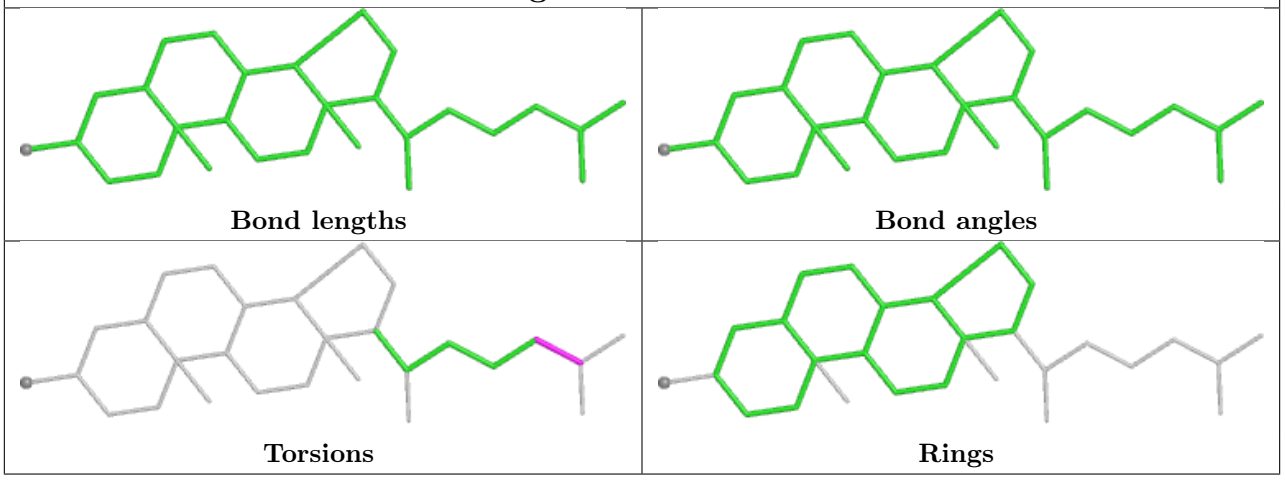
Ligand PC1 b 302



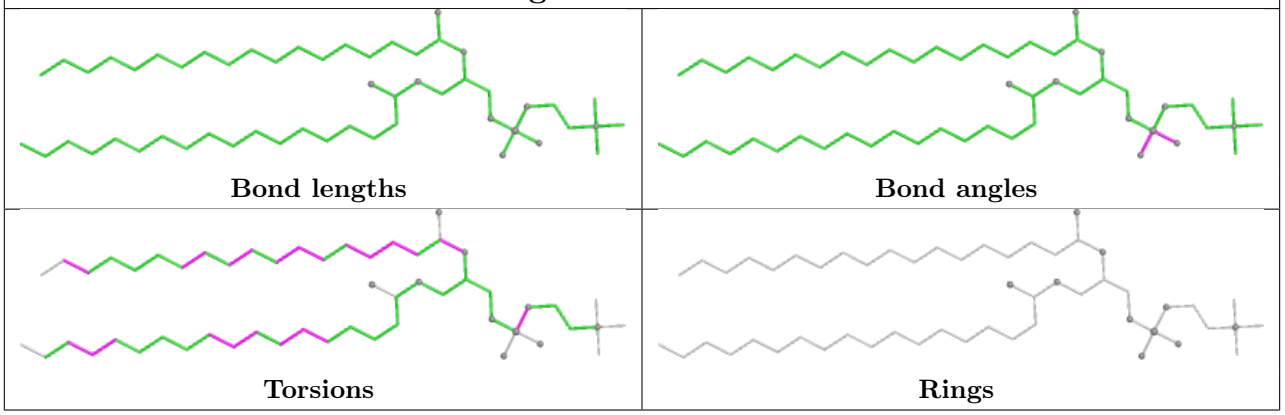
Ligand CLR i 205



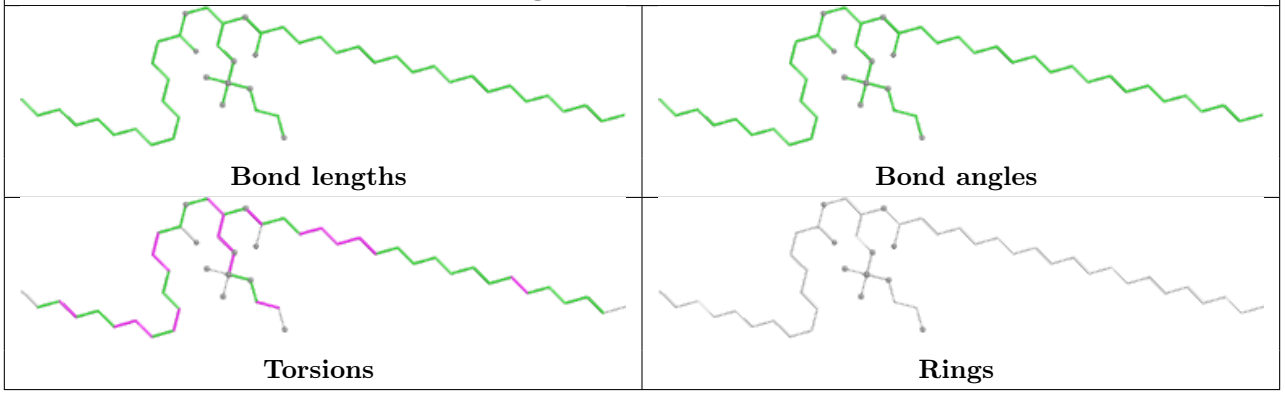
Ligand CLR o 202



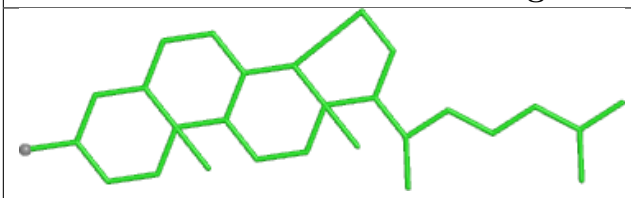
Ligand PC1 P 501



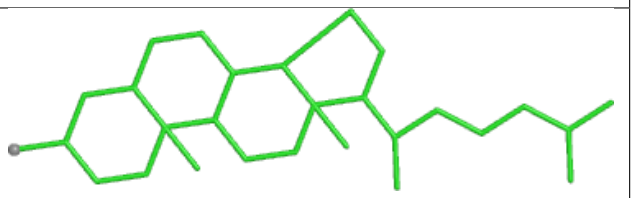
Ligand PTY e 101



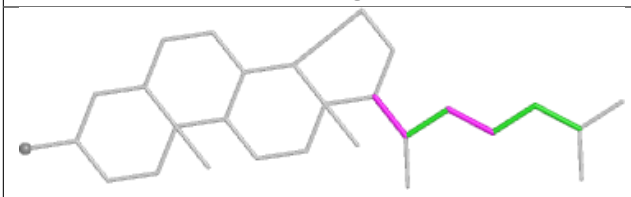
Ligand CLR n 206



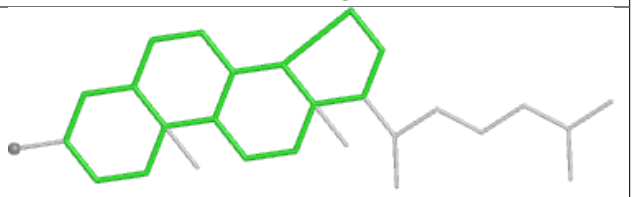
Bond lengths



Bond angles

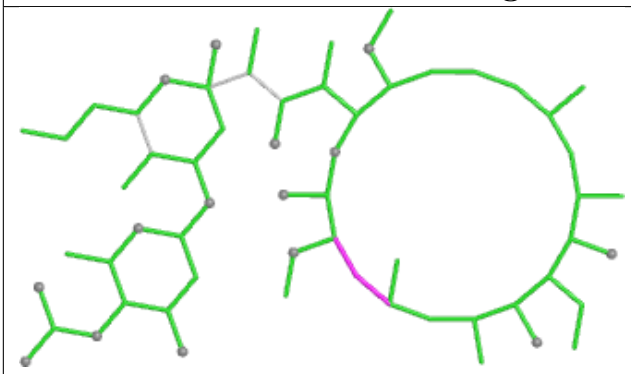


Torsions

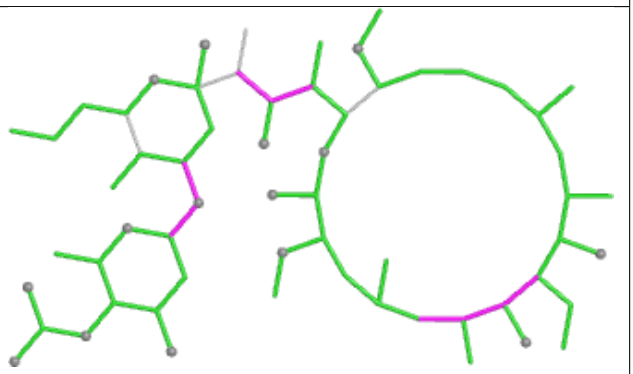


Rings

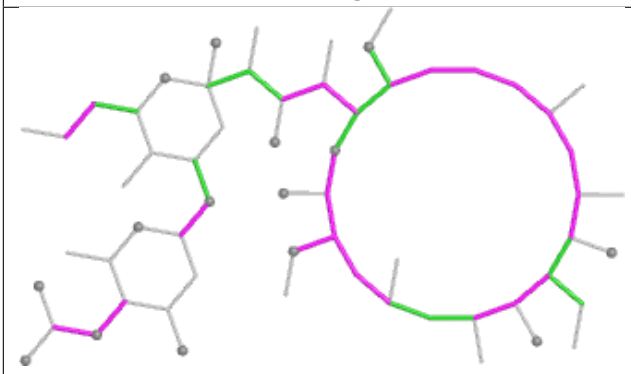
Ligand A1MGD l 201



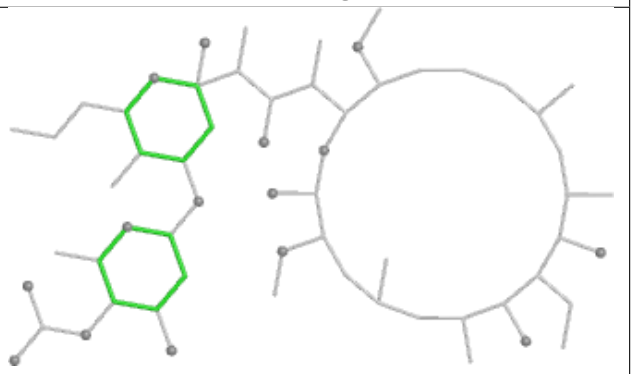
Bond lengths



Bond angles

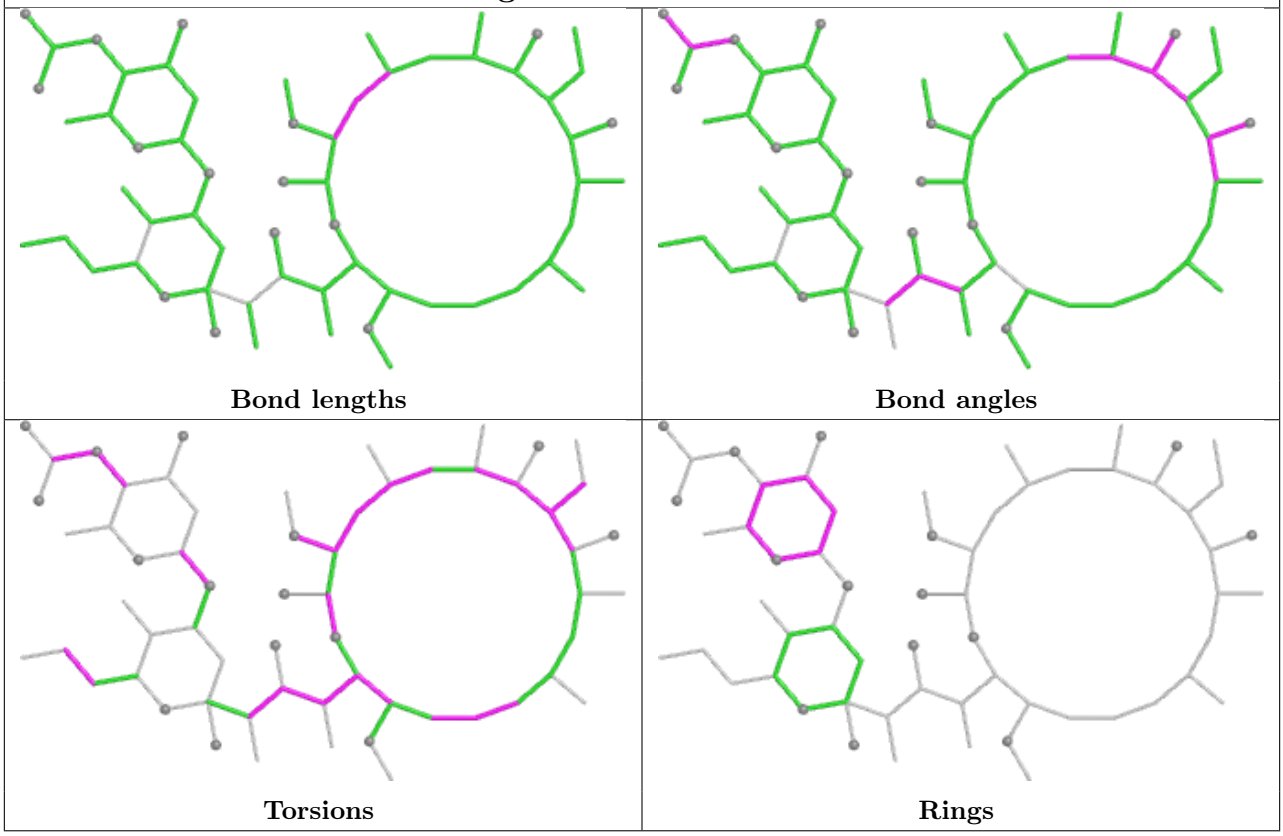


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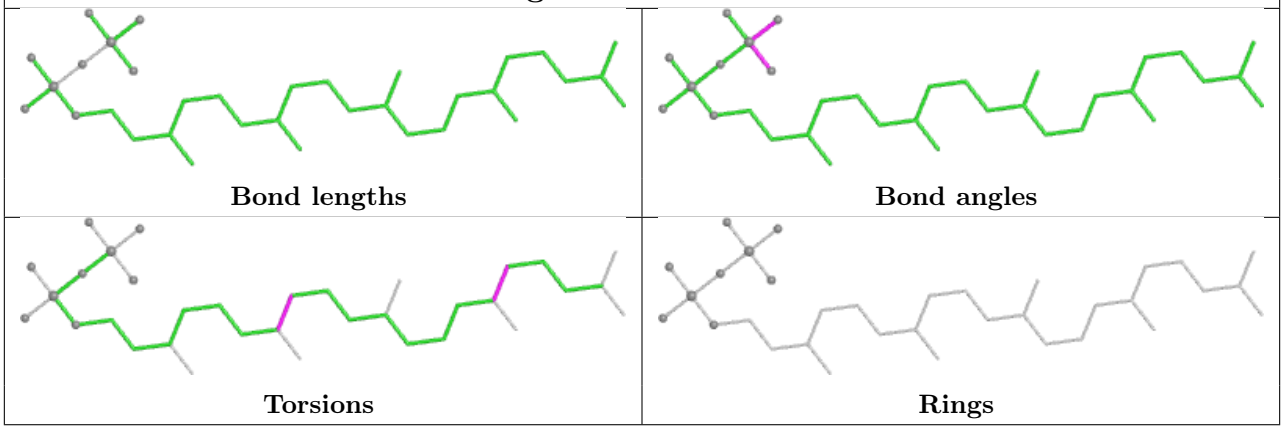


Rings

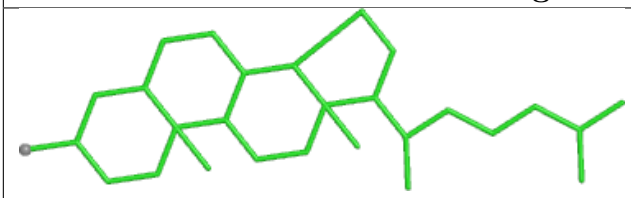
Ligand A1MGD n 202



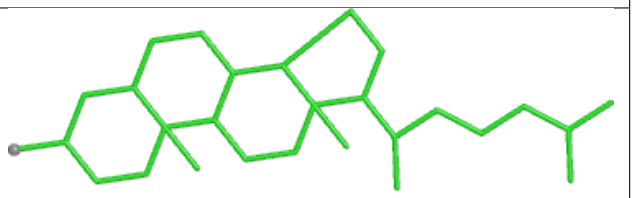
Ligand WJP a 902



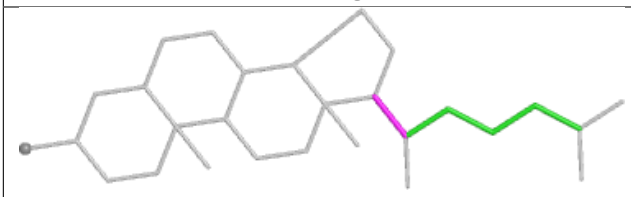
Ligand CLR l 206



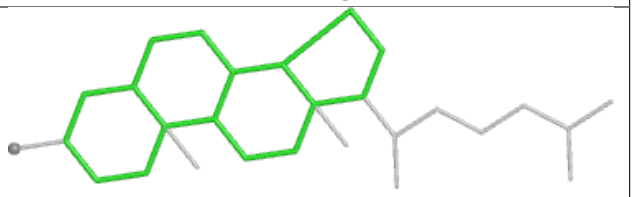
Bond lengths



Bond angles

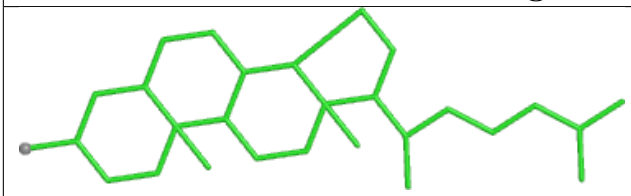


Torsions

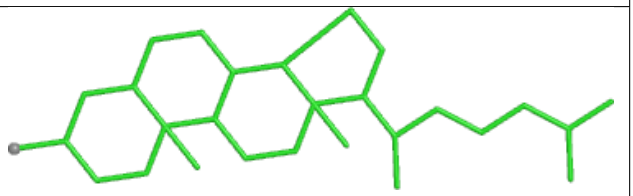


Rings

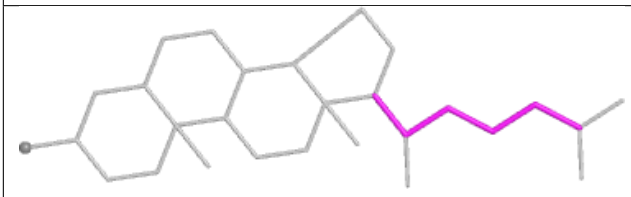
Ligand CLR n 203



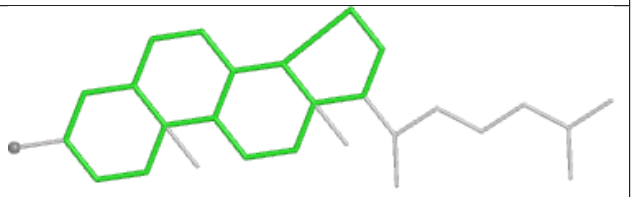
Bond lengths



Bond angles

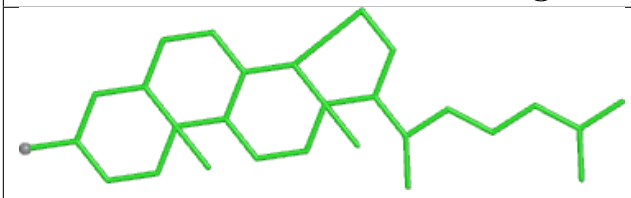


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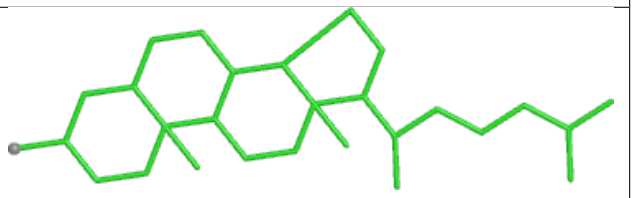


Rings

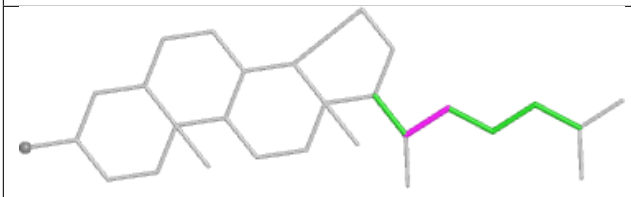
Ligand CLR l 204



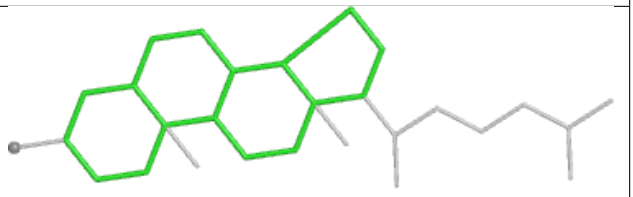
Bond lengths



Bond angles

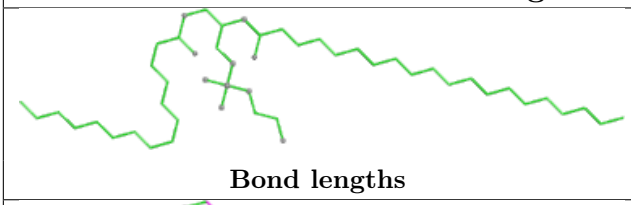


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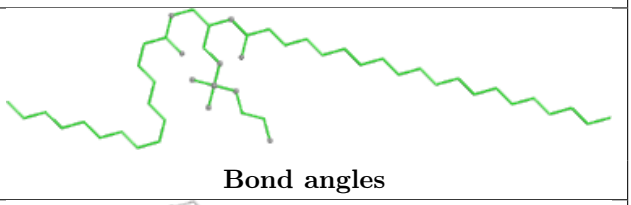


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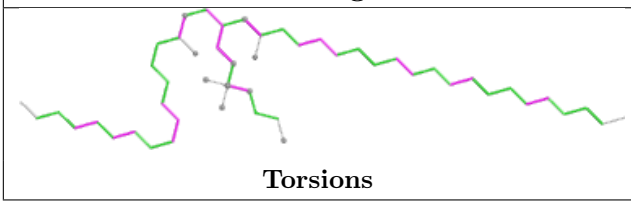
Ligand PTY a 906



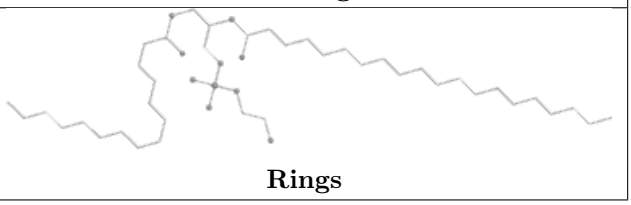
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Bond angles

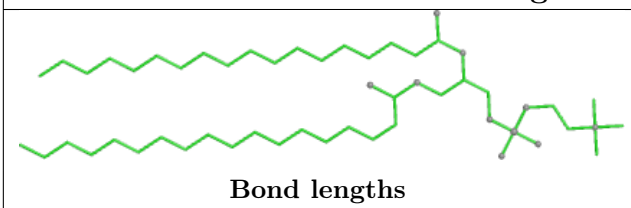


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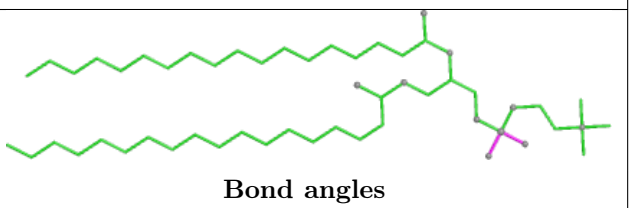


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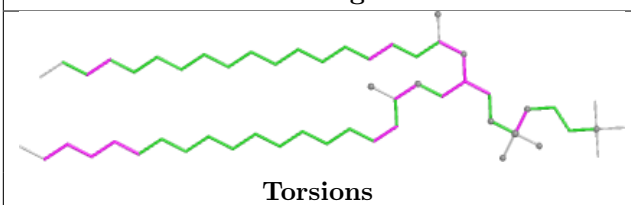
Ligand PC1 b 301



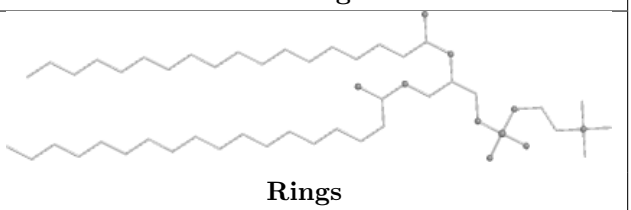
Bond lengths



Bond angles

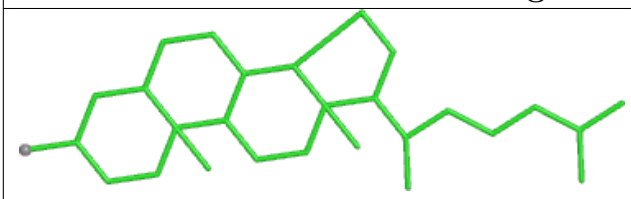


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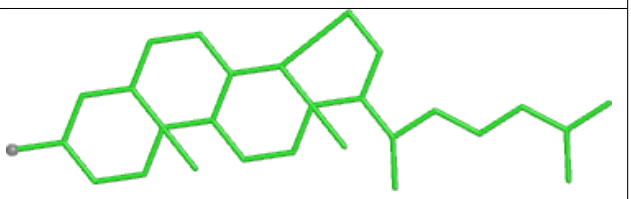


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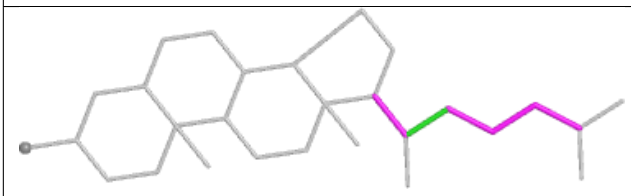
Ligand CLR h 203



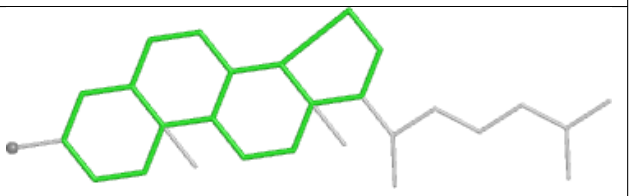
Bond lengths



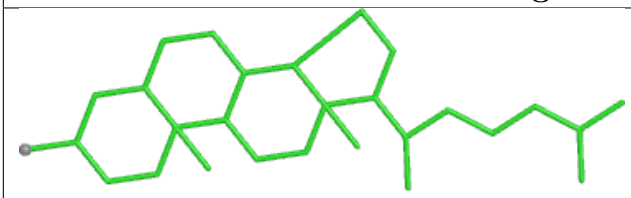
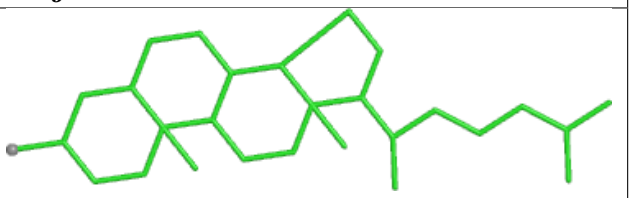
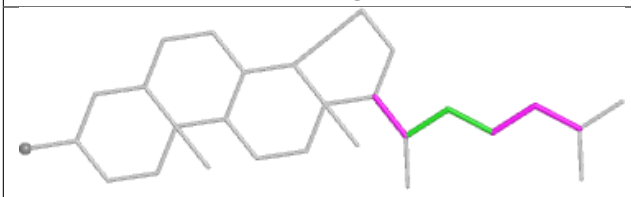
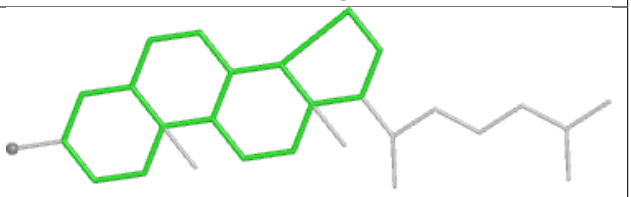
Bond angles

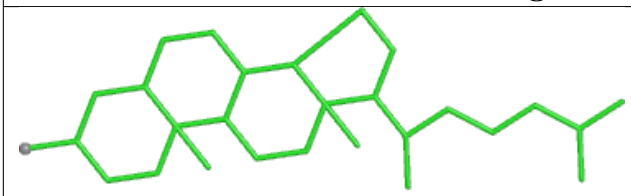
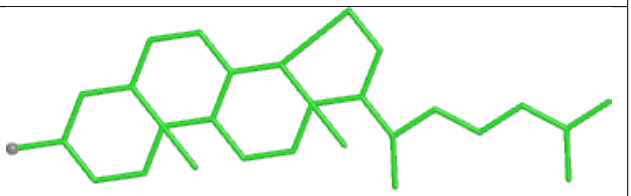
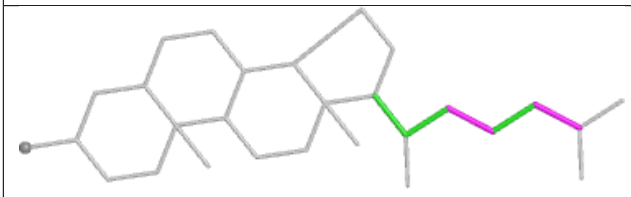
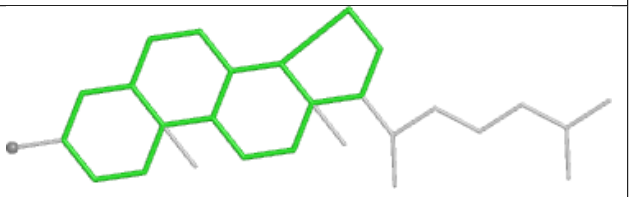


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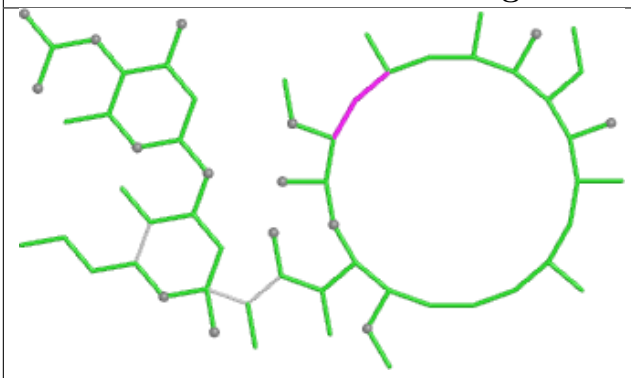


Rings

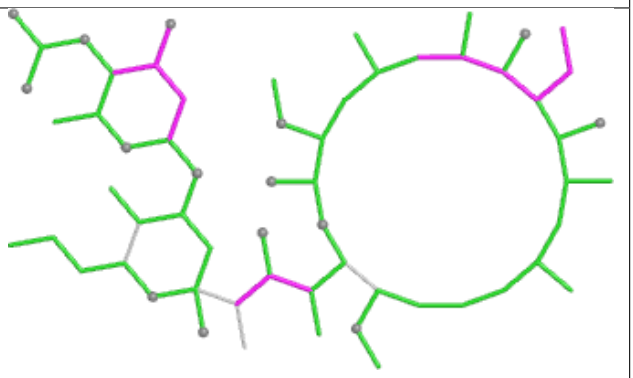
Ligand CLR j 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLR k 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

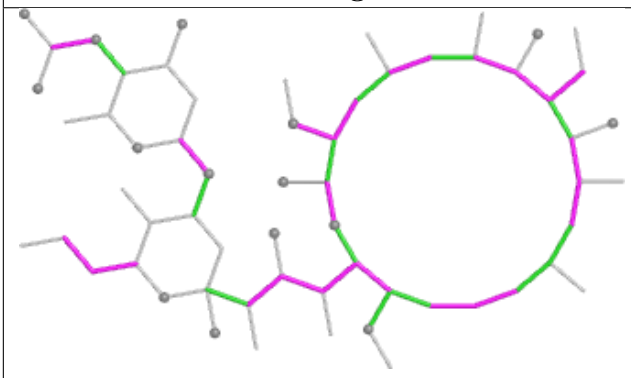
Ligand A1MGD i 201



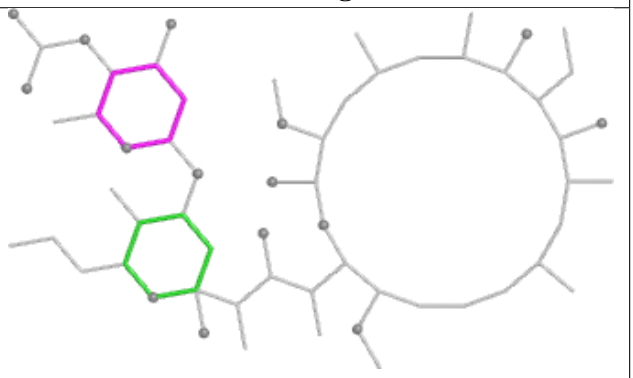
Bond lengths



Bond angles

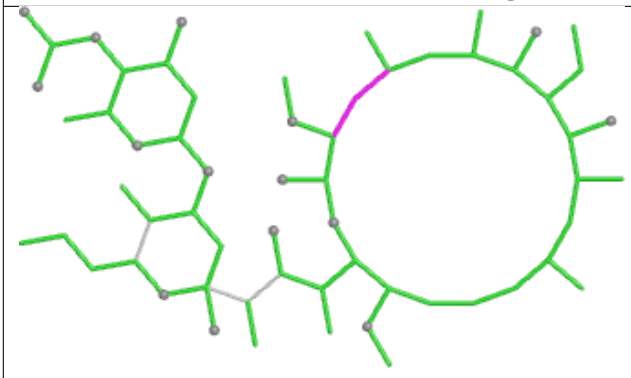


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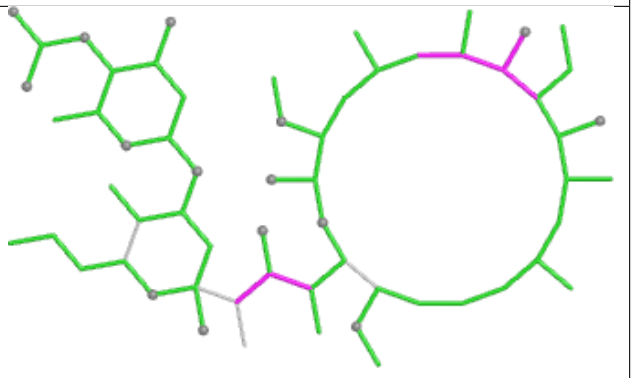


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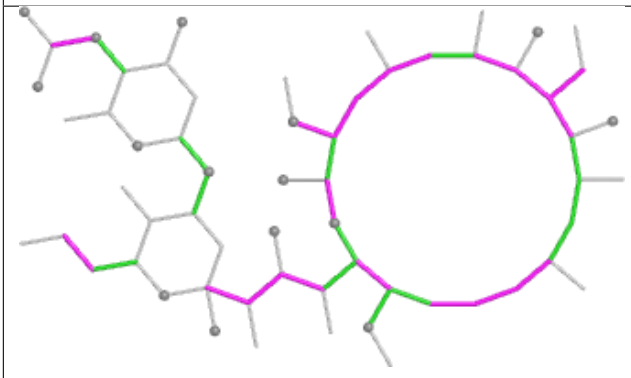
Ligand A1MGD l 202



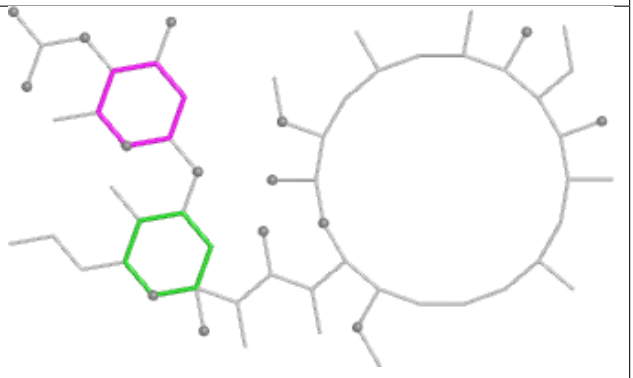
Bond lengths



Bond angles

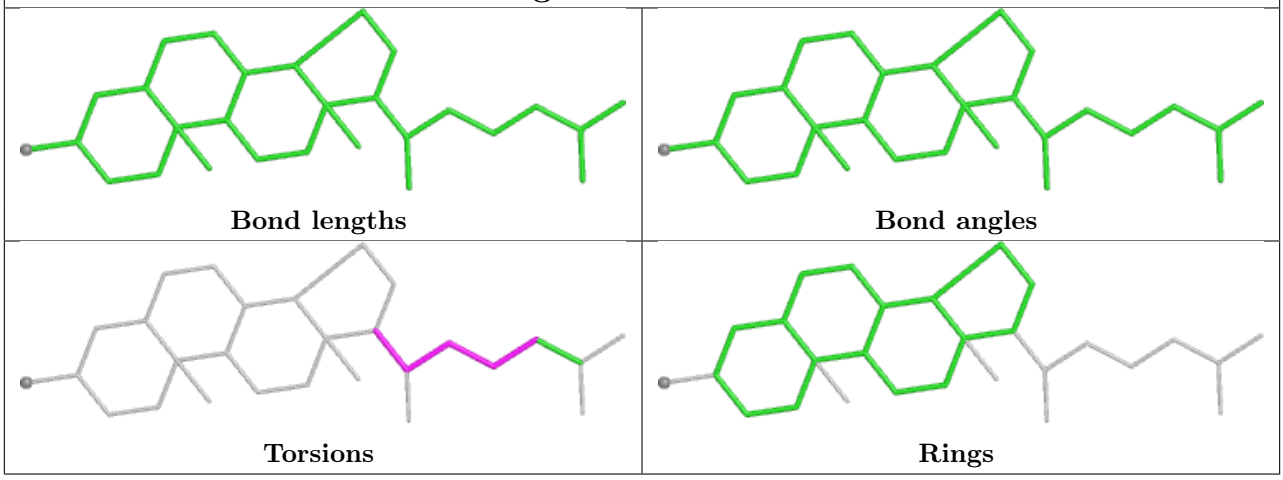


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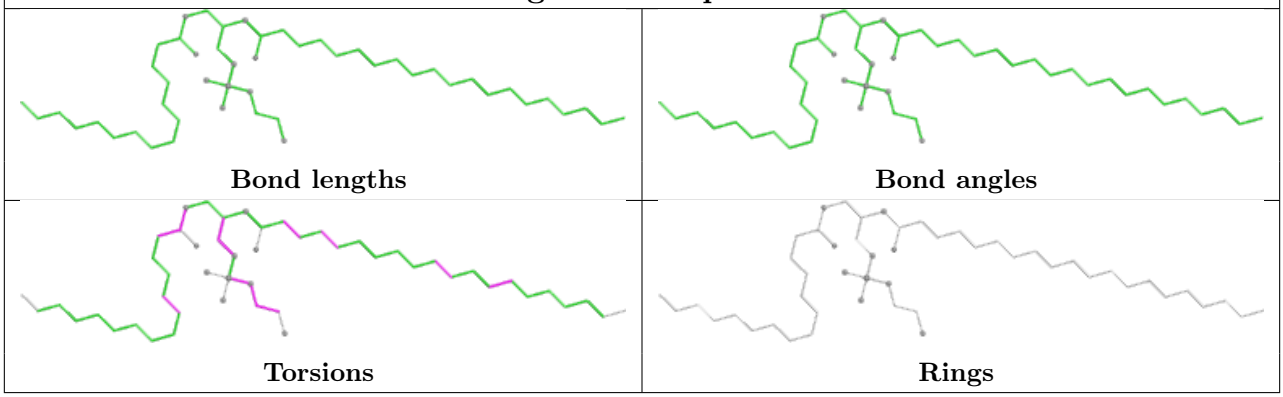


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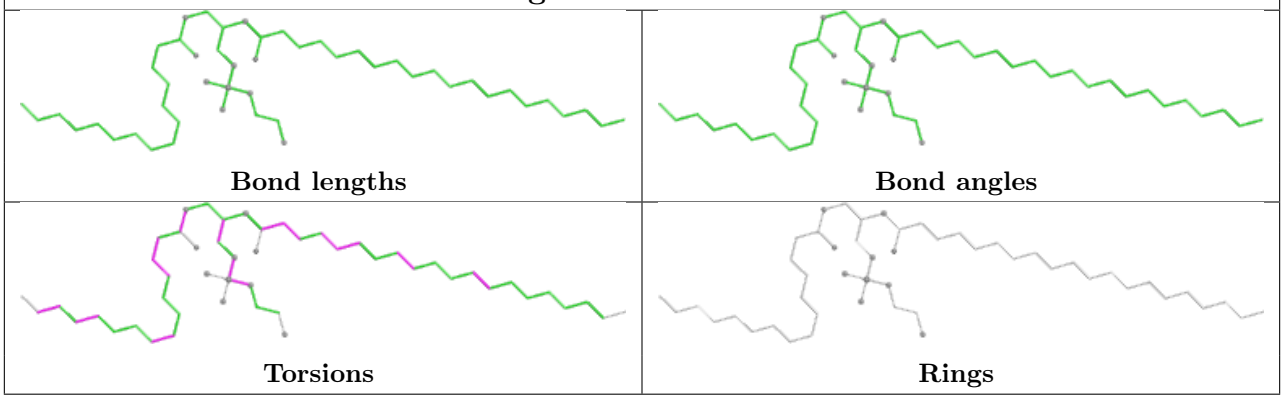
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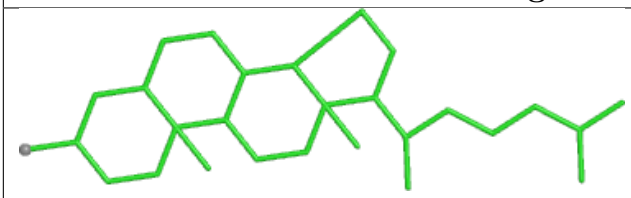
Ligand PTY p 401



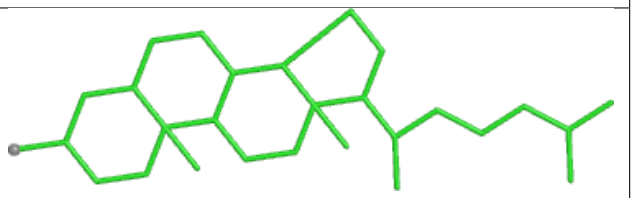
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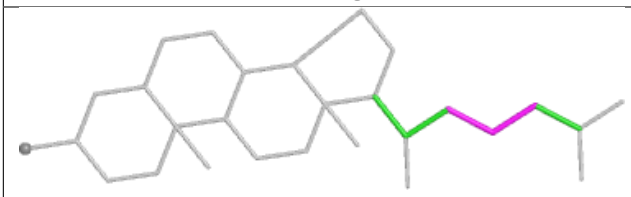
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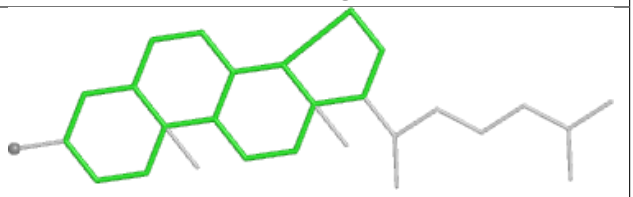
Bond lengths



Bond angles

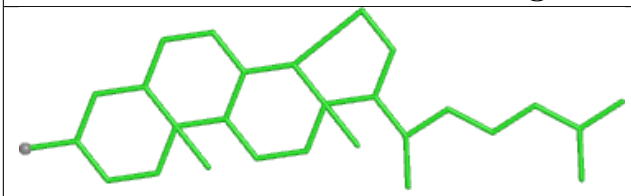


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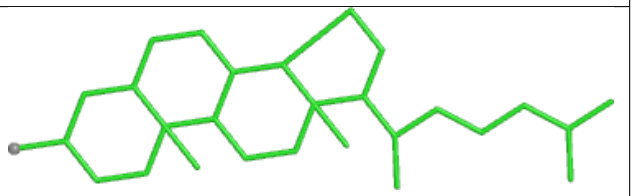


Rings

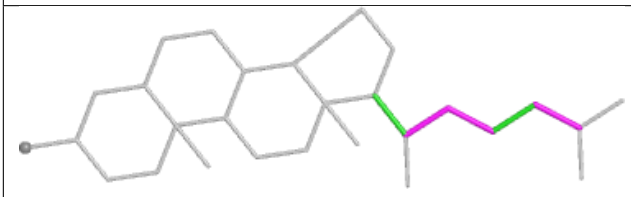
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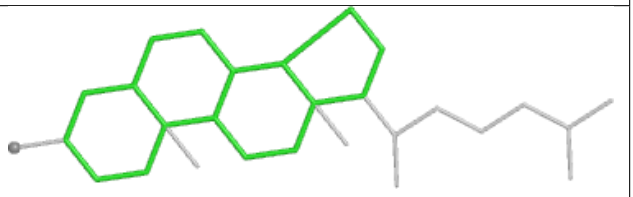
Bond lengths



Bond angles

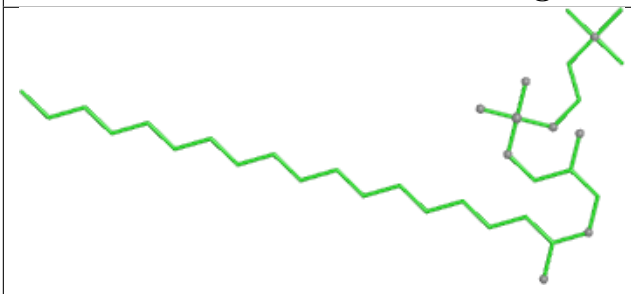


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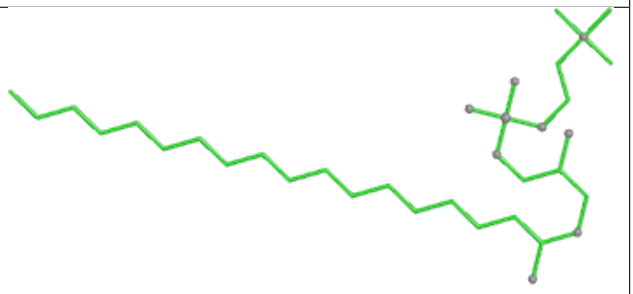


Rings

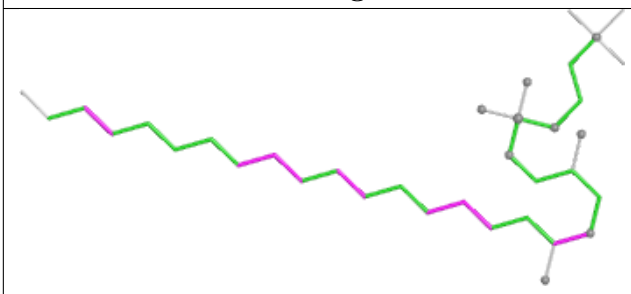
Ligand LP3 a 903



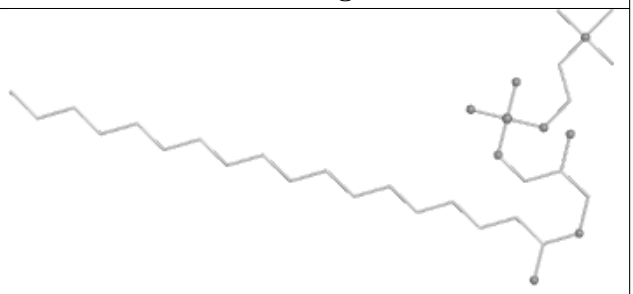
Bond lengths



Bond angles

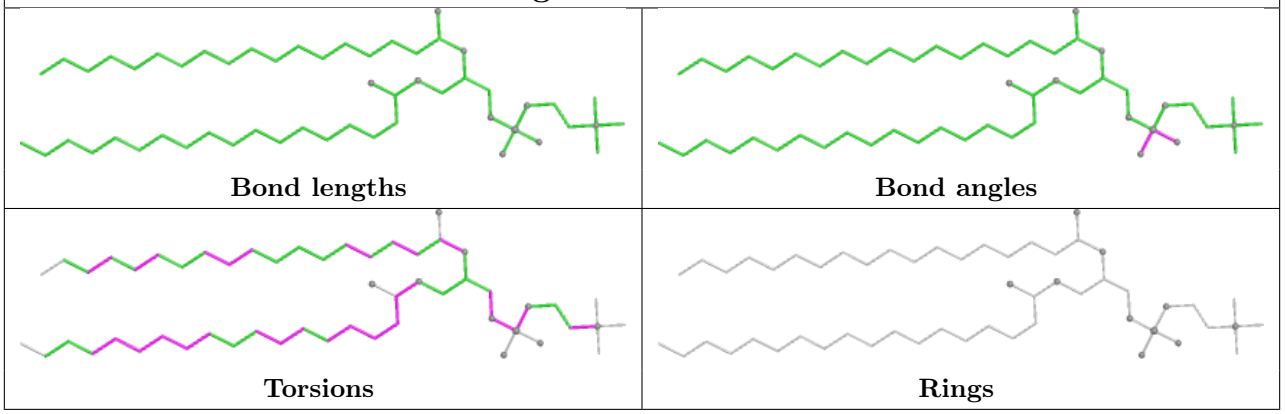


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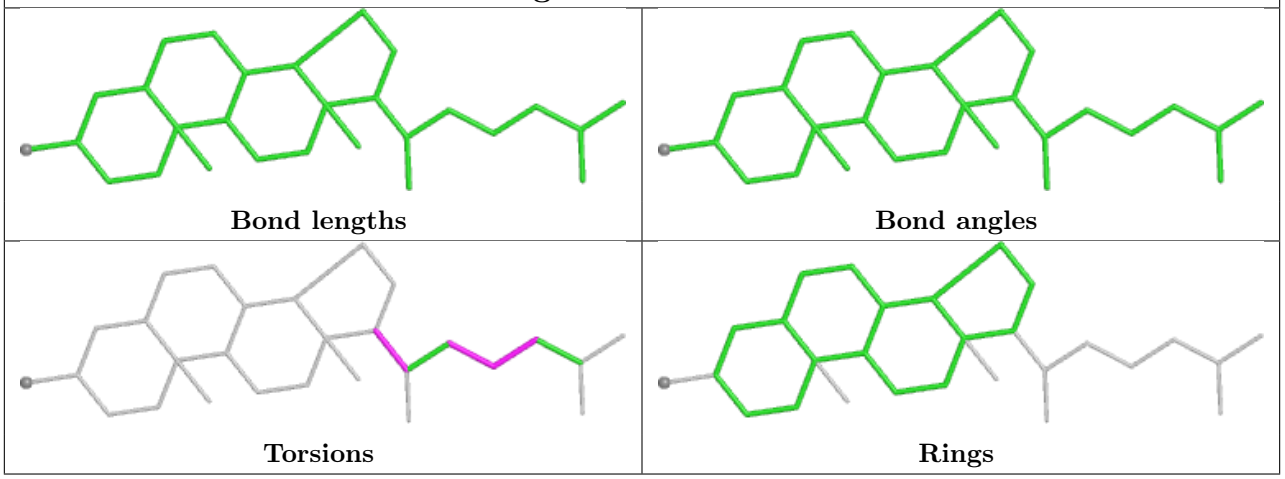


Rings

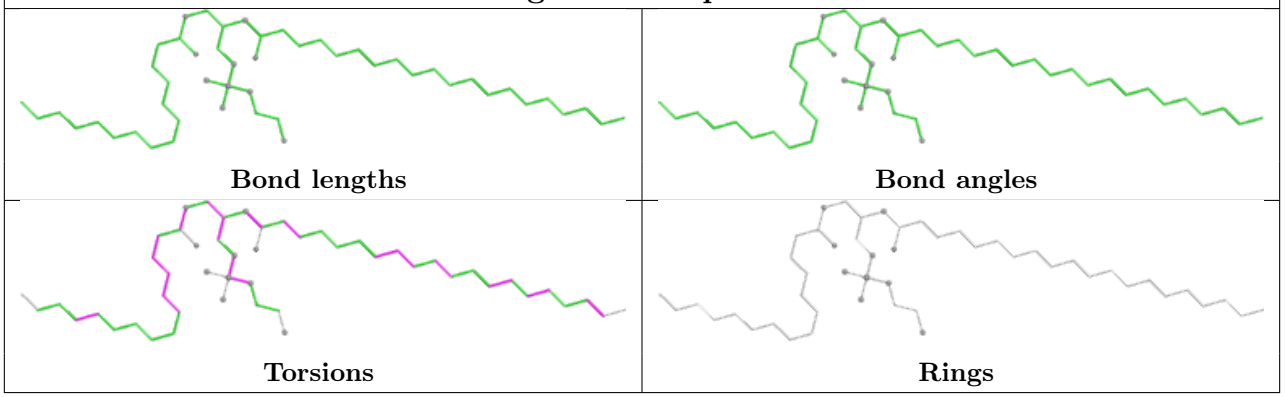
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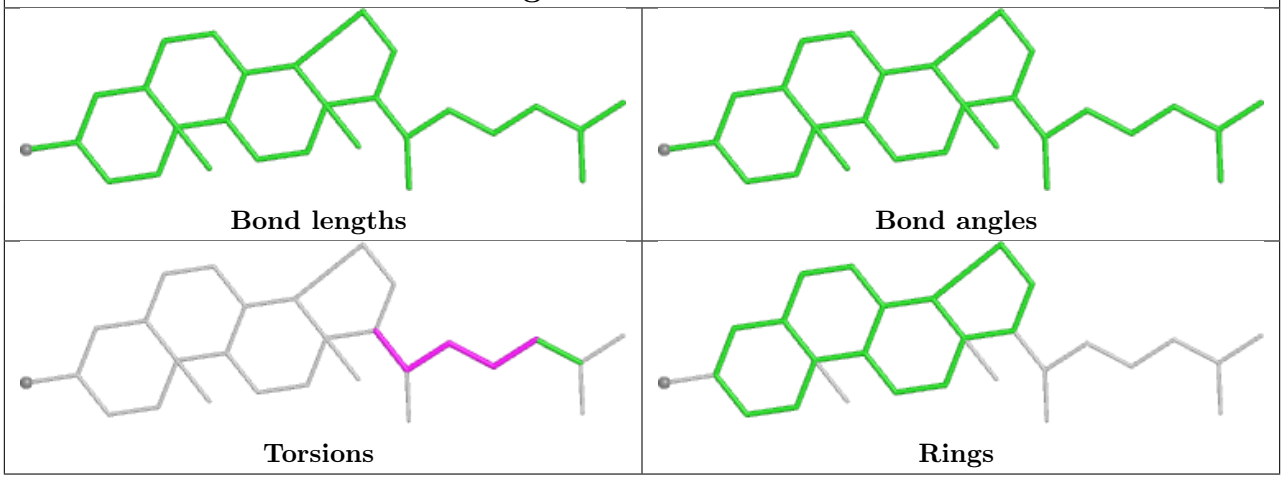
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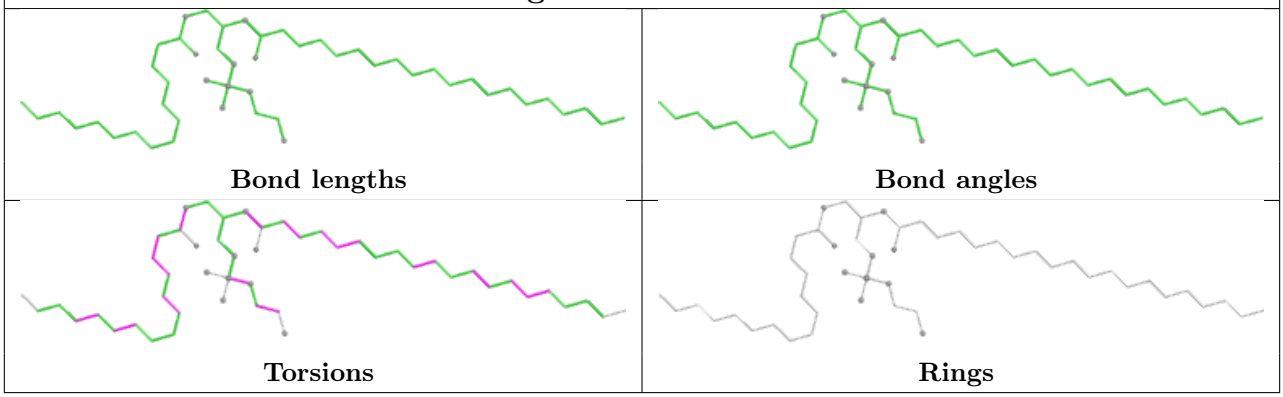
Ligand PTY p 402



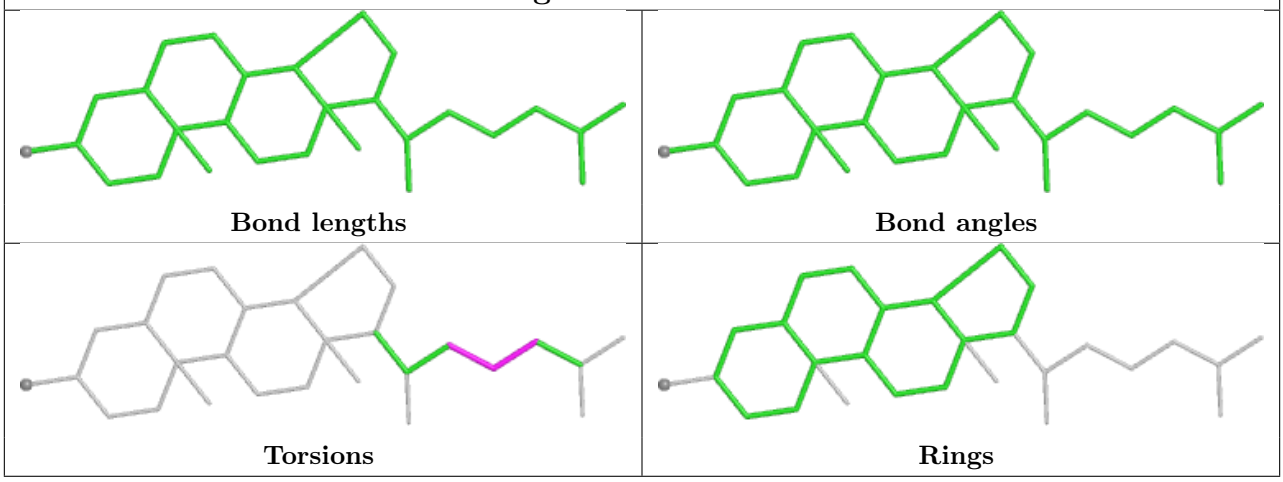
Ligand CLR m 201



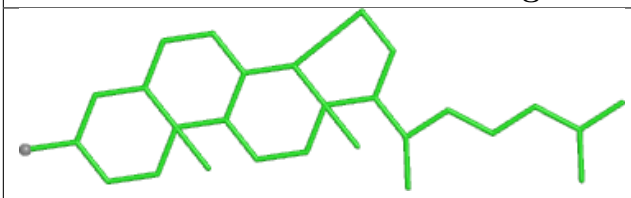
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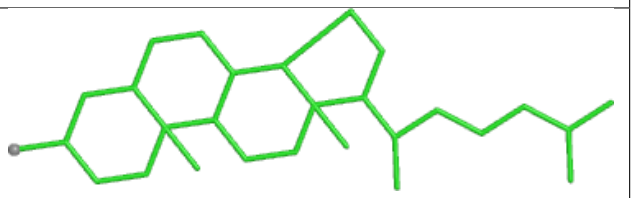
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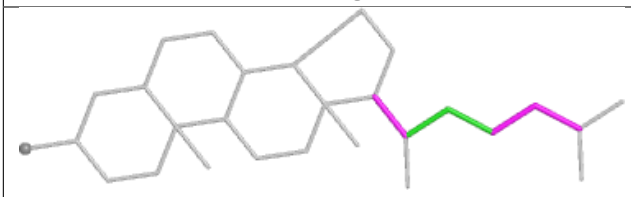
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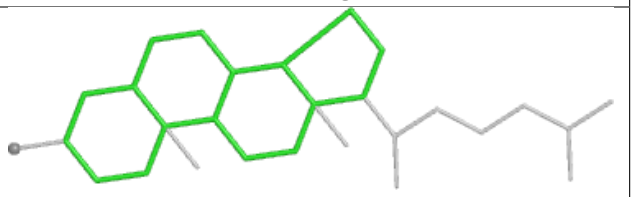
Bond lengths



Bond angles

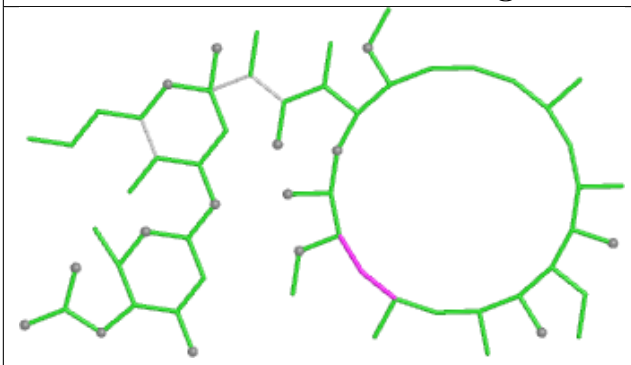


Torsions

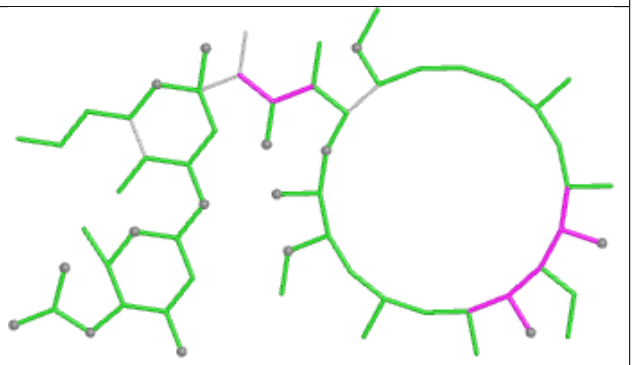


Rings

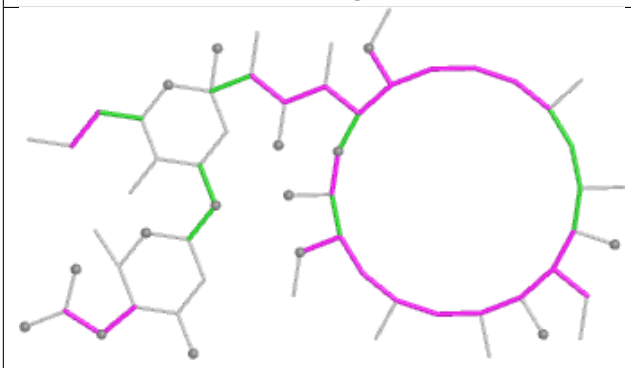
Ligand A1MGD h 201



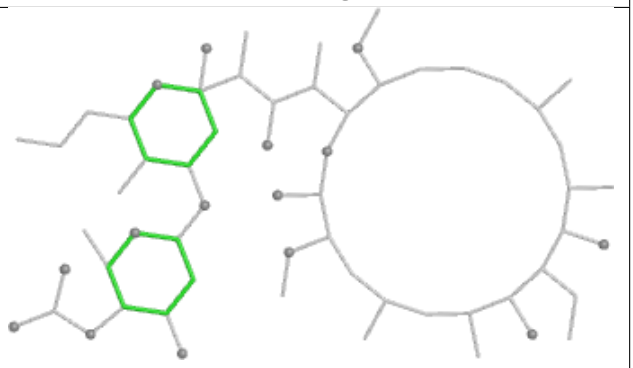
Bond lengths



Bond angles

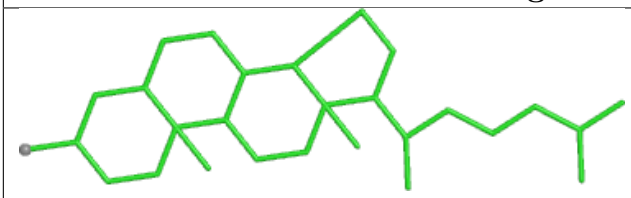


Torsions

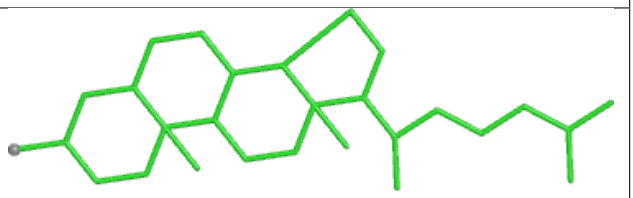


Rings

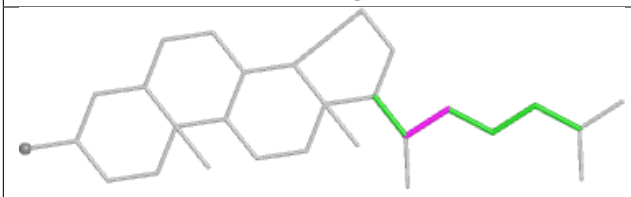
Ligand CLR n 204



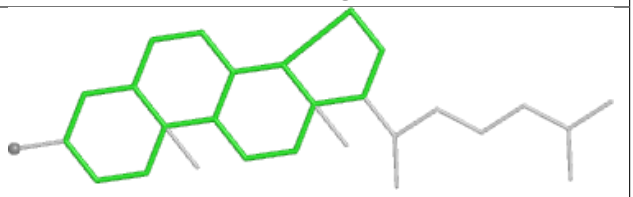
Bond lengths



Bond angles

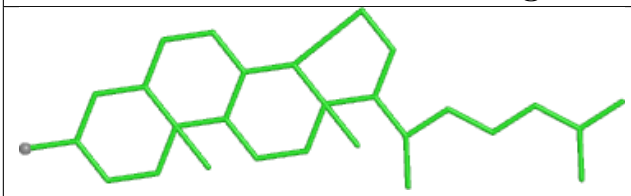


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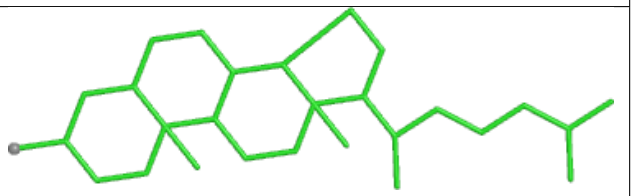


Rings

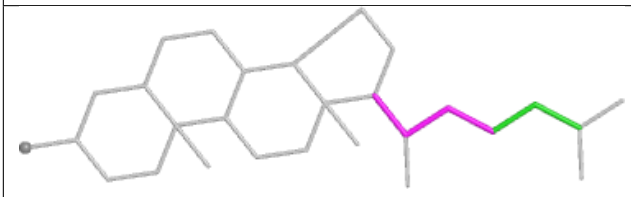
Ligand CLR m 202



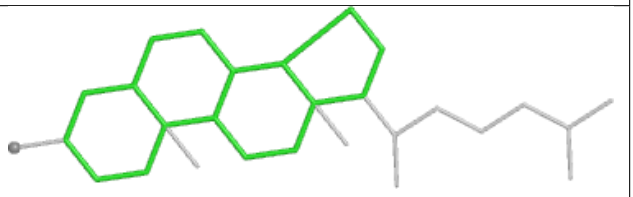
Bond lengths



Bond angles

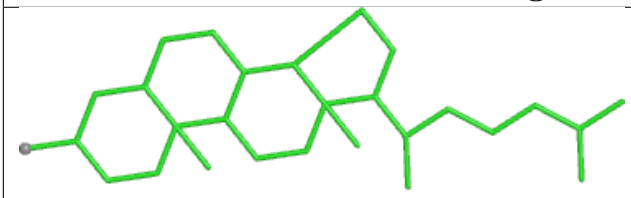


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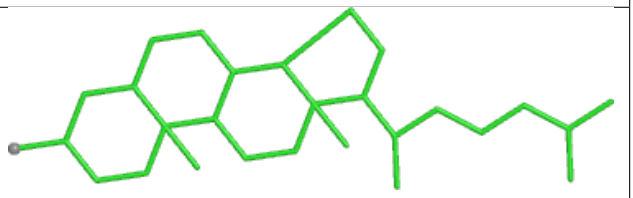


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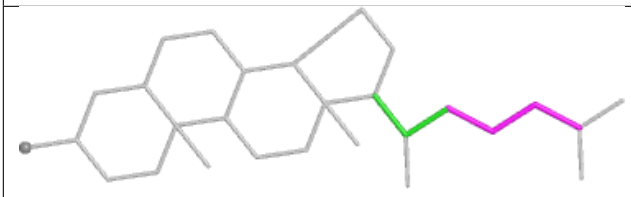
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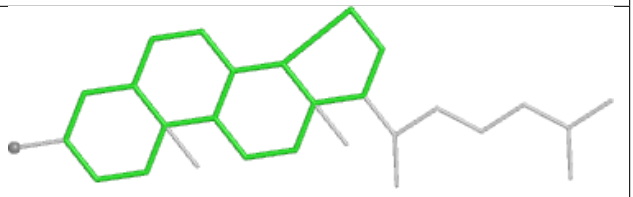
Bond lengths



Bond angles

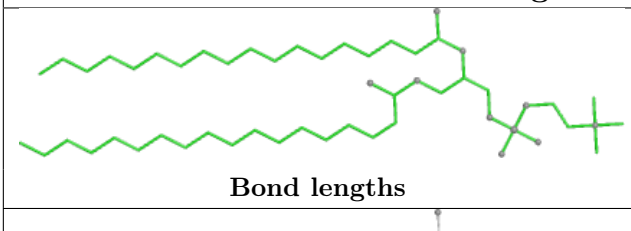


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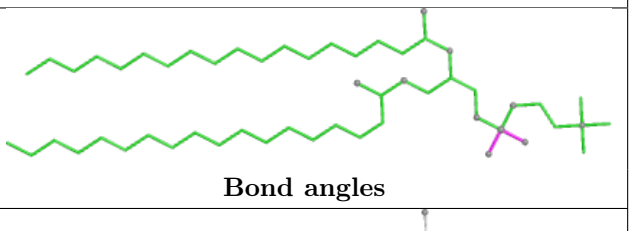


Rings

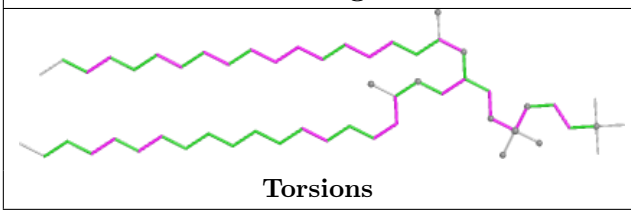
Ligand PC1 k 205



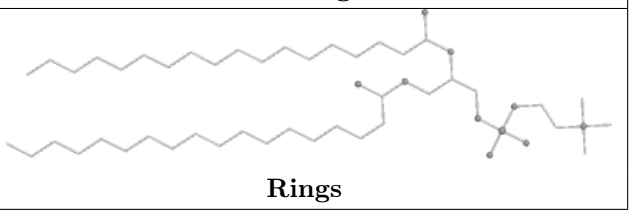
Bond lengths



Bond angles

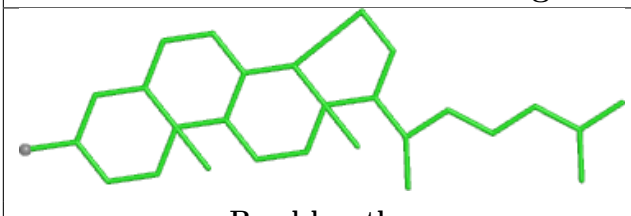


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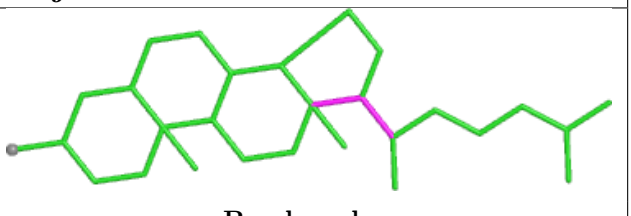


Rings

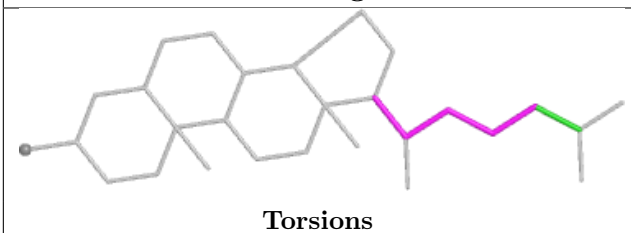
Ligand CLR j 204



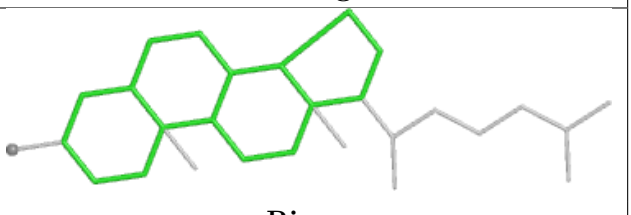
Bond lengths



Bond angles

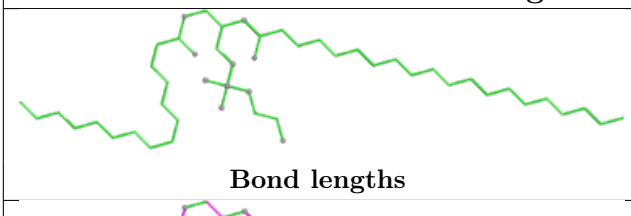


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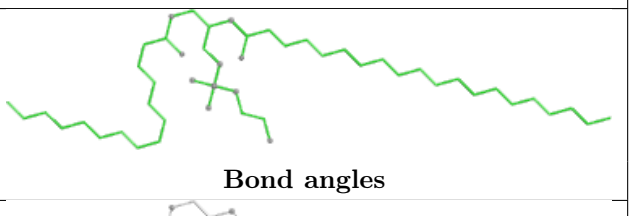


Rings

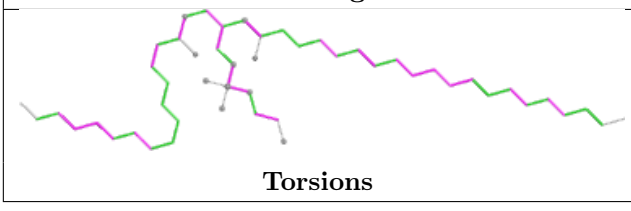
Ligand PTY b 303



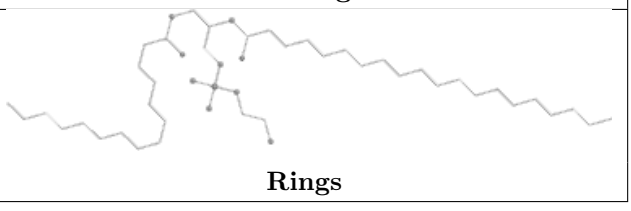
Bond lengths



Bond angles

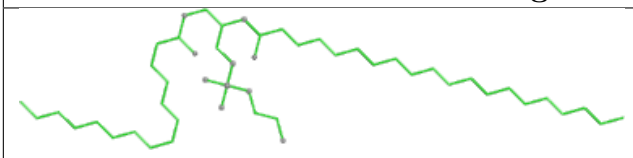


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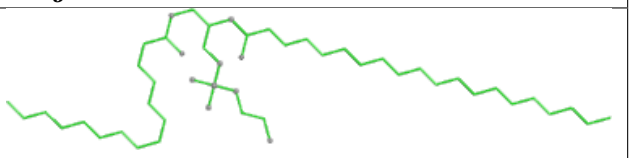


Rings

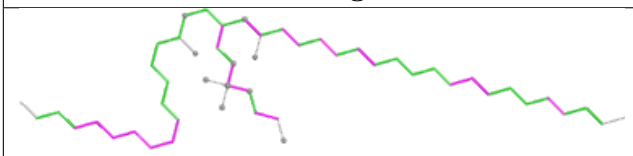
Ligand PTY j 201



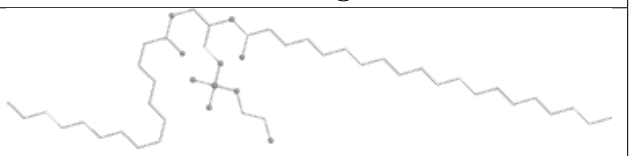
Bond lengths



Bond angles

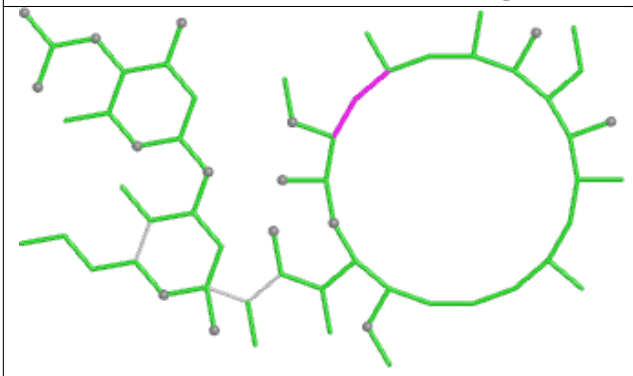


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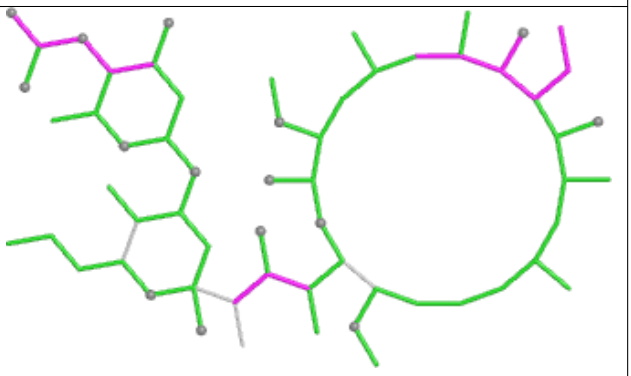


Rings

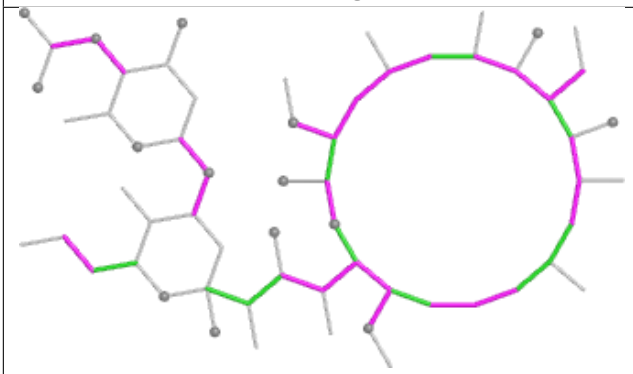
Ligand A1MGD k 201



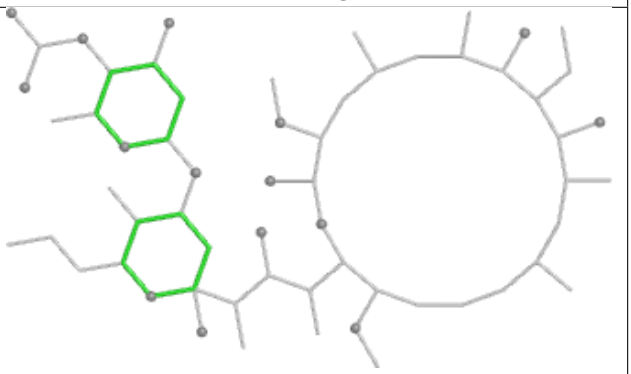
Bond lengths



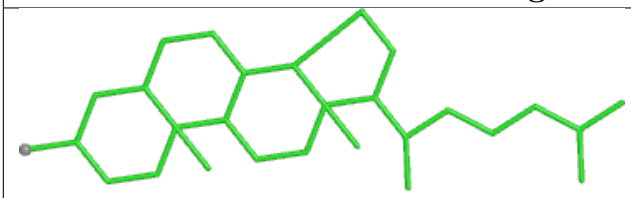
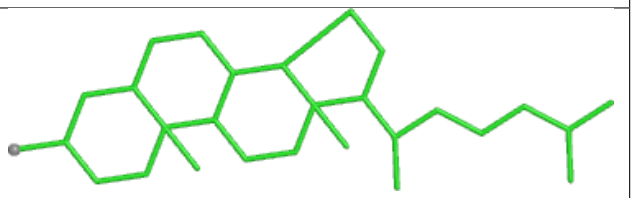
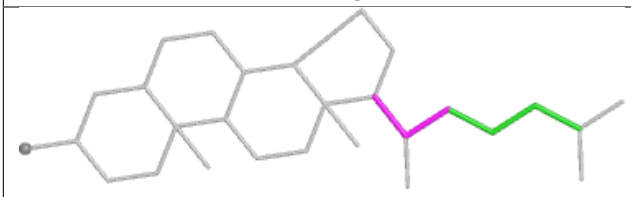
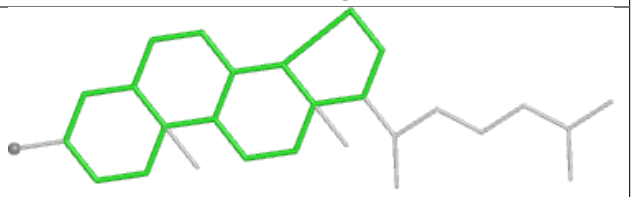
Bond angles

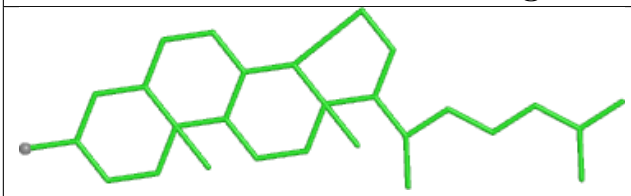
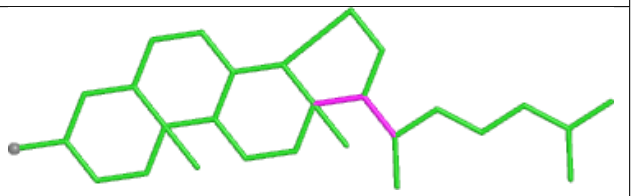
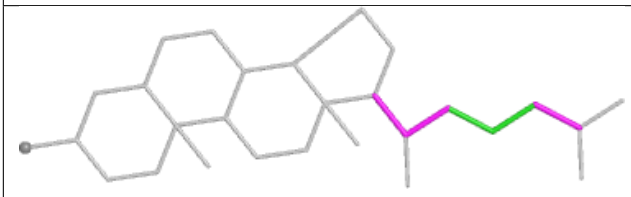
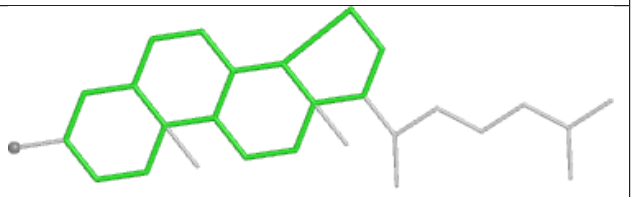


Torsions

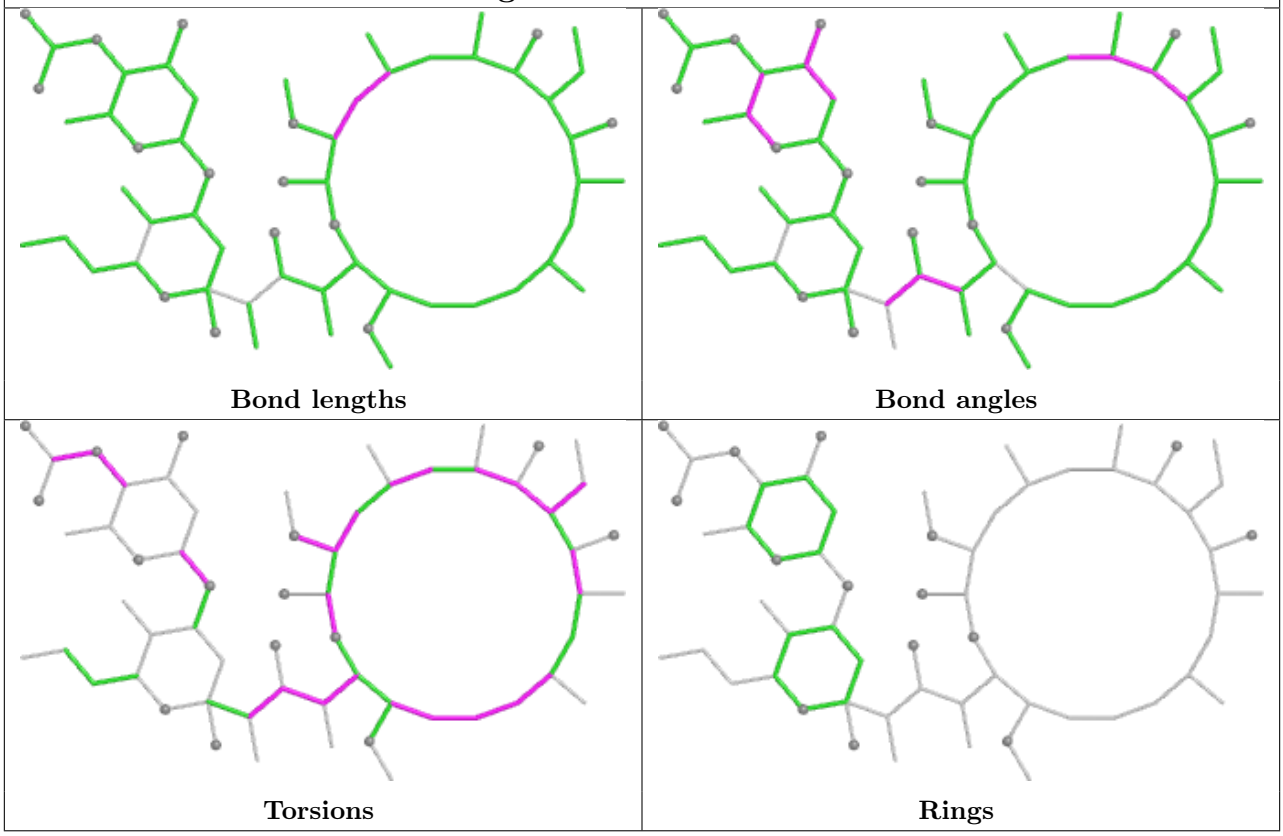


Rings

Ligand CLR k 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLR m 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

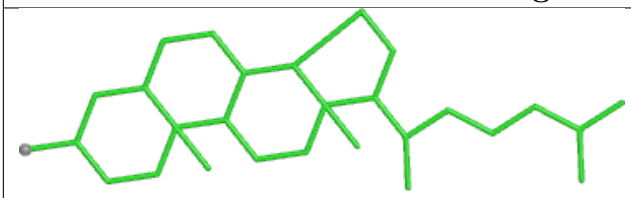
Ligand A1MGD n 201



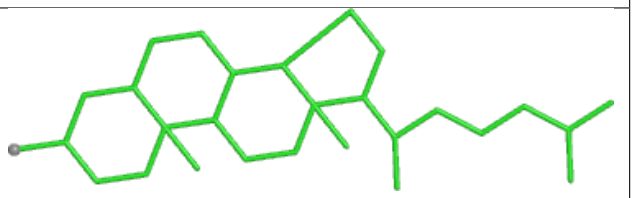
Ligand CLR b 305



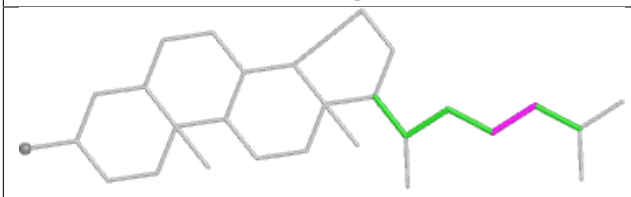
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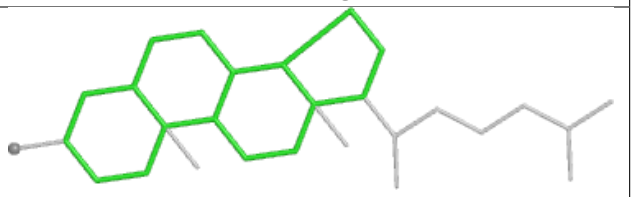
Bond lengths



Bond angles

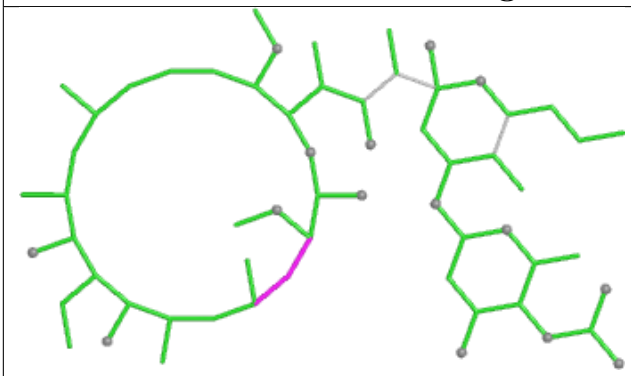


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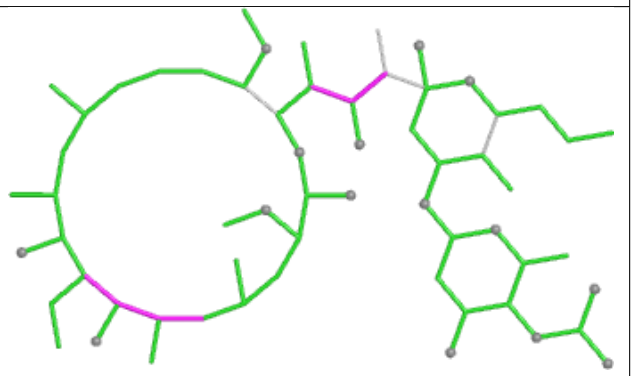


Rings

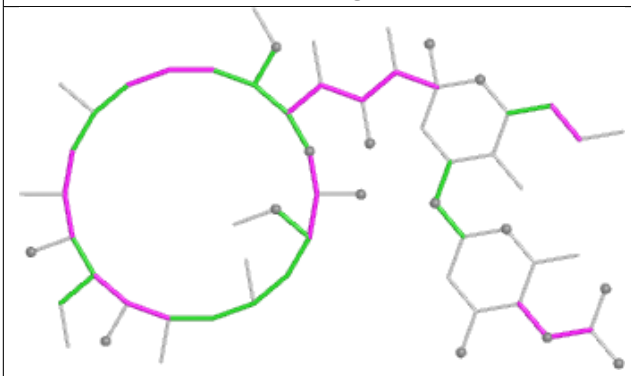
Ligand A1MGD a 901



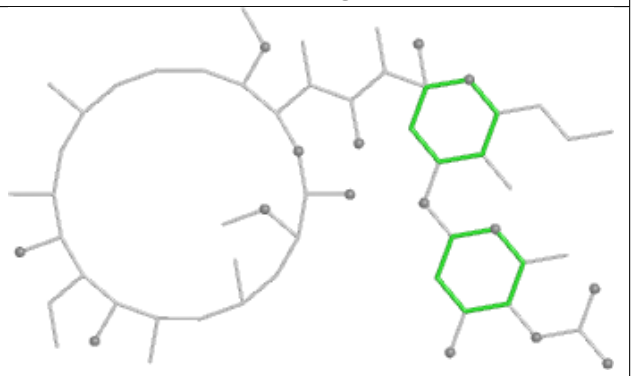
Bond lengths



Bond angles

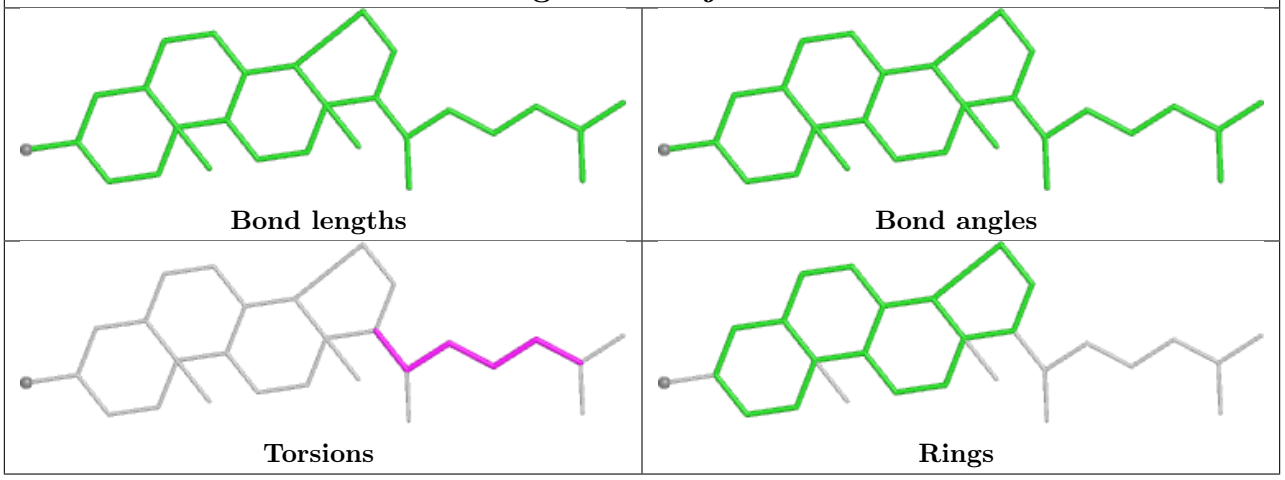


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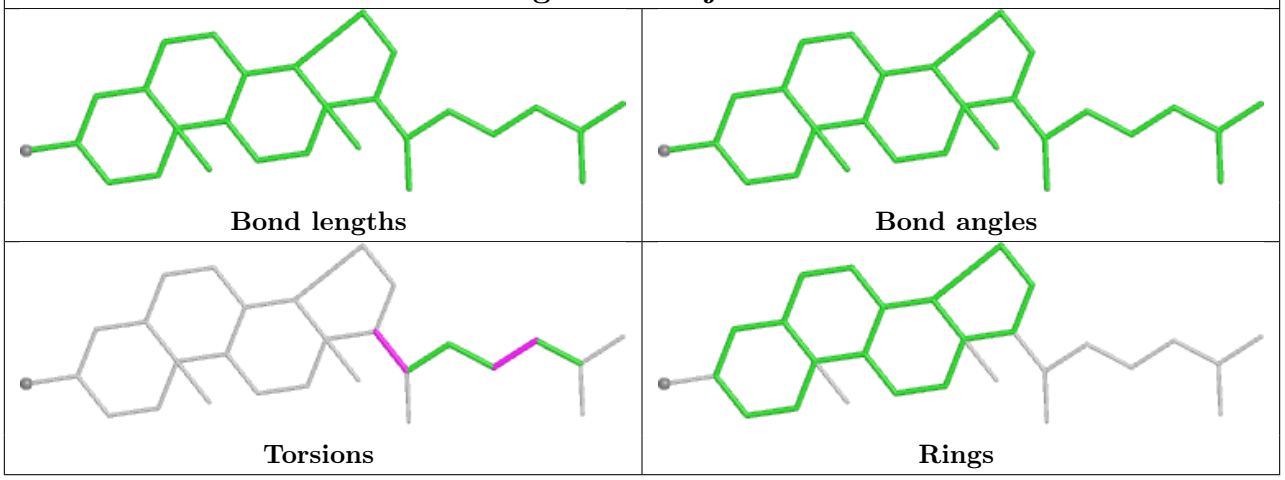


Rings

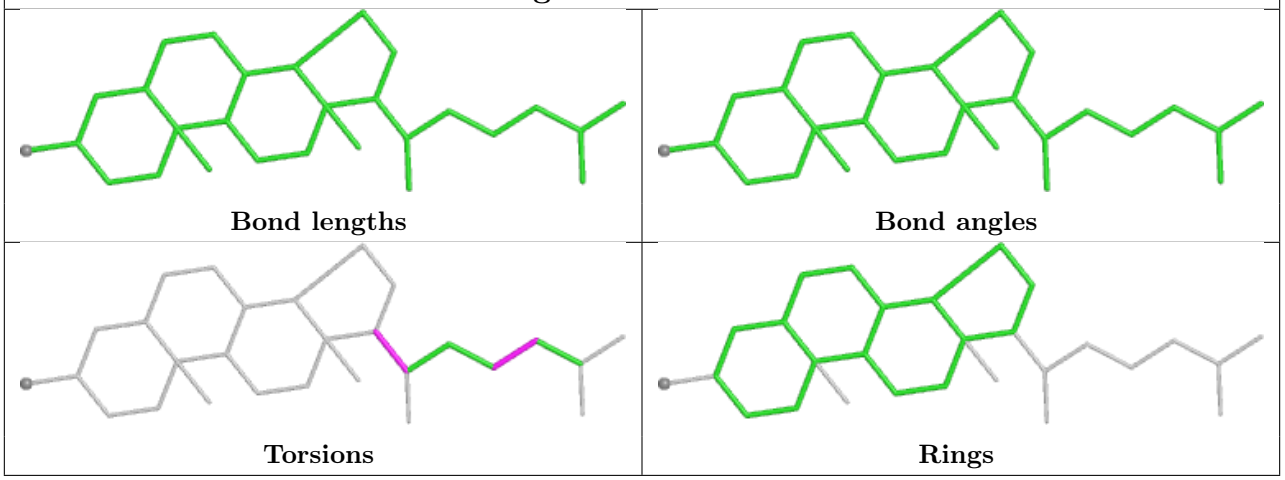
Ligand CLR j 202



Ligand CLR j 205



Ligand CLR i 204



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.

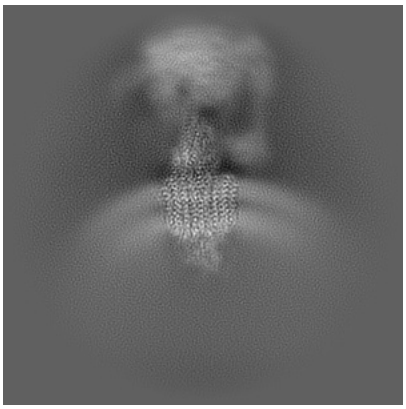
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80481. These allow visual inspection of the internal detail of the map and identification of artifacts.

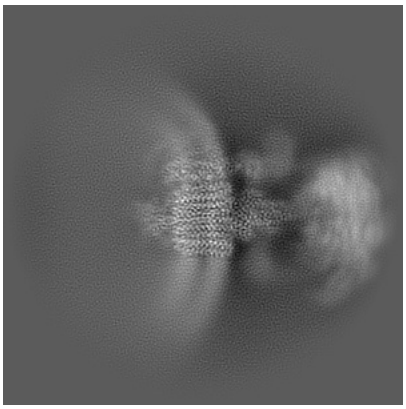
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

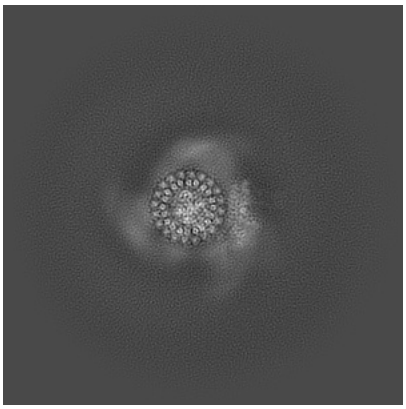
6.1.1 Primary map



X

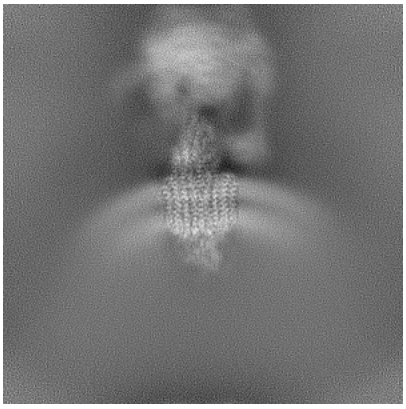


Y

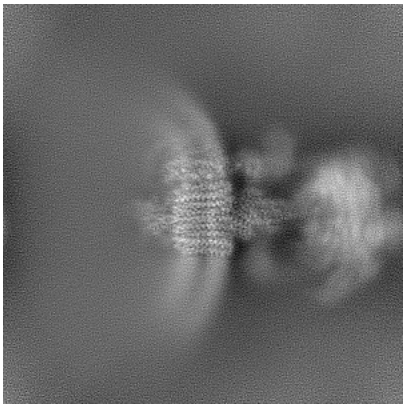


Z

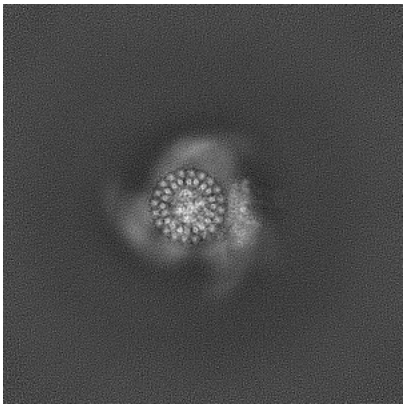
6.1.2 Raw map



X



Y

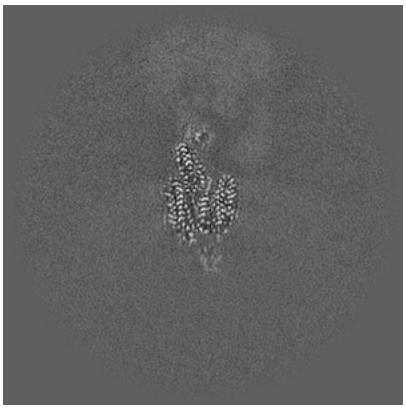


Z

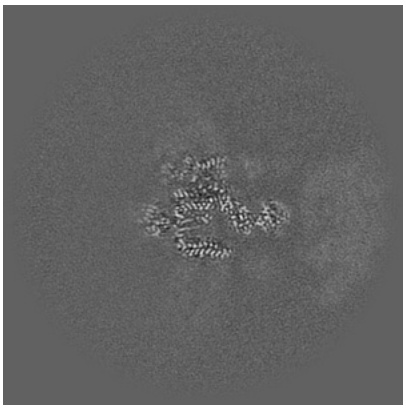
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

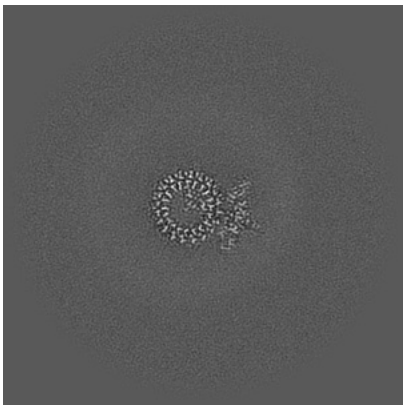
6.2.1 Primary map



X Index: 200

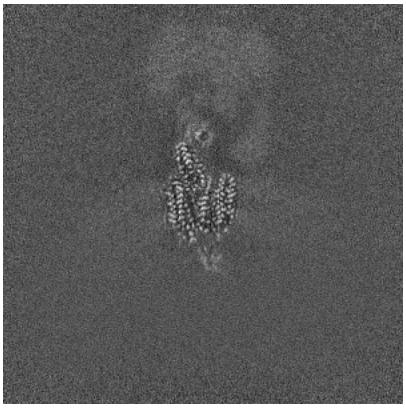


Y Index: 200

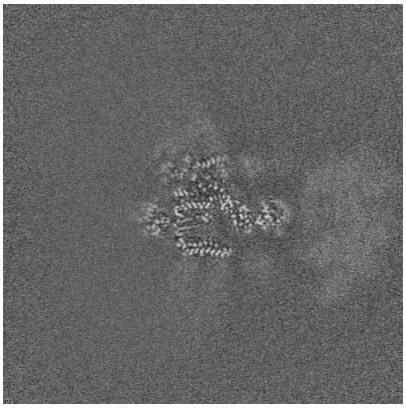


Z Index: 200

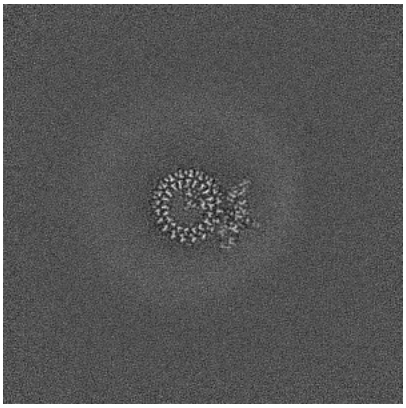
6.2.2 Raw map



X Index: 200



Y Index: 200

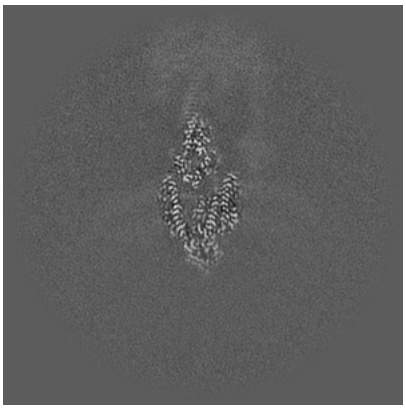


Z Index: 200

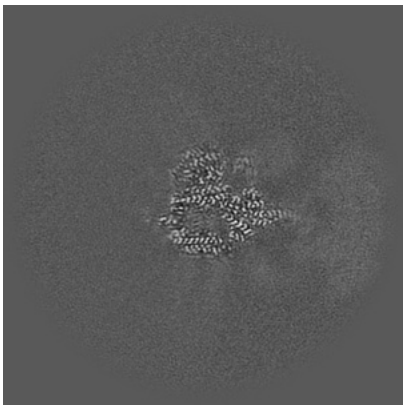
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

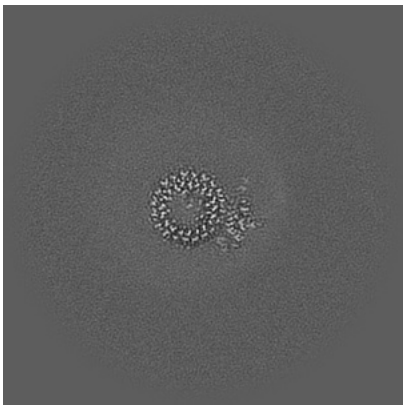
6.3.1 Primary map



X Index: 185

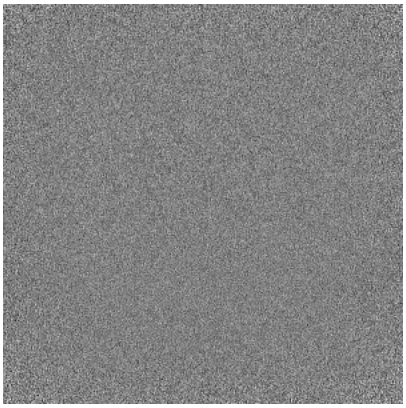


Y Index: 182

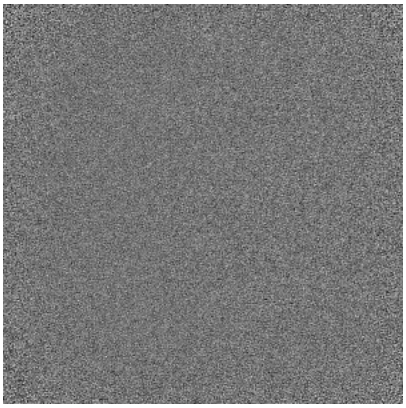


Z Index: 208

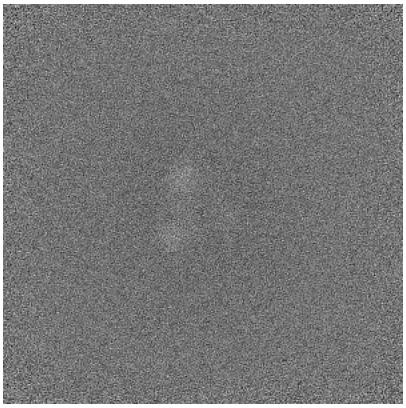
6.3.2 Raw map



X Index: 0



Y Index: 0

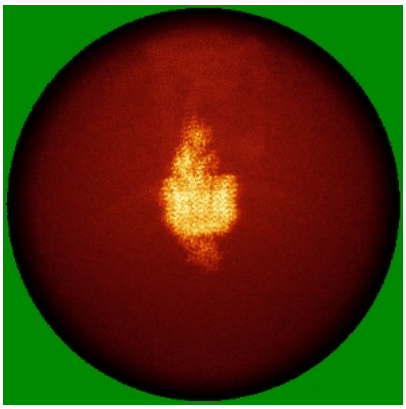


Z Index: 0

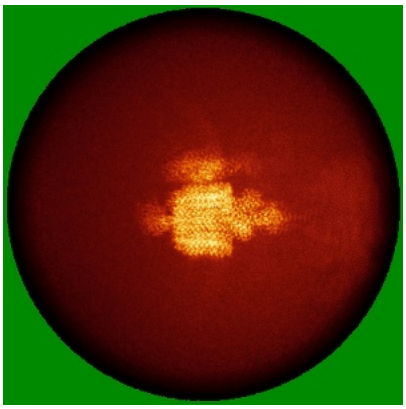
The images above show the largest variance slices of the map in three orthogonal directions.

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

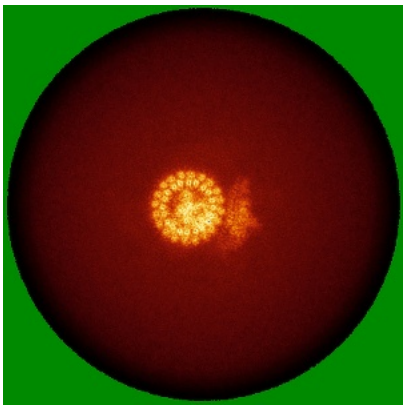
6.4.1 Primary map



X

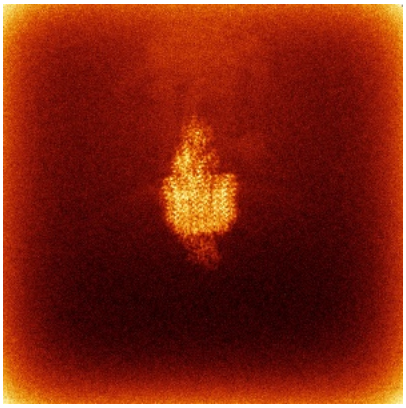


Y

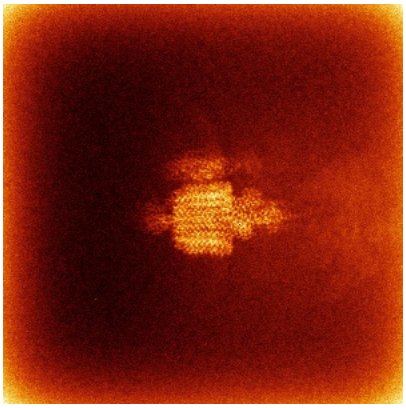


Z

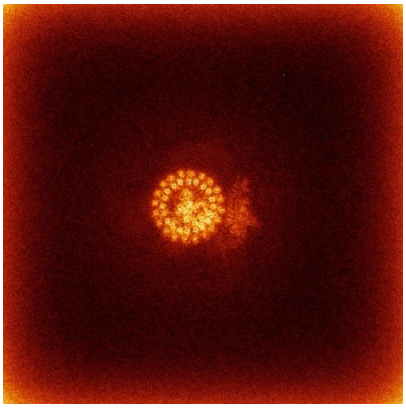
6.4.2 Raw map



X



Y

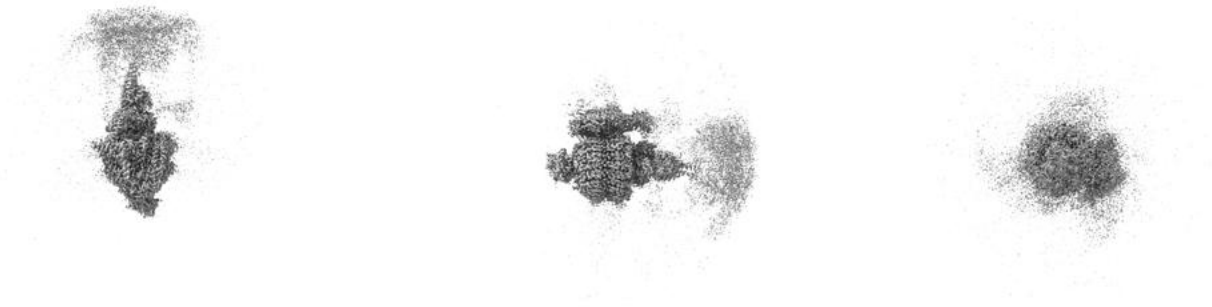


Z

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)

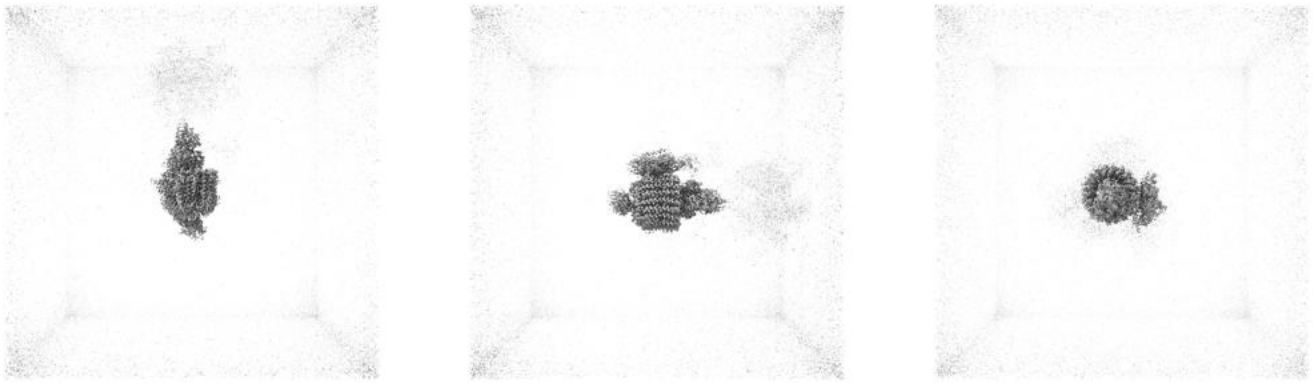
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

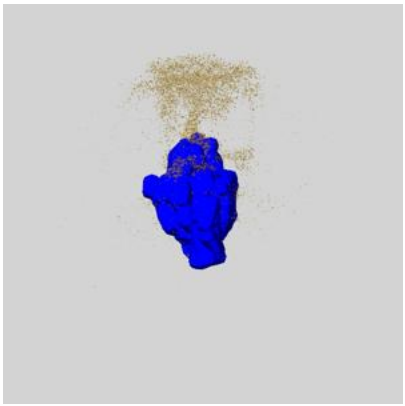
6.6 Mask visualisation (i)

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

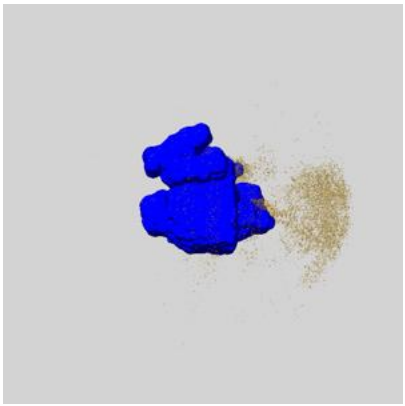
A mask typically either:

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

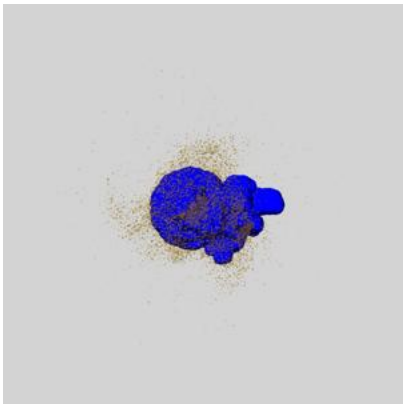
6.6.1 emd_80481_msk_1.map (i)



X



Y

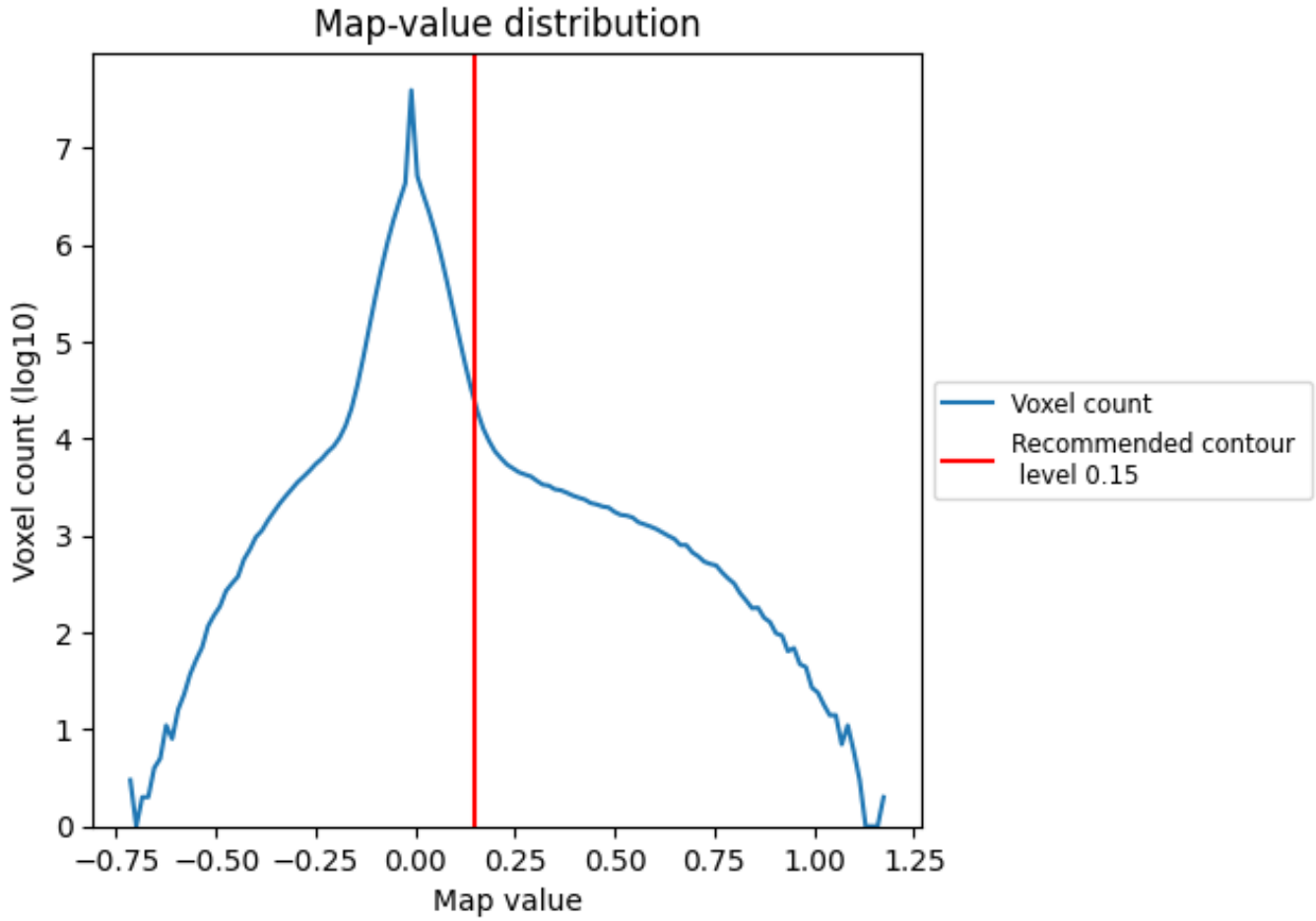


Z

7 Map analysis

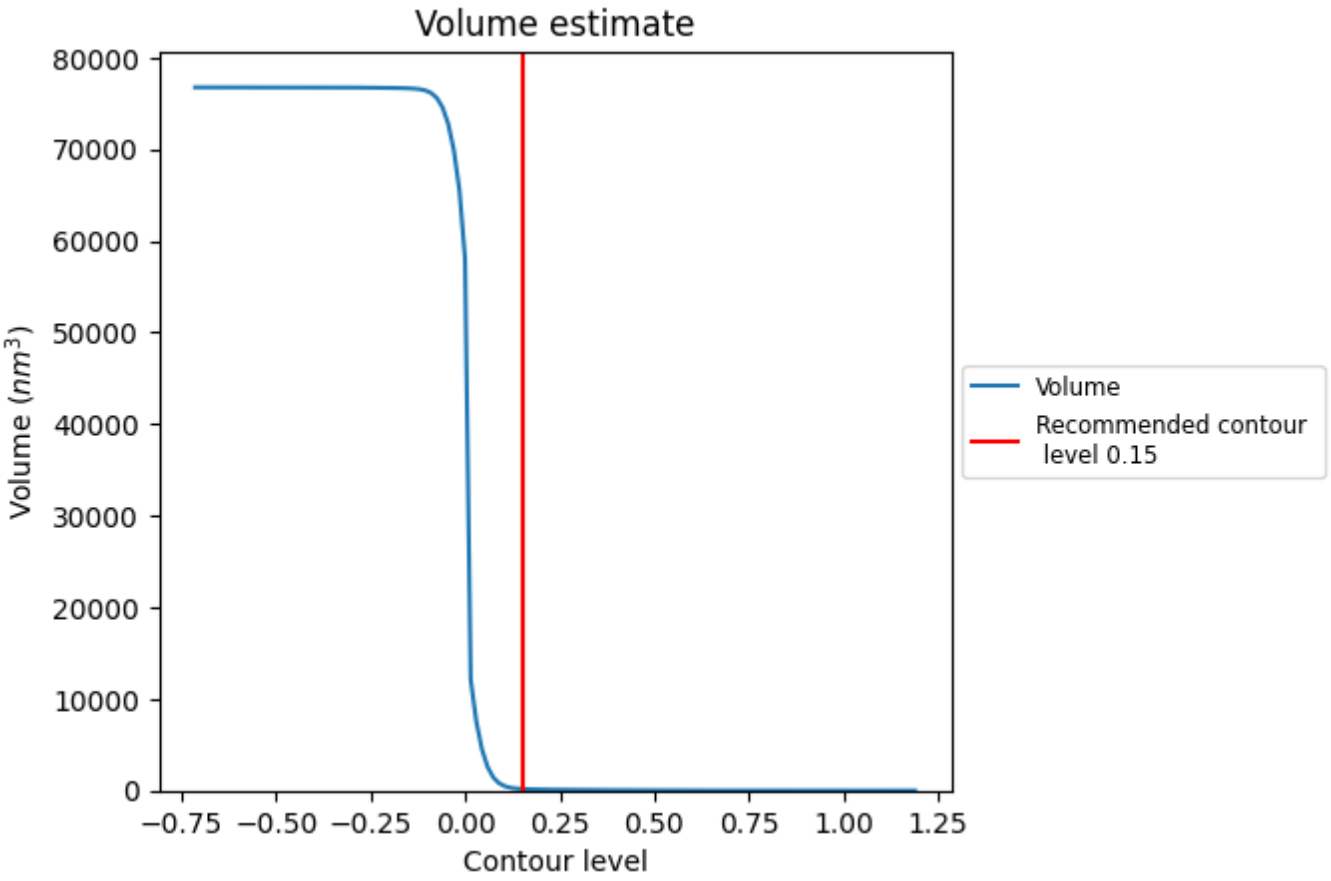
This section contains the results of statistical analysis of the map.

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.

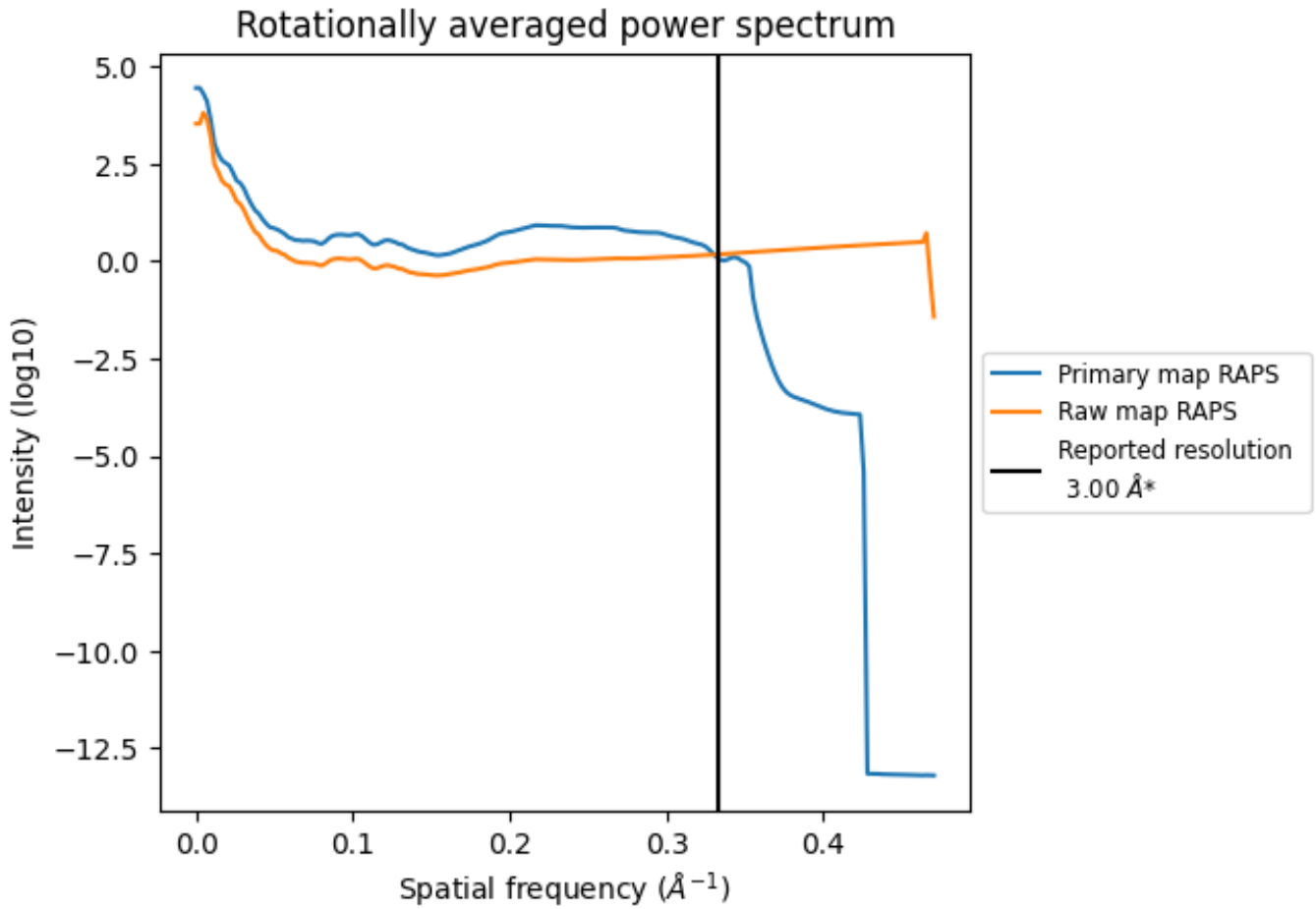
7.2 Volume estimate (i)



The volume at the recommended contour level is 173 nm^3; this corresponds to an approximate mass of 156 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)

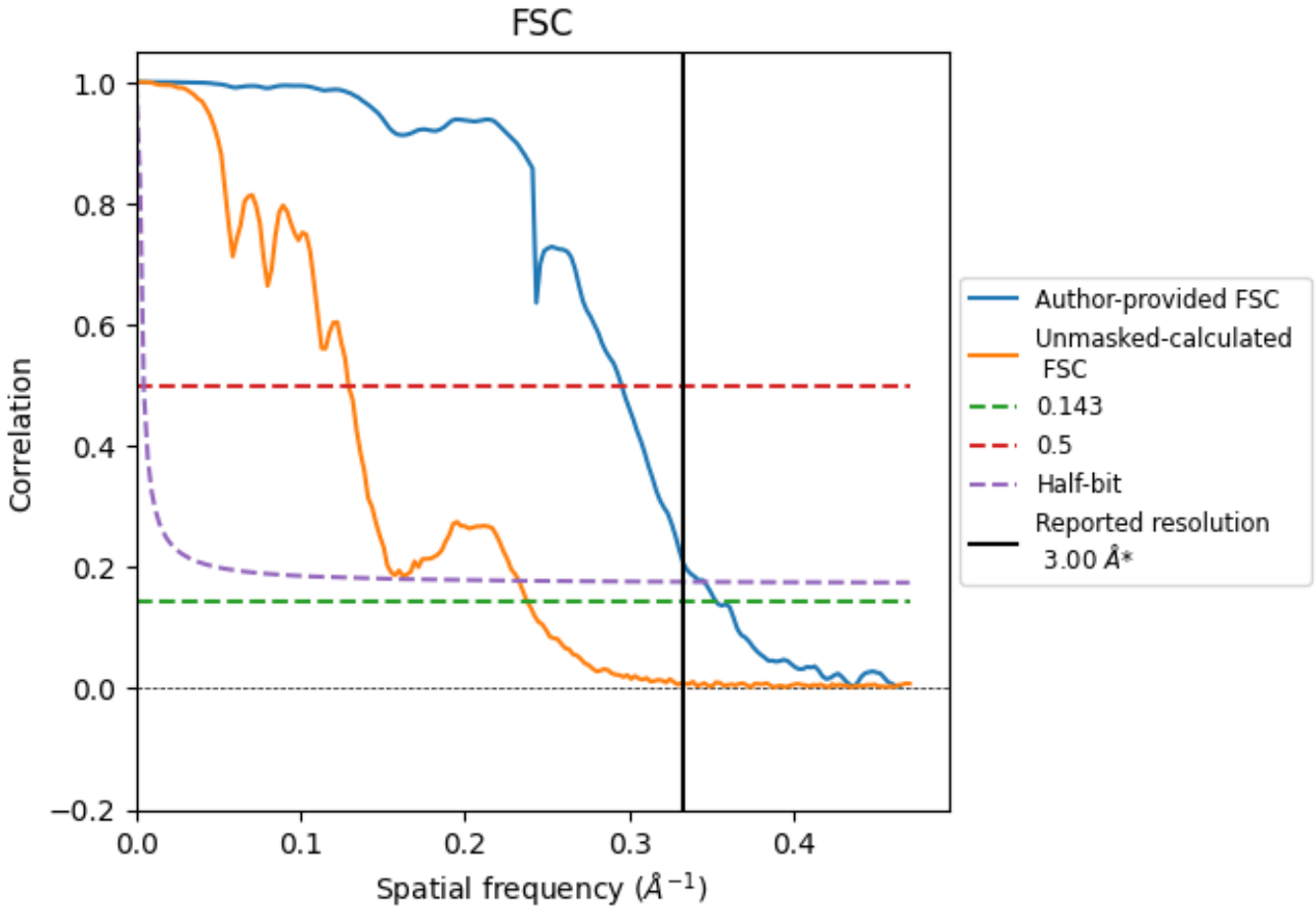


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

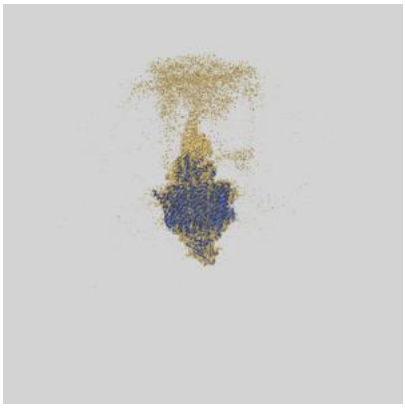
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.83	3.39	2.89
Unmasked-calculated*	4.20	7.74	4.29

*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 4.20 differs from the reported value 3.0 by more than 10 %

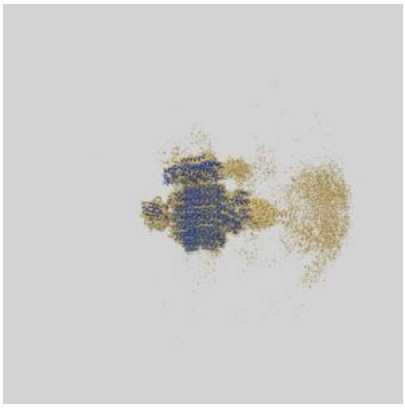
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80481 and PDB model 25YS. Per-residue inclusion information can be found in section 3 on page 12.

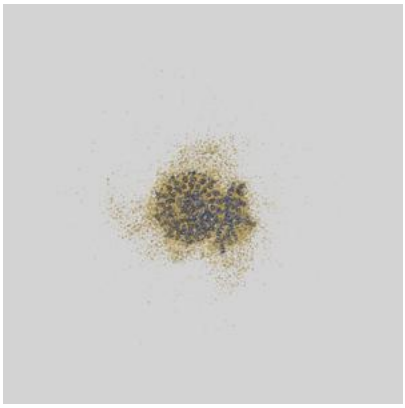
9.1 Map-model overlay



X



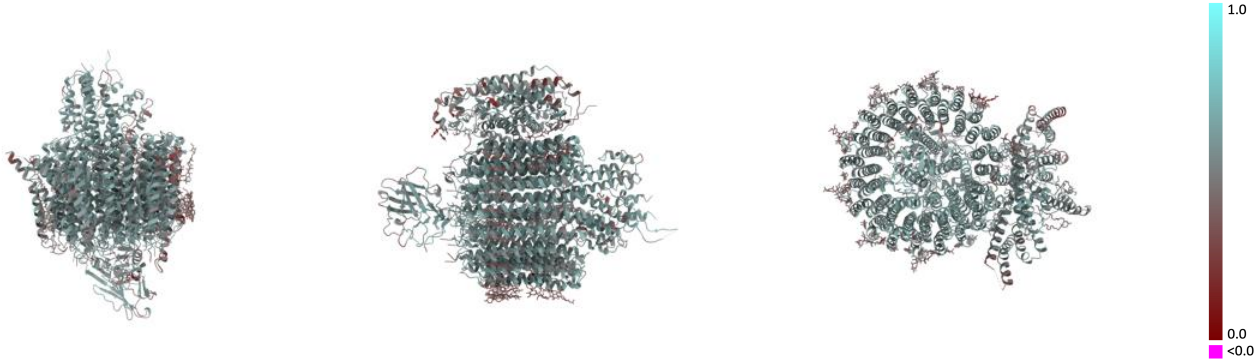
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

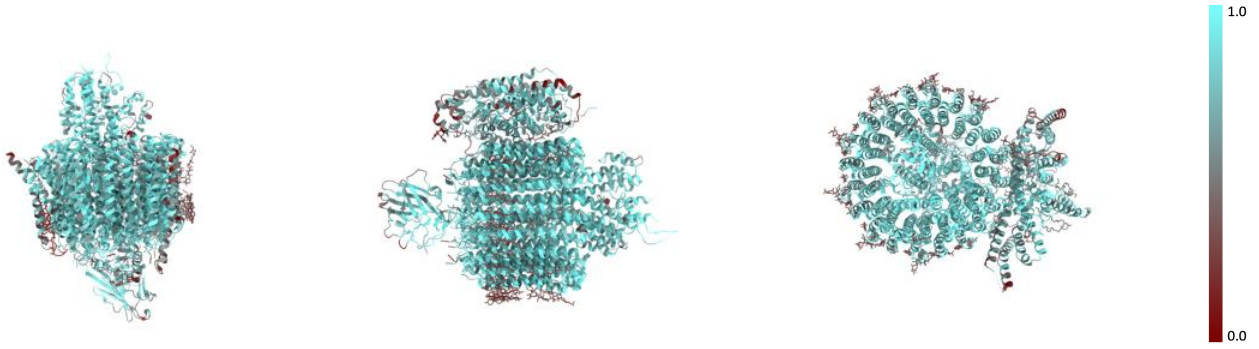
9.2 Q-score mapped to coordinate model



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.

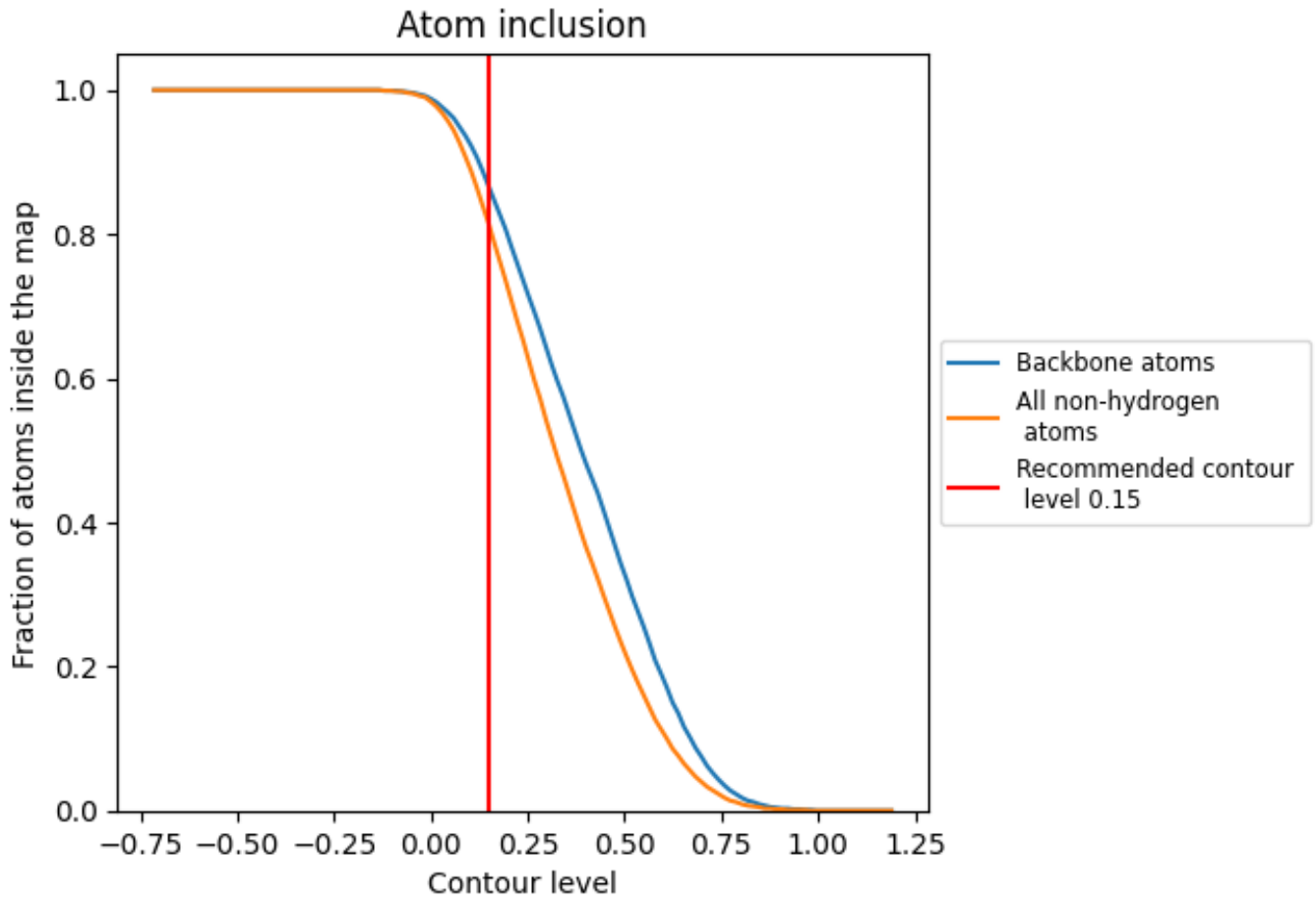
9.3 Atom inclusion mapped to coordinate model



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 81% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.5480
H	0.9360	0.5840
P	0.8180	0.5550
Z	0.4480	0.4150
a	0.7240	0.5250
b	0.8870	0.5870
d	0.8650	0.5670
e	0.7370	0.5070
f	0.5840	0.4510
h	0.8380	0.5460
i	0.8210	0.5460
j	0.8390	0.5550
k	0.8180	0.5520
l	0.7840	0.5260
m	0.8480	0.5630
n	0.8070	0.5420
o	0.8440	0.5590
p	0.8330	0.5450
r	0.9030	0.5780

