wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 04:03 AM EST

PDB ID	:	6WM2
EMDB ID	:	EMD-21847
Title	:	Human V-ATPase in state 1 with SidK and ADP
Authors	:	Wang, L.; Wu, H.; Fu, T.M.
Deposited on	:	2020-04-20
Resolution	:	3.10 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

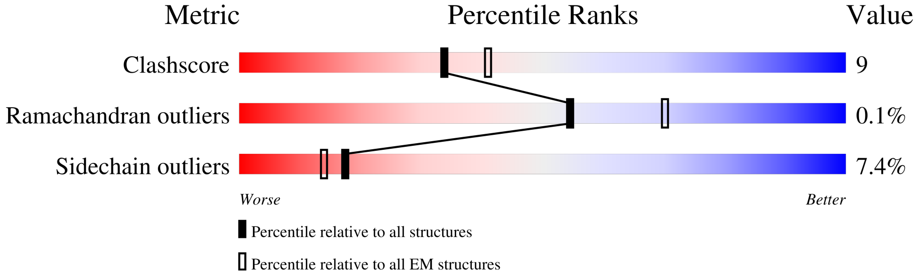
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

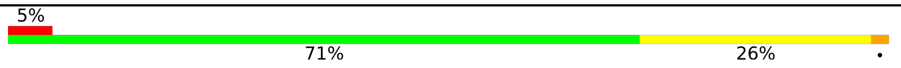
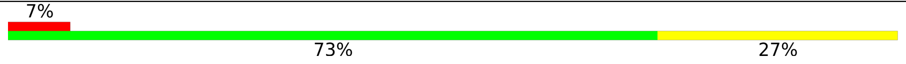
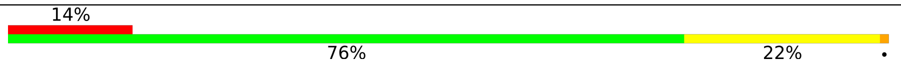
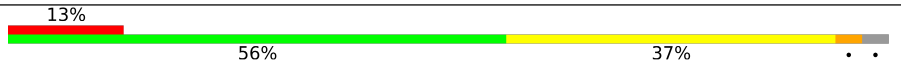
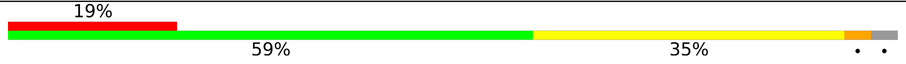
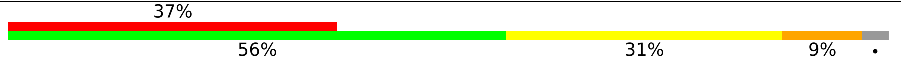
The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	226	
1	I	226	
1	J	226	
2	K	118	
2	L	118	
2	M	118	
3	O	382	
4	P	483	

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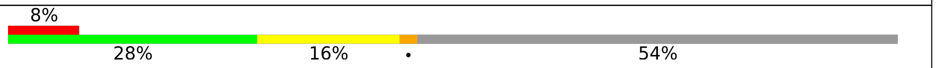
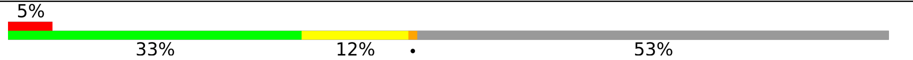
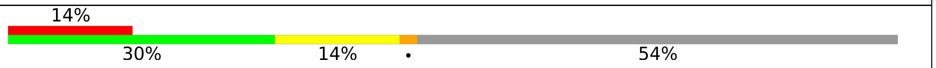
Mol	Chain	Length	Quality of chain
5	R	837	
6	A	617	
6	B	617	
6	C	617	
7	D	511	
7	E	511	
7	F	511	
8	X	573	
8	Y	573	
8	Z	573	
9	G	247	
10	N	119	
11	0	205	
12	1	155	
12	2	155	
12	3	155	
12	4	155	
12	5	155	
12	6	155	
12	7	155	
12	8	155	
12	9	155	
13	Q	351	
14	S	81	
15	T	137	

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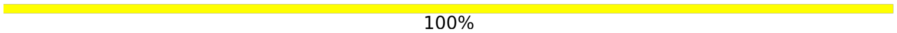
Mol	Chain	Length	Quality of chain
16	U	470	 31% 12% 56%
17	V	350	 13% • 86%
18	W	5	 60% 40%
19	a	4	 100%
20	b	2	 100%
20	c	2	 50% 50%
20	d	2	 100%
20	s	2	 50% 50%
20	u	2	 100%
21	r	11	 36% 64%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	NGA	a	2	X	-	-	-
21	NAG	r	1	X	-	-	-
21	MAN	r	11	X	-	-	-
24	PTY	0	307	X	-	-	-
24	PTY	R	904	X	-	-	-
24	PTY	U	503	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 73243 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 E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	225	1822	1143	322	347	10	0	0
1	I	225	1822	1143	322	347	10	0	0
1	J	225	1822	1143	322	347	10	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit G 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	114	938	573	179	183	3	0	0
2	L	114	938	573	179	183	3	0	0
2	M	114	938	573	179	183	3	0	0

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	O	359	2916	1869	493	545	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	427	3508	2228	605	648	27	0	0

- Molecule 5 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	753	6141	4013	1020	1068	40	0	0

- Molecule 6 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	600	4652	2949	785	890	28	0	0
6	B	600	4656	2952	786	890	28	0	0
6	C	600	4656	2952	786	890	28	0	0

- Molecule 7 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	460	3600	2284	616	680	20	0	0
7	E	460	3589	2278	616	676	19	0	0
7	F	460	3596	2282	616	678	20	0	0

- Molecule 8 is a protein called SidK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	X	262	2111	1339	354	408	10	0	0
8	Y	267	2136	1355	359	411	11	0	0
8	Z	262	2105	1333	354	408	10	0	0

- Molecule 9 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	213	1713	1087	309	312	5	0	0

- Molecule 10 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	110	875	552	157	164	2	0	0

- Molecule 11 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	0	204	1495	988	238	259	10	0	0

- Molecule 12 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1	150	1065	698	169	191	7	0	0
12	2	150	1065	698	169	191	7	0	0
12	3	150	1065	698	169	191	7	0	0
12	4	150	1065	698	169	191	7	0	0
12	5	150	1065	698	169	191	7	0	0
12	6	150	1065	698	169	191	7	0	0
12	7	150	1059	695	166	191	7	0	0
12	8	150	1065	698	169	191	7	0	0
12	9	150	1065	698	169	191	7	0	0

- Molecule 13 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	350	2829	1825	461	530	13	0	0

- Molecule 14 is a protein called V-type proton ATPase subunit e 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	S	77	631	436	97	93	5	0	0

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	T	85	654	431	101	115	7	0	0

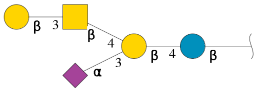
- Molecule 16 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	U	205	1664	1089	265	300	10	0	0

- Molecule 17 is a protein called Renin receptor.

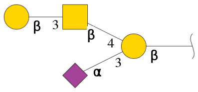
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	V	50	417	283	58	73	3	0	0

- Molecule 18 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	W	5	68	37	2	29	0	0

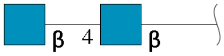
- Molecule 19 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	a	4	56	31	2	23	0	0

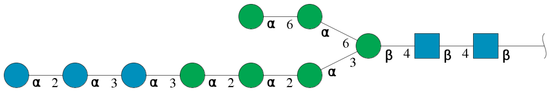
- Molecule 20 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.



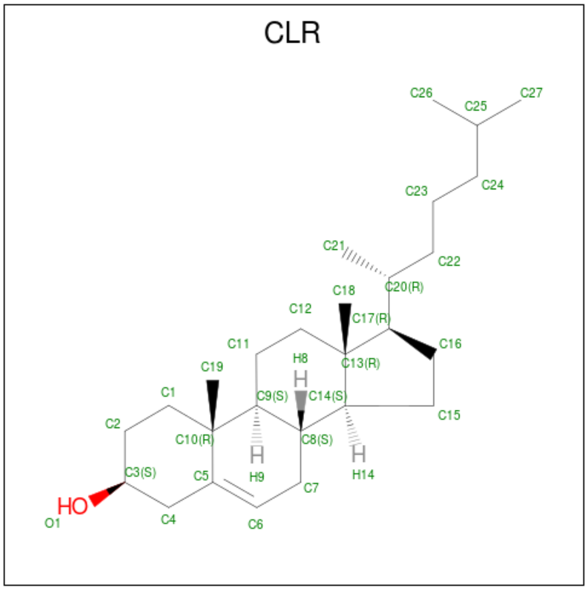
Mol	Chain	Residues	Atoms	AltConf	Trace
20	u	2	Total C N O 28 16 2 10	0	0
20	b	2	Total C N O 28 16 2 10	0	0
20	c	2	Total C N O 28 16 2 10	0	0
20	d	2	Total C N O 28 16 2 10	0	0
20	s	2	Total C N O 28 16 2 10	0	0

- Molecule 21 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)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



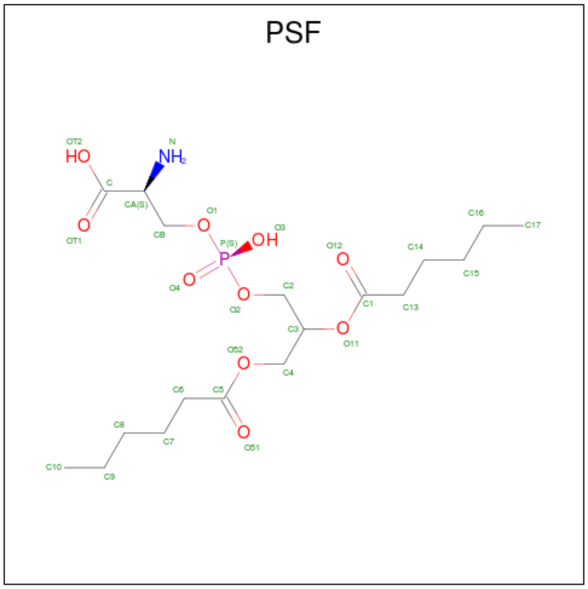
Mol	Chain	Residues	Atoms	AltConf	Trace
21	r	11	Total C N O 127 70 2 55	0	0

- Molecule 22 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



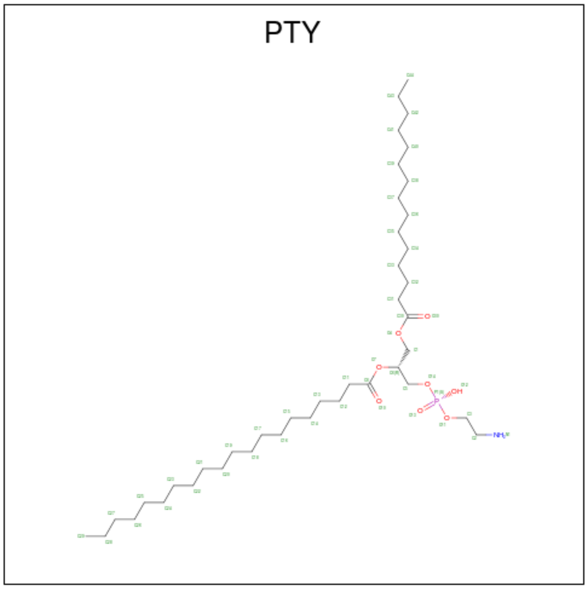
Mol	Chain	Residues	Atoms	AltConf
22	R	1	Total C O 28 27 1	0
22	0	1	Total C O 28 27 1	0
22	5	1	Total C O 28 27 1	0
22	V	1	Total C O 28 27 1	0

- Molecule 23 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
23	R	1	Total C N O P 30 18 1 10 1	0

- Molecule 24 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
24	R	1	Total C N O P 61 47 1 12 1	0
24	R	1	Total C N O P 61 47 1 12 1	0
24	0	1	Total C N O P 65 47 1 15 2	0
24	0	1	Total C N O P 65 47 1 15 2	0
24	2	1	Total C N O P 29 20 1 7 1	0
24	5	1	Total C N O P 35 25 1 8 1	0
24	6	1	Total C O P 21 13 7 1	0
24	7	1	Total C N O P 42 32 1 8 1	0
24	8	1	Total C N O P 83 68 1 13 1	0
24	8	1	Total C N O P 83 68 1 13 1	0

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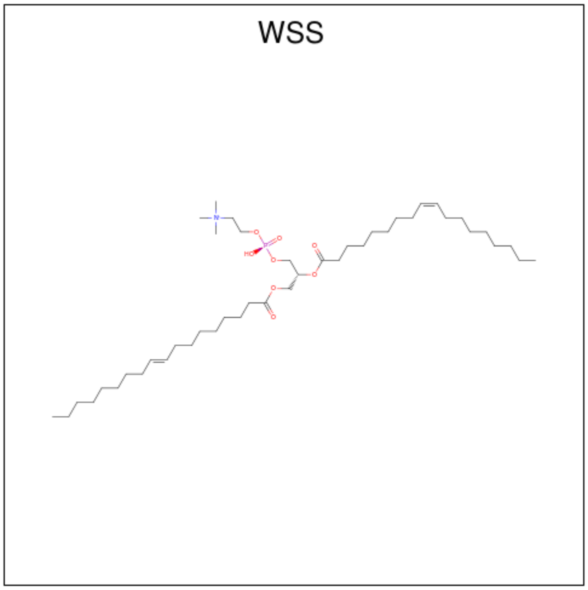
Mol	Chain	Residues	Atoms	AltConf
24	Q	1	Total C N O P 30 20 1 8 1	0
24	U	1	Total C O 26 21 5	0
24	V	1	Total C N O P 29 20 1 7 1	0

- Molecule 25 is tri(methyl)-[2-[[(2 {R})-2-[({Z})-octadec-9-enoyl]oxy-3-[({E})-1-oxidanylideneoctadec-9-enoxy]propoxy]-oxidanyl-phosphoryl]oxyethyl]azanium (three-letter code: WSS) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
25	R	1	Total C N O P 40 30 1 8 1	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	0	1	Total C N O P 142 103 3 32 4	0
25	1	1	Total C N O P 34 24 1 8 1	0
25	3	1	Total C O P 41 32 8 1	0

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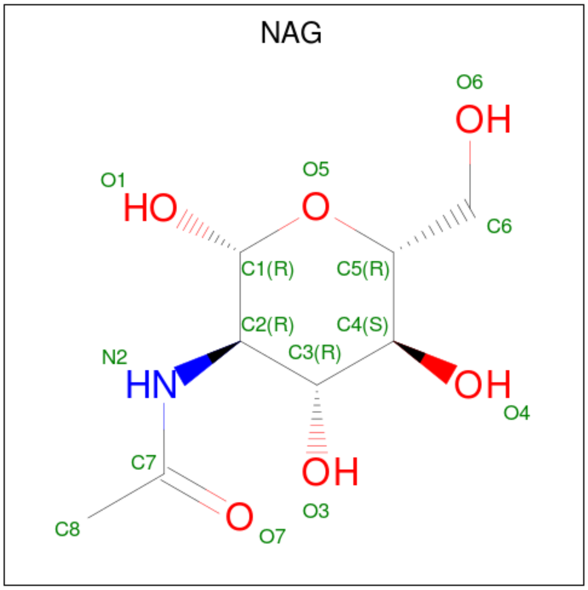
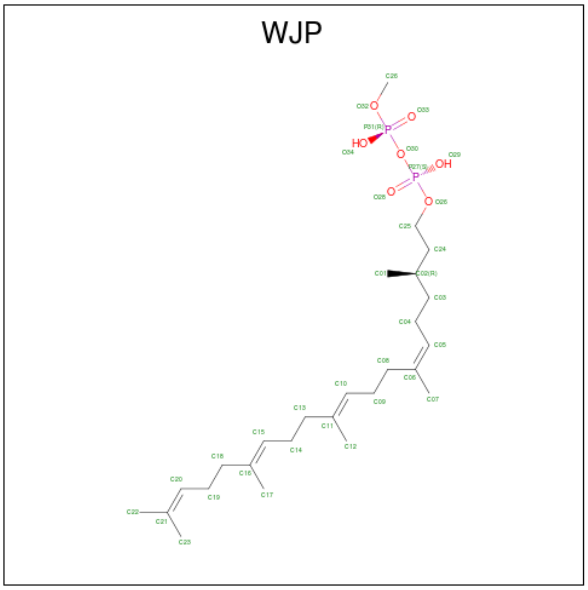
Mol	Chain	Residues	Atoms					AltConf
25	U	1	Total 76	C 56	N 2	O 16	P 2	0
25	U	1	Total 76	C 56	N 2	O 16	P 2	0
25	V	1	Total 37	C 27	N 1	O 8	P 1	0

- Molecule 26 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



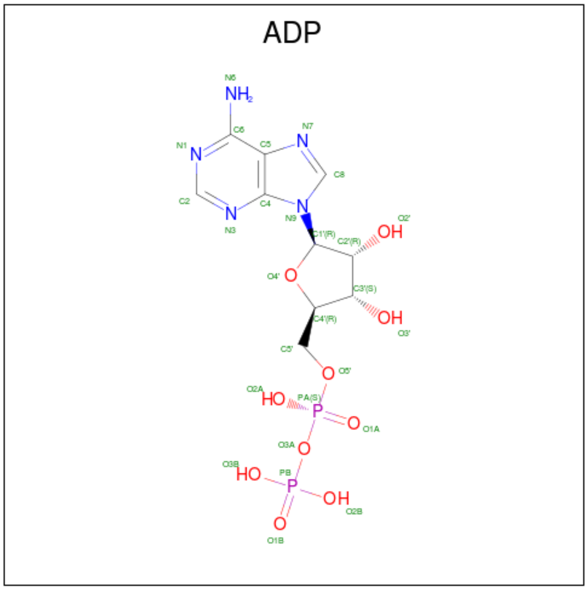
Mol	Chain	Residues	Atoms				AltConf
26	R	1	Total 14	C 8	N 1	O 5	0
26	U	1	Total 14	C 8	N 1	O 5	0

- Molecule 27 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicosa-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (three-letter code: WJP) (formula: $C_{26}H_{48}O_7P_2$) (labeled as "Ligand of Interest" by depositor).



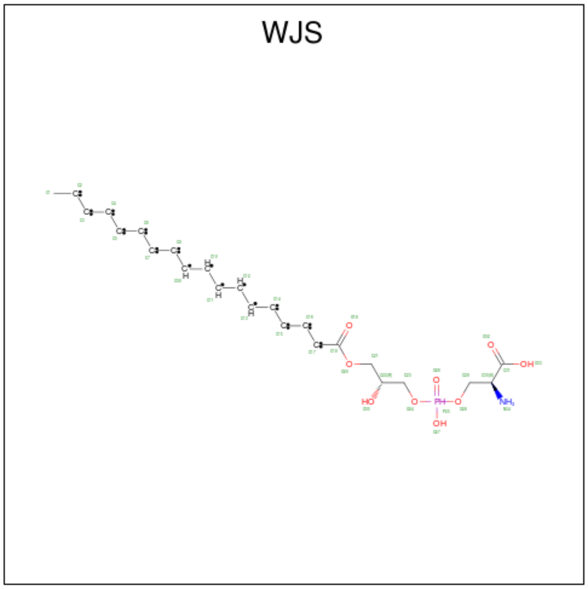
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	R	1	34	25	7	2	0

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
28	C	1	27	10	5	10	2	0

- Molecule 29 is (2 {S})-2-$l^{4}-azanyl-3-[[(2 {R})-3-octadecanoyloxy-2-oxidanyl-propoxy]-oxidanyl-oxidanylidene-$l^{6}-phosphanyl]oxy-propanoic acid (three-letter code: WJS) (formula: $C_{24}H_{20}NO_9P$).



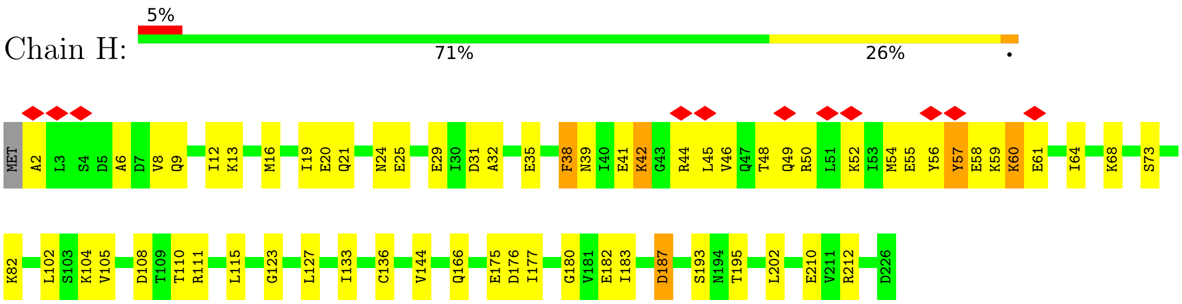
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	3	1	27	16	1	9	1	0

3 Residue-property plots ⓘ

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.

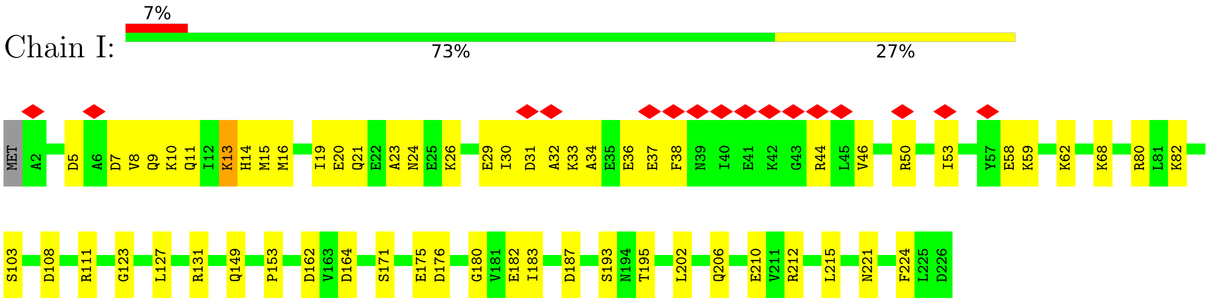
- Molecule 1: V-type proton ATPase subunit E 1

Chain H:



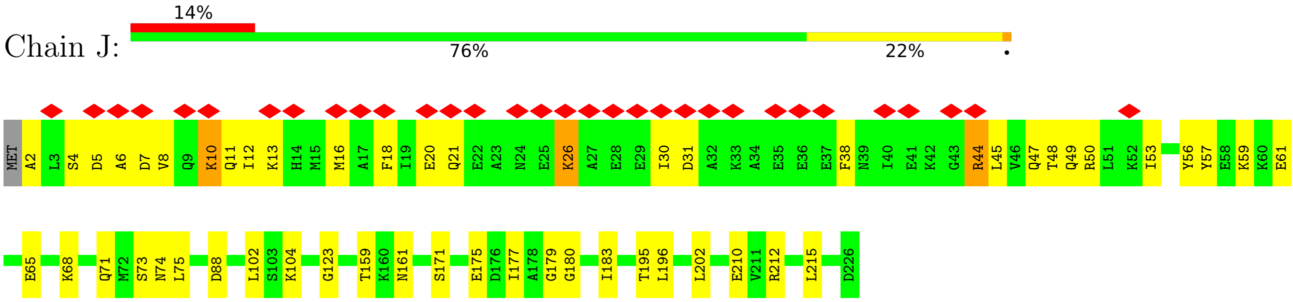
- Molecule 1: V-type proton ATPase subunit E 1

Chain I:



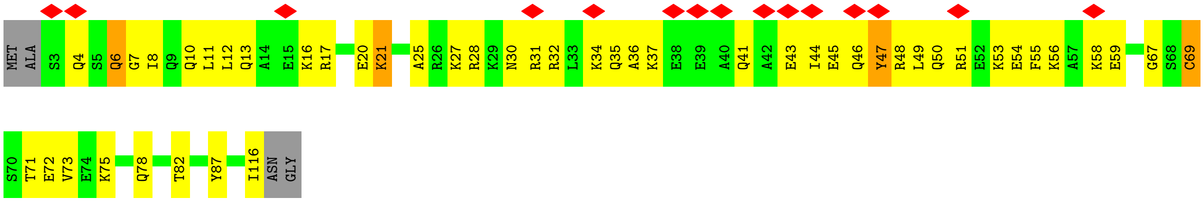
- Molecule 1: V-type proton ATPase subunit E 1

Chain J:



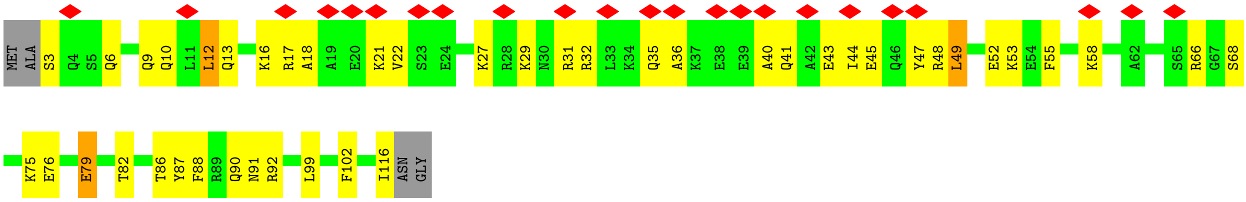
- Molecule 2: V-type proton ATPase subunit G 1

Chain K:



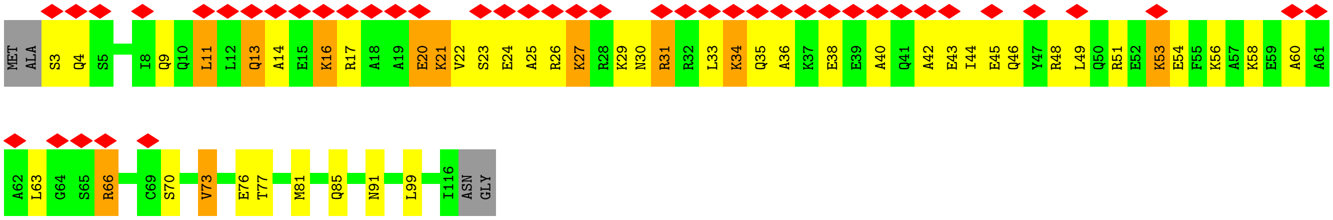
- Molecule 2: V-type proton ATPase subunit G 1

Chain L:



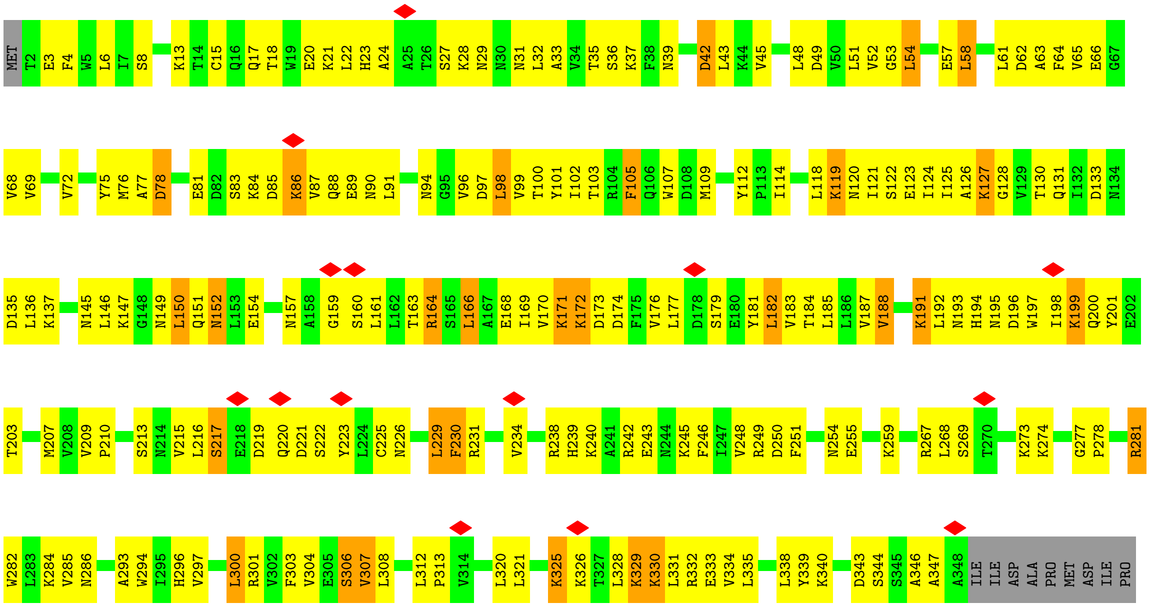
- Molecule 2: V-type proton ATPase subunit G 1

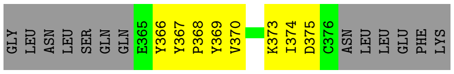
Chain M:



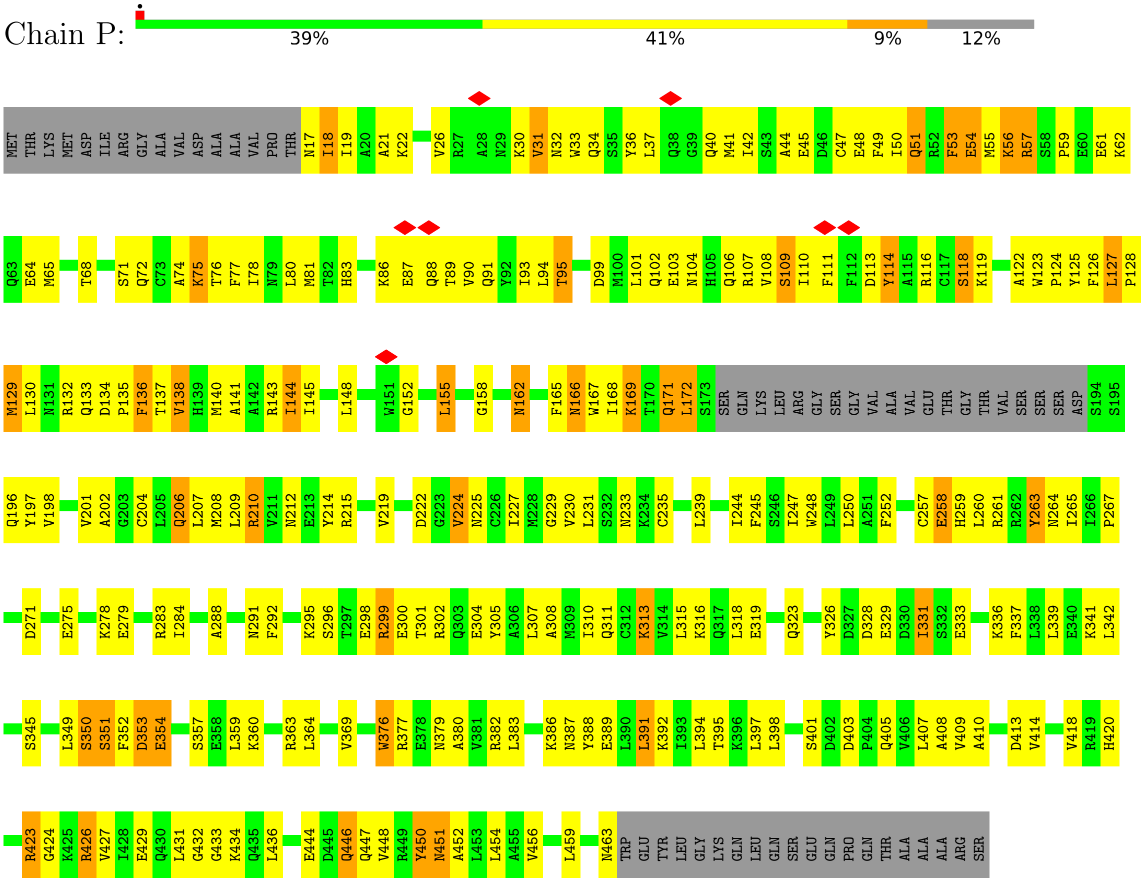
- Molecule 3: V-type proton ATPase subunit C 1

Chain O:

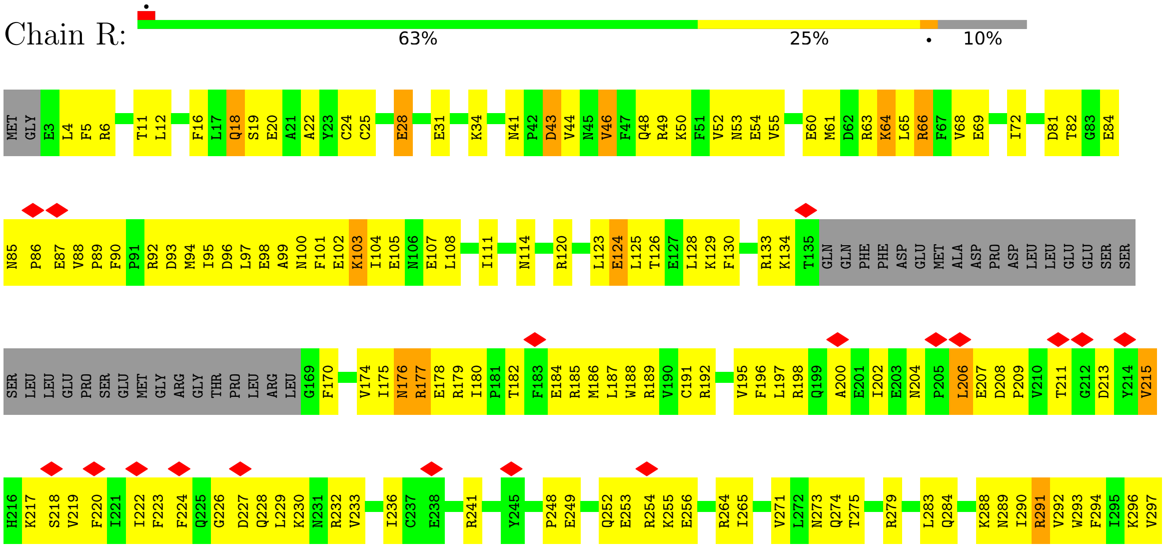


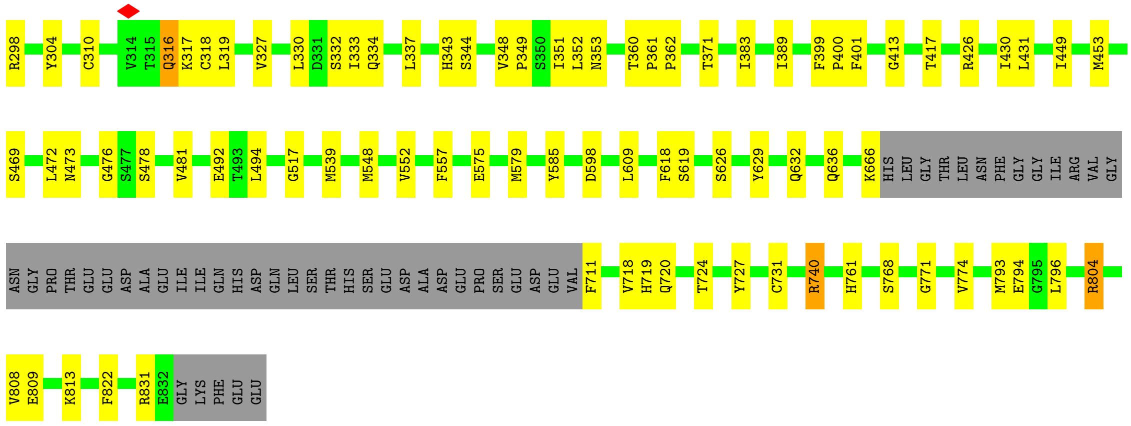


- Molecule 4: V-type proton ATPase subunit H

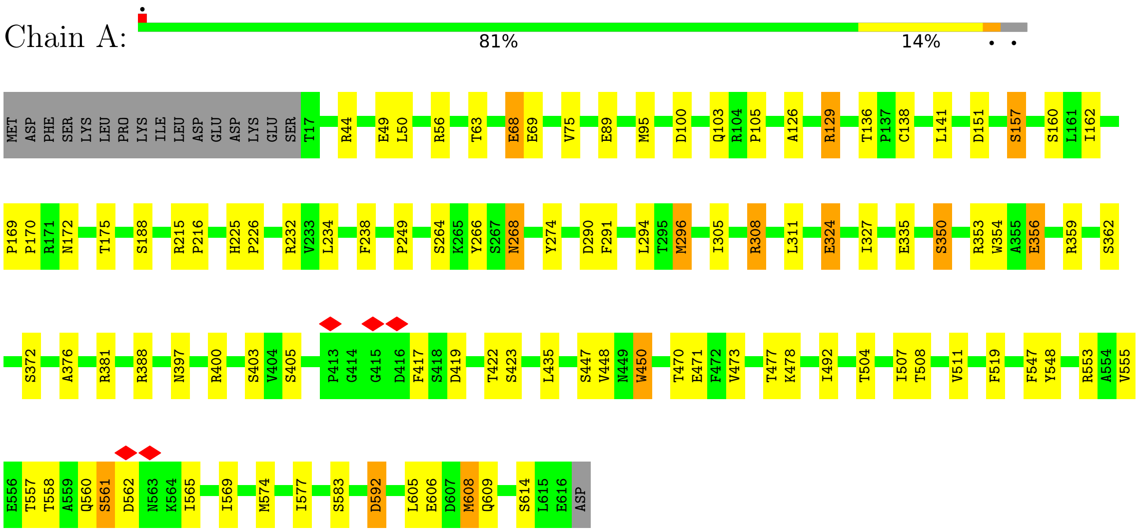


- Molecule 5: V-type proton ATPase 116 kDa subunit a isoform 1

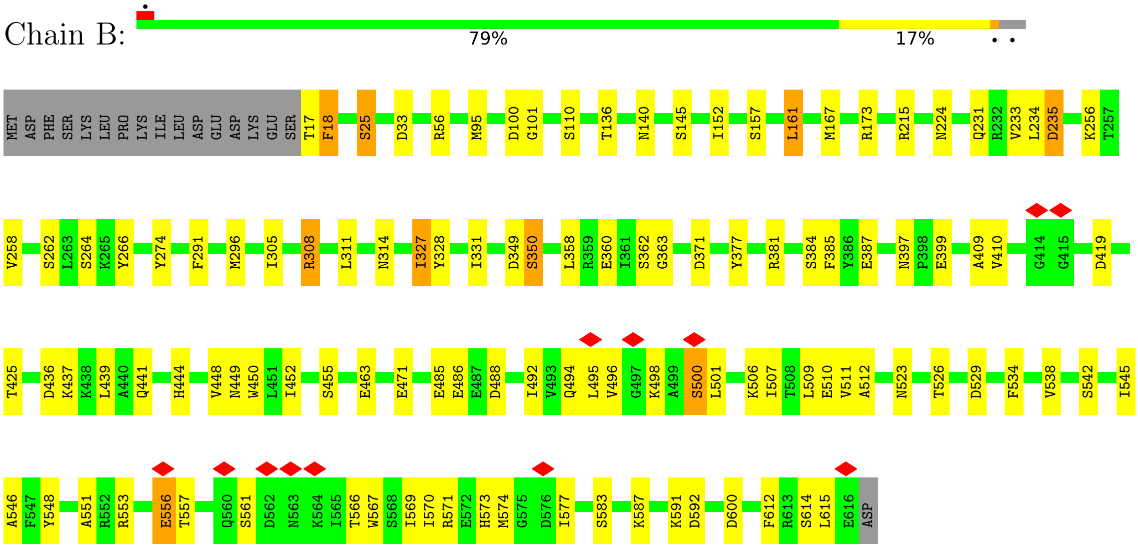




- Molecule 6: V-type proton ATPase catalytic subunit A

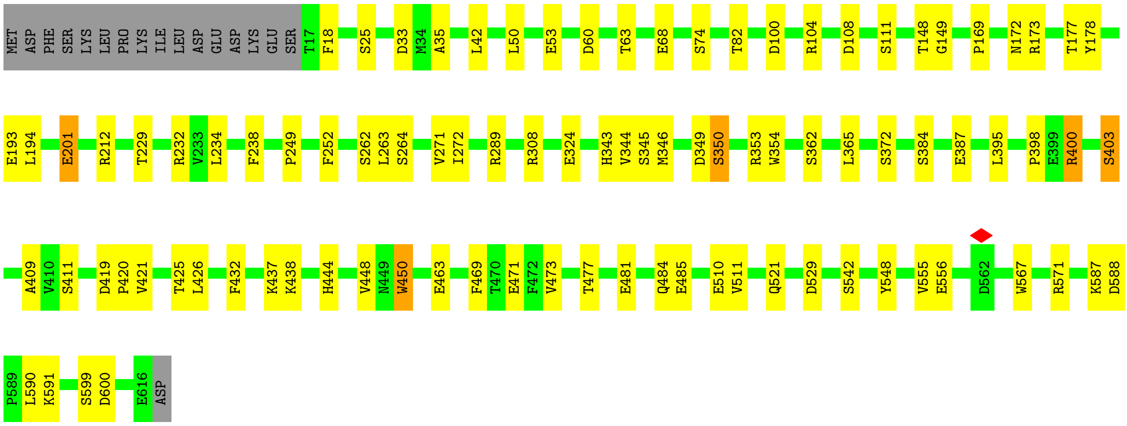


- Molecule 6: V-type proton ATPase catalytic subunit A



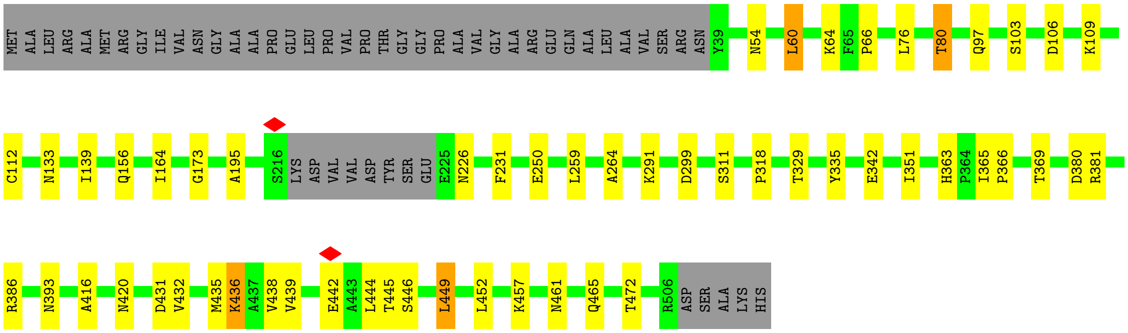
- Molecule 6: V-type proton ATPase catalytic subunit A

Chain C:



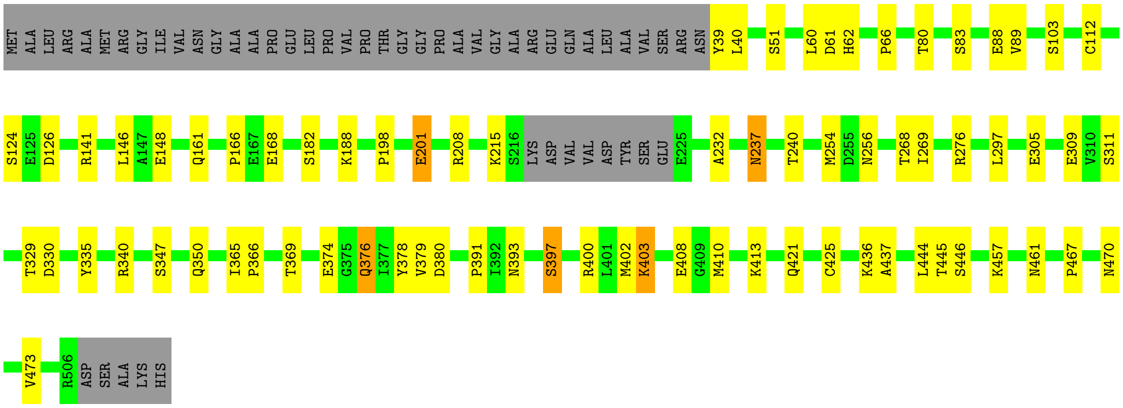
- Molecule 7: V-type proton ATPase subunit B, brain isoform

Chain D:



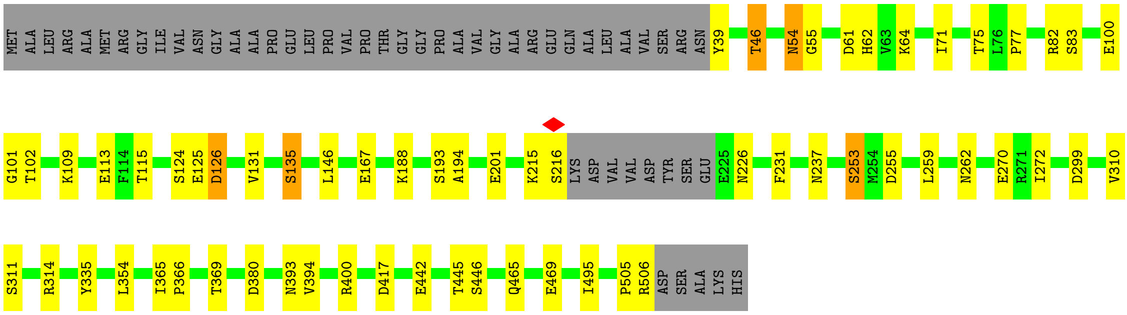
- Molecule 7: V-type proton ATPase subunit B, brain isoform

Chain E:



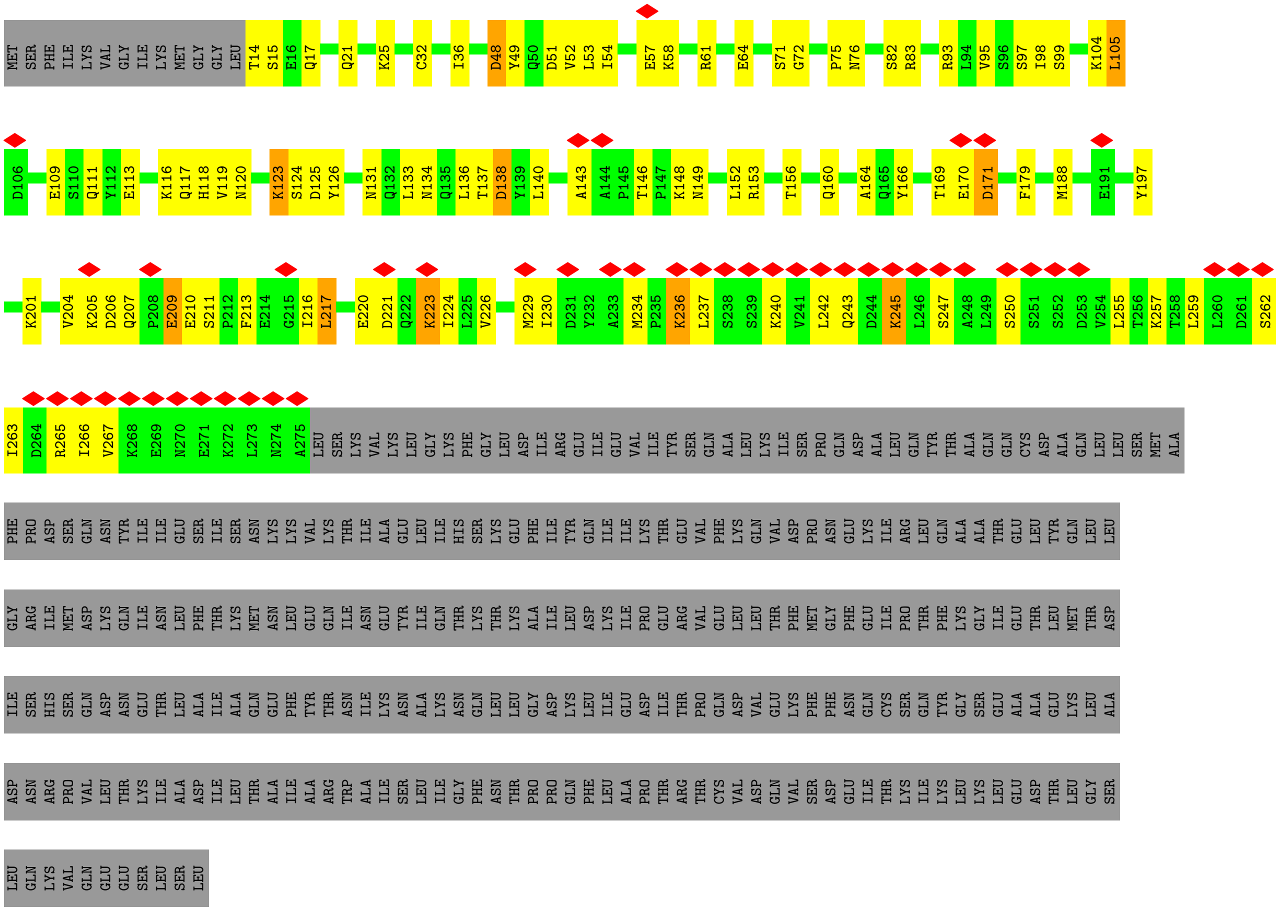
- Molecule 7: V-type proton ATPase subunit B, brain isoform

Chain F:



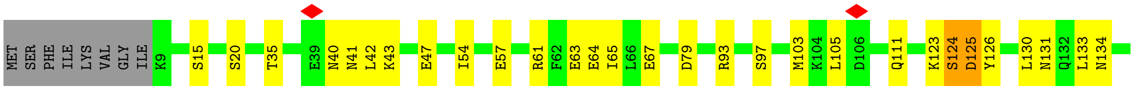
- Molecule 8: SidK

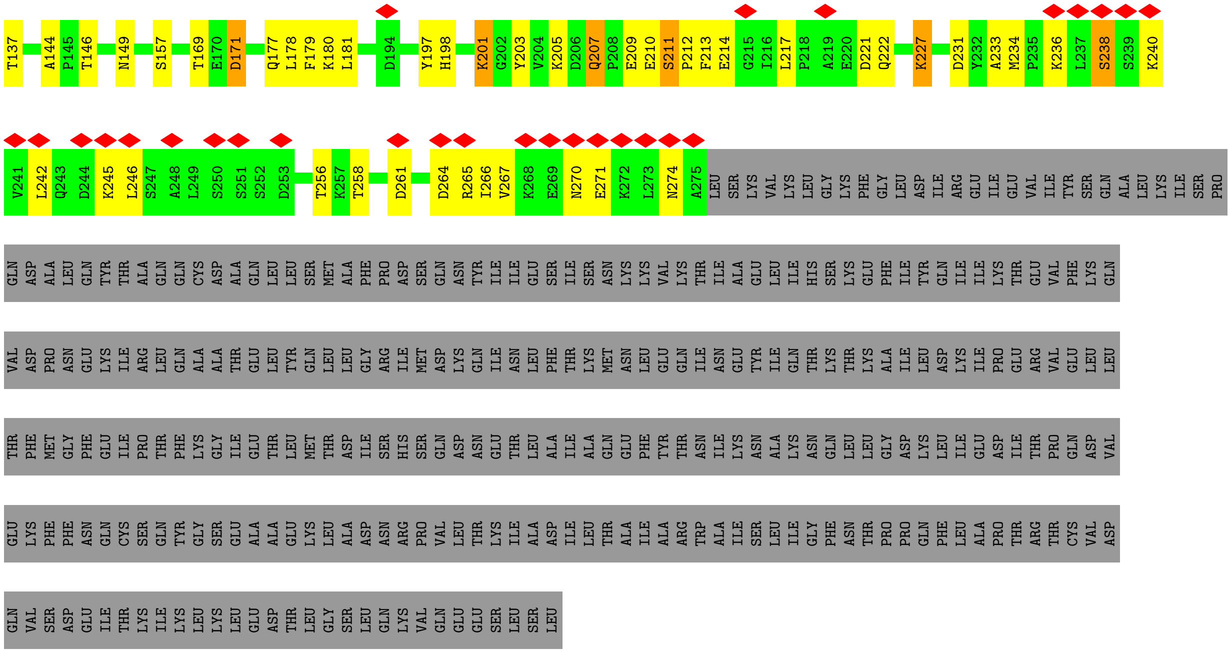
Chain X:



- Molecule 8: SidK

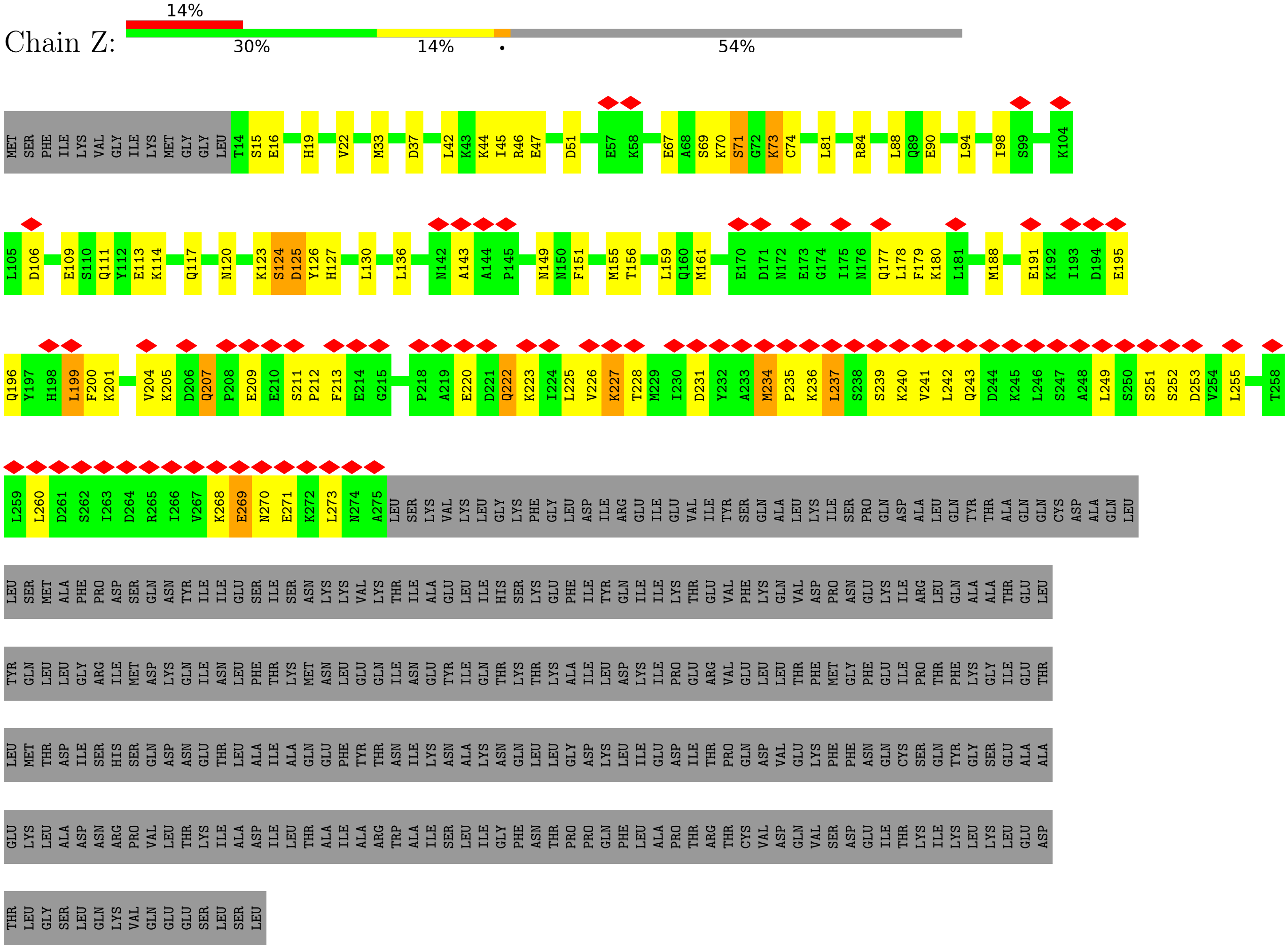
Chain Y:



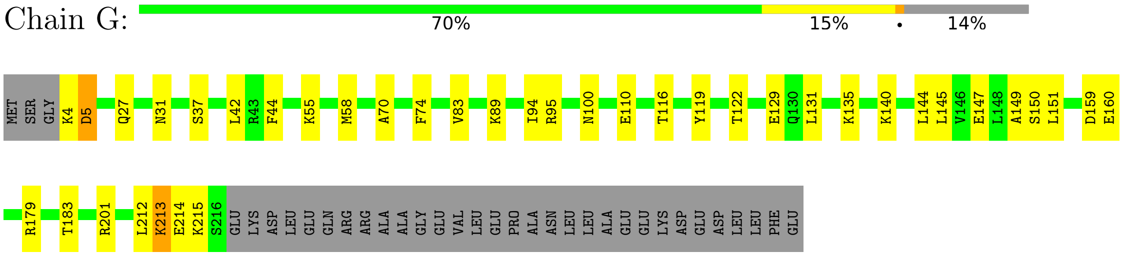


- Molecule 8: SidK

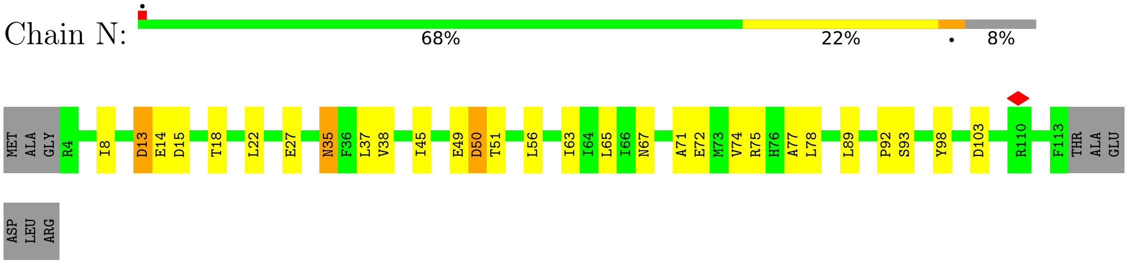
Chain Z:



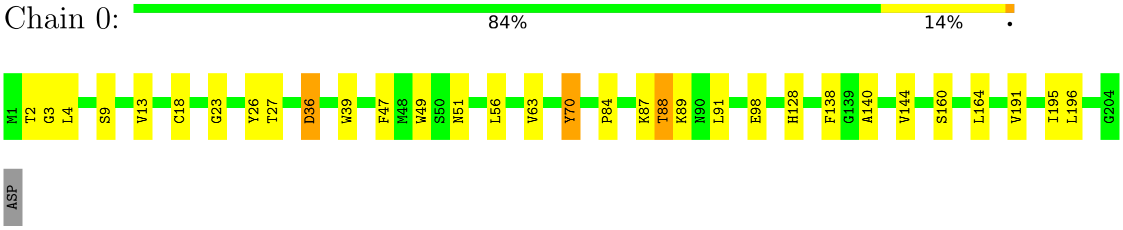
- Molecule 9: V-type proton ATPase subunit D



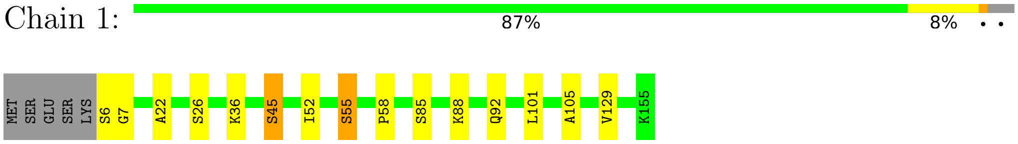
- Molecule 10: V-type proton ATPase subunit F



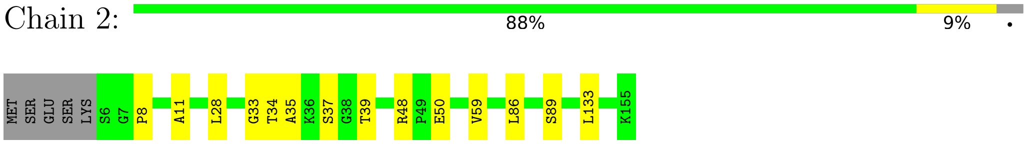
- Molecule 11: V-type proton ATPase 21 kDa proteolipid subunit



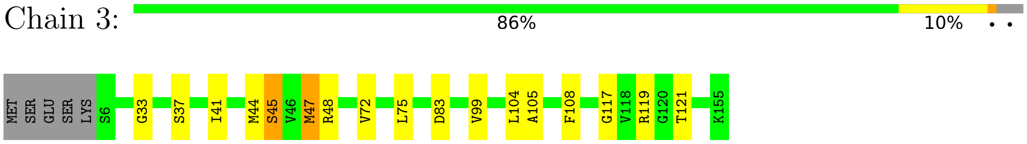
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

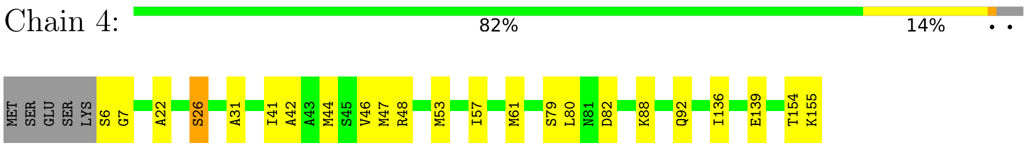


- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit



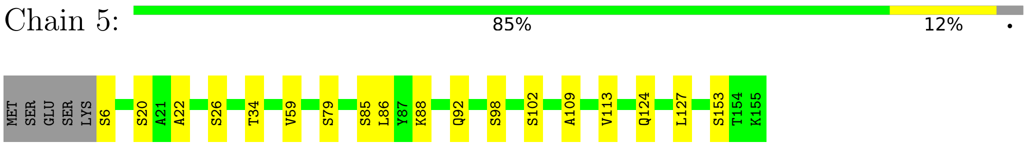
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 4:



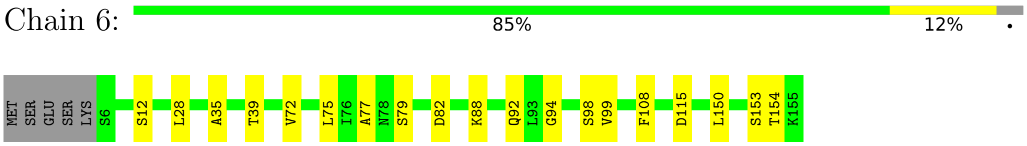
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 5:



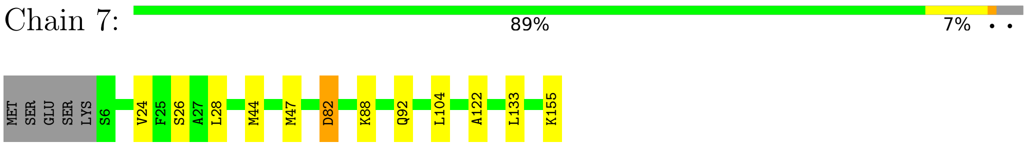
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 6:



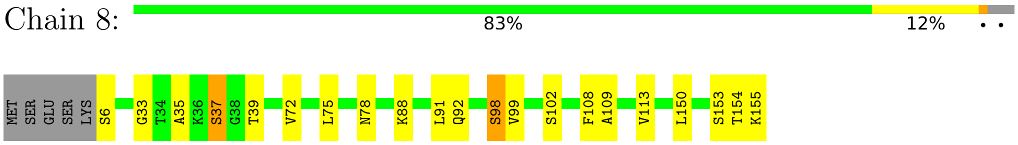
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 7:



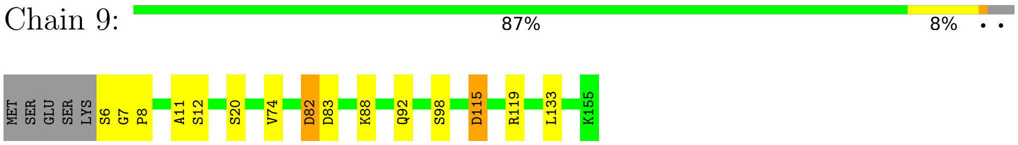
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 8:



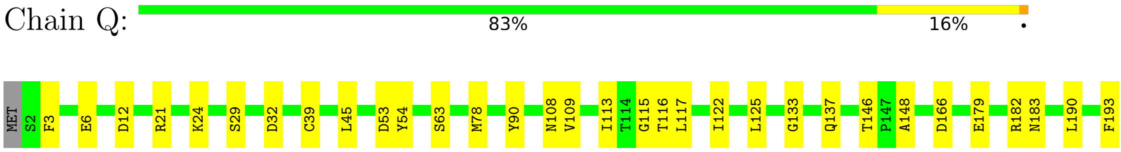
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain 9:

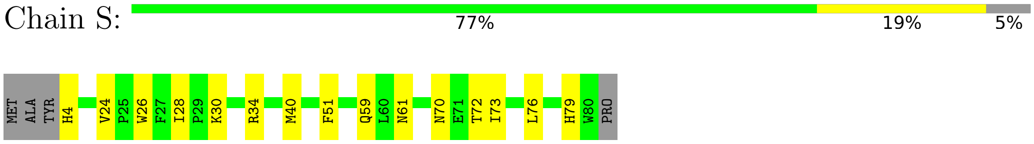


- Molecule 13: V-type proton ATPase subunit d 1

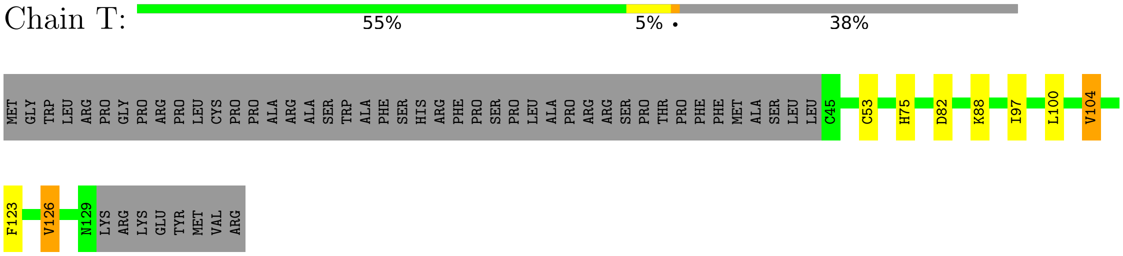
Chain Q:



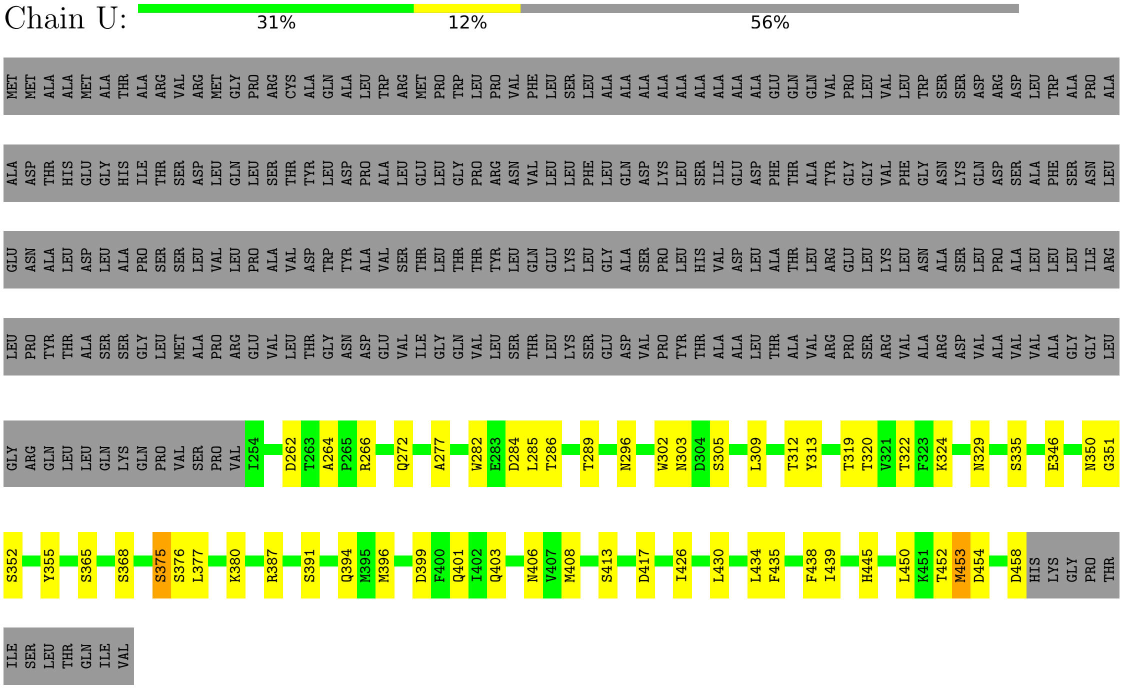
- Molecule 14: V-type proton ATPase subunit e 1



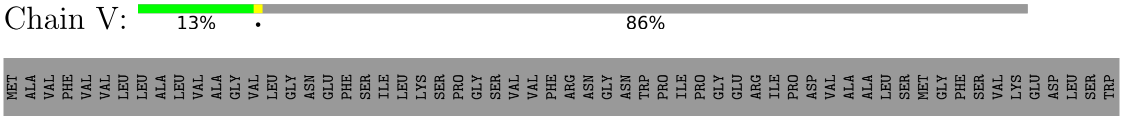
- Molecule 15: Ribonuclease kappa

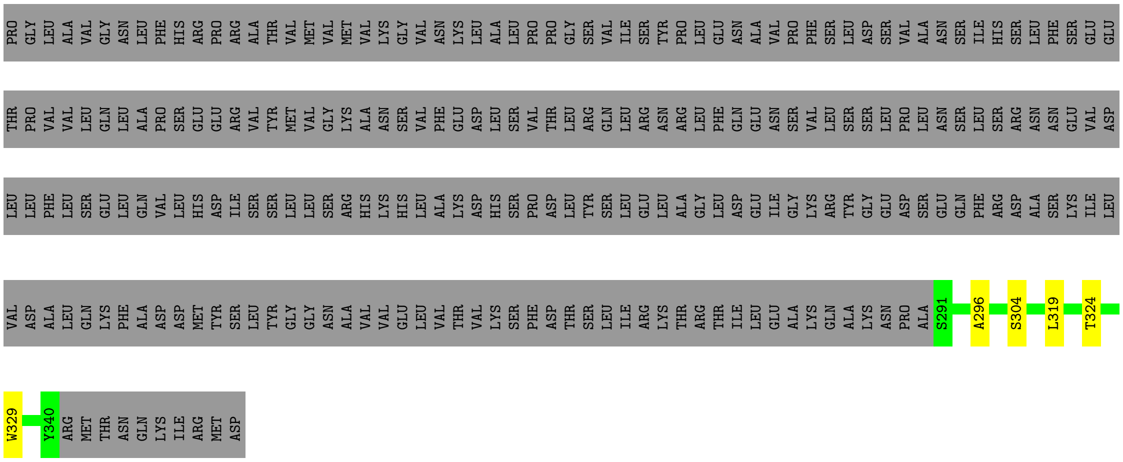


- Molecule 16: V-type proton ATPase subunit S1



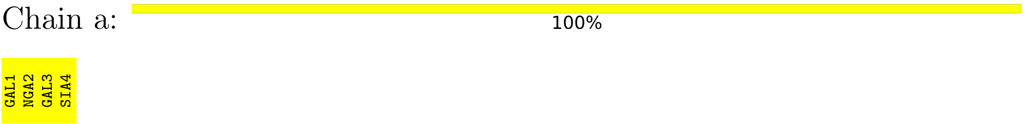
- Molecule 17: Renin receptor



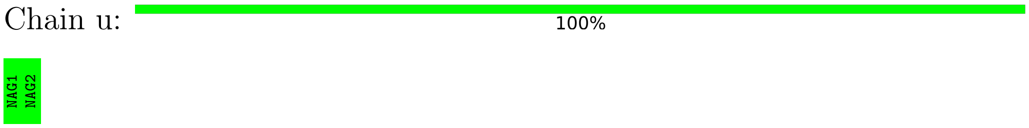


- Molecule 18: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

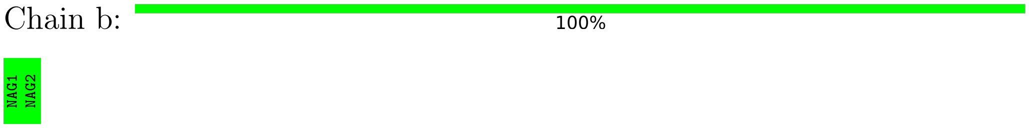
- Molecule 19: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose



- Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



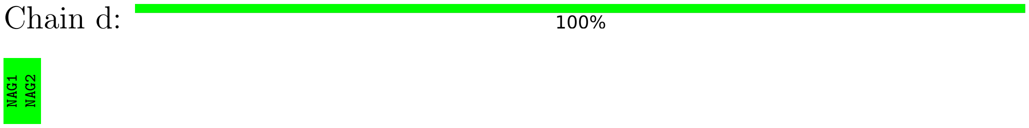
- Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

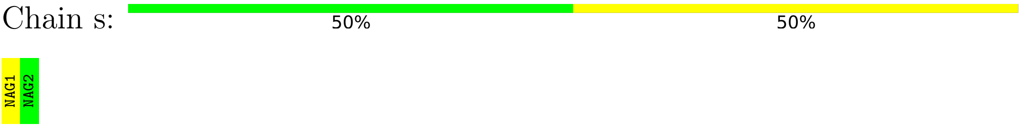
- Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



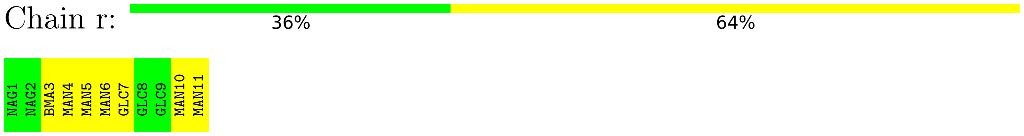
- Molecule 20: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:



- Molecule 21: 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)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	30.271	Depositor
Minimum map value	-15.824	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	2.8	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, PSF, NGA, BGC, MAN, NAG, SIA, WJP, WSS, GLC, WJS, PTY, CLR, BMA, ADP

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	H	0.32	0/1839	0.47	0/2462
1	I	0.33	0/1839	0.46	0/2462
1	J	0.32	0/1839	0.45	0/2462
2	K	0.31	0/945	0.49	0/1258
2	L	0.33	0/945	0.49	1/1258 (0.1%)
2	M	0.34	0/945	0.50	0/1258
3	O	0.29	0/2970	0.56	1/4013 (0.0%)
4	P	0.31	0/3576	0.51	0/4819
5	R	0.40	0/6299	0.48	0/8523
6	A	0.41	0/4748	0.46	0/6431
6	B	0.39	0/4752	0.47	0/6435
6	C	0.43	0/4752	0.47	0/6435
7	D	0.43	0/3671	0.47	0/4973
7	E	0.43	0/3660	0.47	0/4960
7	F	0.42	0/3667	0.47	0/4968
8	X	0.29	0/2145	0.47	0/2893
8	Y	0.28	0/2170	0.43	0/2926
8	Z	0.28	0/2138	0.46	0/2884
9	G	0.37	0/1731	0.50	0/2316
10	N	0.34	0/889	0.51	0/1200
11	0	0.47	0/1529	0.48	0/2079
12	1	0.47	0/1080	0.48	0/1461
12	2	0.46	0/1080	0.48	0/1461
12	3	0.46	0/1080	0.46	0/1461
12	4	0.48	0/1080	0.47	0/1461
12	5	0.46	0/1080	0.47	0/1461
12	6	0.43	0/1080	0.48	0/1461
12	7	0.43	0/1074	0.46	0/1454
12	8	0.45	0/1080	0.48	0/1461
12	9	0.47	0/1080	0.48	0/1461
13	Q	0.49	0/2895	0.46	0/3922
14	S	0.42	0/657	0.45	0/902

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	T	0.38	0/670	0.44	0/911
16	U	0.41	0/1718	0.48	0/2337
17	V	0.50	0/431	0.43	0/591
All	All	0.39	0/73134	0.48	2/98820 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	300	LEU	CA-CB-CG	5.27	127.41	115.30
2	L	12	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	O	312	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1822	0	1886	42	0
1	I	1822	0	1886	44	0
1	J	1822	0	1886	32	0
2	K	938	0	947	31	0
2	L	938	0	947	36	0
2	M	938	0	947	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	2916	0	2955	162	0
4	P	3508	0	3483	196	0
5	R	6141	0	6161	145	0
6	A	4652	0	4631	45	0
6	B	4656	0	4642	56	0
6	C	4656	0	4642	46	0
7	D	3600	0	3605	26	0
7	E	3589	0	3590	39	0
7	F	3596	0	3601	32	0
8	X	2111	0	2134	52	0
8	Y	2136	0	2158	40	0
8	Z	2105	0	2127	51	0
9	G	1713	0	1818	21	0
10	N	875	0	878	23	0
11	0	1495	0	1537	22	0
12	1	1065	0	1131	8	0
12	2	1065	0	1131	8	0
12	3	1065	0	1131	14	0
12	4	1065	0	1131	13	0
12	5	1065	0	1131	9	0
12	6	1065	0	1131	8	0
12	7	1059	0	1120	9	0
12	8	1065	0	1131	12	0
12	9	1065	0	1131	8	0
13	Q	2829	0	2757	30	0
14	S	631	0	646	10	0
15	T	654	0	641	4	0
16	U	1664	0	1584	45	0
17	V	417	0	405	4	0
18	W	68	0	58	3	0
19	a	56	0	47	0	0
20	b	28	0	25	0	0
20	c	28	0	25	0	0
20	d	28	0	25	0	0
20	s	28	0	25	0	0
20	u	28	0	25	0	0
21	r	127	0	106	0	0
22	0	28	0	46	1	0
22	5	28	0	46	16	0
22	R	28	0	46	1	0
22	V	28	0	46	11	0
23	R	30	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	0	65	0	85	4	0
24	2	29	0	40	1	0
24	5	35	0	46	6	0
24	6	21	0	19	7	0
24	7	42	0	60	7	0
24	8	83	0	129	10	0
24	Q	30	0	33	6	0
24	R	61	0	85	2	0
24	U	26	0	33	21	0
24	V	29	0	40	9	0
25	0	142	0	0	1	0
25	1	34	0	0	0	0
25	3	41	0	0	0	0
25	R	40	0	0	5	0
25	U	76	0	0	0	0
25	V	37	0	0	0	0
26	R	14	0	13	0	0
26	U	14	0	13	0	0
27	R	34	0	0	0	0
28	C	27	0	12	1	0
29	3	27	0	0	5	0
All	All	73243	0	73822	1307	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1307 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)
5:R:473:ASN:ND2	25:R:905:WSS:C4	1.82	1.39
5:R:473:ASN:HD22	25:R:905:WSS:C4	1.38	1.33
16:U:438:PHE:CE2	24:U:503:PTY:H181	1.71	1.25
16:U:438:PHE:HE2	24:U:503:PTY:C18	1.56	1.17
24:6:201:PTY:O13	24:7:201:PTY:C2	1.95	1.14

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	H	223/226 (99%)	213 (96%)	10 (4%)	0	100	100
1	I	223/226 (99%)	218 (98%)	5 (2%)	0	100	100
1	J	223/226 (99%)	221 (99%)	2 (1%)	0	100	100
2	K	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
2	L	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
2	M	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
3	O	355/382 (93%)	325 (92%)	29 (8%)	1 (0%)	41	73
4	P	423/483 (88%)	379 (90%)	41 (10%)	3 (1%)	22	57
5	R	745/837 (89%)	698 (94%)	47 (6%)	0	100	100
6	A	598/617 (97%)	572 (96%)	26 (4%)	0	100	100
6	B	598/617 (97%)	562 (94%)	36 (6%)	0	100	100
6	C	598/617 (97%)	567 (95%)	30 (5%)	1 (0%)	47	79
7	D	456/511 (89%)	432 (95%)	24 (5%)	0	100	100
7	E	456/511 (89%)	434 (95%)	22 (5%)	0	100	100
7	F	456/511 (89%)	440 (96%)	16 (4%)	0	100	100
8	X	260/573 (45%)	248 (95%)	12 (5%)	0	100	100
8	Y	265/573 (46%)	250 (94%)	15 (6%)	0	100	100
8	Z	260/573 (45%)	238 (92%)	22 (8%)	0	100	100
9	G	211/247 (85%)	201 (95%)	10 (5%)	0	100	100
10	N	108/119 (91%)	97 (90%)	11 (10%)	0	100	100
11	0	202/205 (98%)	199 (98%)	3 (2%)	0	100	100
12	1	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	2	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	3	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	4	148/155 (96%)	144 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	5	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
12	6	148/155 (96%)	139 (94%)	9 (6%)	0	100	100
12	7	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
12	8	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	9	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
13	Q	348/351 (99%)	333 (96%)	15 (4%)	0	100	100
14	S	75/81 (93%)	70 (93%)	5 (7%)	0	100	100
15	T	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
16	U	203/470 (43%)	187 (92%)	16 (8%)	0	100	100
17	V	48/350 (14%)	44 (92%)	4 (8%)	0	100	100
All	All	9085/11192 (81%)	8610 (95%)	470 (5%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	P	109	SER
4	P	30	LYS
6	C	35	ALA
3	O	313	PRO
4	P	31	VAL

5.3.2 Protein sidechains ⓘ

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	H	198/199 (100%)	182 (92%)	16 (8%)	11	39
1	I	198/199 (100%)	188 (95%)	10 (5%)	24	56
1	J	198/199 (100%)	185 (93%)	13 (7%)	16	47
2	K	99/101 (98%)	88 (89%)	11 (11%)	6	24
2	L	99/101 (98%)	92 (93%)	7 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	99/101 (98%)	81 (82%)	18 (18%)	1	7
3	O	323/344 (94%)	274 (85%)	49 (15%)	3	12
4	P	385/429 (90%)	320 (83%)	65 (17%)	2	9
5	R	673/746 (90%)	622 (92%)	51 (8%)	13	41
6	A	507/525 (97%)	470 (93%)	37 (7%)	14	43
6	B	508/525 (97%)	471 (93%)	37 (7%)	14	43
6	C	508/525 (97%)	479 (94%)	29 (6%)	20	52
7	D	393/430 (91%)	376 (96%)	17 (4%)	29	62
7	E	390/430 (91%)	369 (95%)	21 (5%)	22	53
7	F	392/430 (91%)	376 (96%)	16 (4%)	30	64
8	X	238/519 (46%)	210 (88%)	28 (12%)	5	21
8	Y	239/519 (46%)	215 (90%)	24 (10%)	7	28
8	Z	237/519 (46%)	212 (90%)	25 (10%)	7	26
9	G	183/212 (86%)	168 (92%)	15 (8%)	11	38
10	N	94/100 (94%)	90 (96%)	4 (4%)	29	62
11	0	153/155 (99%)	147 (96%)	6 (4%)	32	65
12	1	107/112 (96%)	103 (96%)	4 (4%)	34	66
12	2	107/112 (96%)	106 (99%)	1 (1%)	78	91
12	3	107/112 (96%)	104 (97%)	3 (3%)	43	73
12	4	107/112 (96%)	102 (95%)	5 (5%)	26	59
12	5	107/112 (96%)	102 (95%)	5 (5%)	26	59
12	6	107/112 (96%)	100 (94%)	7 (6%)	17	47
12	7	106/112 (95%)	104 (98%)	2 (2%)	57	81
12	8	107/112 (96%)	102 (95%)	5 (5%)	26	59
12	9	107/112 (96%)	102 (95%)	5 (5%)	26	59
13	Q	303/306 (99%)	288 (95%)	15 (5%)	24	57
14	S	69/72 (96%)	66 (96%)	3 (4%)	29	62
15	T	70/116 (60%)	65 (93%)	5 (7%)	14	44
16	U	182/397 (46%)	171 (94%)	11 (6%)	19	49
17	V	45/308 (15%)	44 (98%)	1 (2%)	52	78
All	All	7745/9515 (81%)	7174 (93%)	571 (7%)	17	42

5 of 571 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Z	191	GLU
9	G	42	LEU
8	Z	179	PHE
12	6	79	SER
5	R	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
9	G	88	ASN
9	G	206	GLN
14	S	67	GLN
4	P	457	GLN
4	P	439	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

30 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	$\#\|Z\| > 2$
18	BGC	W	1	18	12,12,12	0.55	0	17,17,17	1.39	4 (23%)
18	GAL	W	2	18	11,11,12	0.77	0	15,15,17	1.44	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	NGA	W	3	18	14,14,15	0.43	0	17,19,21	1.94	6 (35%)
18	GAL	W	4	18	11,11,12	0.33	0	15,15,17	0.86	1 (6%)
18	SIA	W	5	18	20,20,21	0.60	0	24,28,31	1.37	2 (8%)
19	GAL	a	1	19	11,11,12	0.59	0	15,15,17	1.41	2 (13%)
19	NGA	a	2	19	14,14,15	0.70	0	17,19,21	1.85	4 (23%)
19	GAL	a	3	19	11,11,12	0.58	0	15,15,17	1.79	2 (13%)
19	SIA	a	4	19	20,20,21	0.73	1 (5%)	24,28,31	1.13	2 (8%)
20	NAG	b	1	16,20	14,14,15	0.23	0	17,19,21	0.51	0
20	NAG	b	2	20	14,14,15	0.27	0	17,19,21	0.47	0
20	NAG	c	1	16,20	14,14,15	0.53	0	17,19,21	0.74	0
20	NAG	c	2	20	14,14,15	0.24	0	17,19,21	0.85	1 (5%)
20	NAG	d	1	20	14,14,15	0.44	0	17,19,21	0.34	0
20	NAG	d	2	20	14,14,15	0.18	0	17,19,21	0.45	0
21	NAG	r	1	21,27	14,14,15	0.37	0	17,19,21	0.49	0
21	MAN	r	10	21	11,11,12	0.57	0	15,15,17	1.10	1 (6%)
21	MAN	r	11	21	11,11,12	0.37	0	15,15,17	0.82	1 (6%)
21	NAG	r	2	21	14,14,15	0.43	0	17,19,21	0.49	0
21	BMA	r	3	21	11,11,12	0.86	0	15,15,17	1.03	1 (6%)
21	MAN	r	4	21	11,11,12	0.91	1 (9%)	15,15,17	1.06	1 (6%)
21	MAN	r	5	21	11,11,12	0.95	1 (9%)	15,15,17	1.23	2 (13%)
21	MAN	r	6	21	11,11,12	0.86	1 (9%)	15,15,17	0.90	1 (6%)
21	GLC	r	7	21	11,11,12	0.78	0	15,15,17	0.90	1 (6%)
21	GLC	r	8	21	11,11,12	0.64	0	15,15,17	0.90	0
21	GLC	r	9	21	11,11,12	0.66	0	15,15,17	0.75	0
20	NAG	s	1	14,20	14,14,15	0.25	0	17,19,21	0.66	1 (5%)
20	NAG	s	2	20	14,14,15	0.21	0	17,19,21	0.50	0
20	NAG	u	1	16,20	14,14,15	0.22	0	17,19,21	0.53	0
20	NAG	u	2	20	14,14,15	0.29	0	17,19,21	0.46	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
18	BGC	W	1	18	-	1/2/22/22	0/1/1/1
18	GAL	W	2	18	-	0/2/19/22	0/1/1/1
18	NGA	W	3	18	-	2/6/23/26	0/1/1/1
18	GAL	W	4	18	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SIA	W	5	18	-	2/18/34/38	0/1/1/1
19	GAL	a	1	19	-	0/2/19/22	0/1/1/1
19	NGA	a	2	19	1/1/5/7	3/6/23/26	0/1/1/1
19	GAL	a	3	19	-	1/2/19/22	0/1/1/1
19	SIA	a	4	19	-	13/18/34/38	0/1/1/1
20	NAG	b	1	16,20	-	1/6/23/26	0/1/1/1
20	NAG	b	2	20	-	4/6/23/26	0/1/1/1
20	NAG	c	1	16,20	-	3/6/23/26	0/1/1/1
20	NAG	c	2	20	-	2/6/23/26	0/1/1/1
20	NAG	d	1	20	-	3/6/23/26	0/1/1/1
20	NAG	d	2	20	-	2/6/23/26	0/1/1/1
21	NAG	r	1	21,27	1/1/5/7	2/6/23/26	0/1/1/1
21	MAN	r	10	21	-	2/2/19/22	0/1/1/1
21	MAN	r	11	21	1/1/4/5	0/2/19/22	0/1/1/1
21	NAG	r	2	21	-	2/6/23/26	0/1/1/1
21	BMA	r	3	21	-	0/2/19/22	0/1/1/1
21	MAN	r	4	21	-	2/2/19/22	0/1/1/1
21	MAN	r	5	21	-	2/2/19/22	0/1/1/1
21	MAN	r	6	21	-	2/2/19/22	0/1/1/1
21	GLC	r	7	21	-	1/2/19/22	0/1/1/1
21	GLC	r	8	21	-	0/2/19/22	0/1/1/1
21	GLC	r	9	21	-	0/2/19/22	0/1/1/1
20	NAG	s	1	14,20	-	2/6/23/26	0/1/1/1
20	NAG	s	2	20	-	3/6/23/26	0/1/1/1
20	NAG	u	1	16,20	-	2/6/23/26	0/1/1/1
20	NAG	u	2	20	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	4	SIA	O1B-C1	-2.83	1.21	1.30
21	r	6	MAN	O5-C1	-2.62	1.39	1.43
21	r	4	MAN	O5-C1	-2.55	1.39	1.43
21	r	5	MAN	O5-C1	-2.02	1.40	1.43

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	2	NGA	C1-O5-C5	4.82	118.72	112.19
19	a	3	GAL	C1-C2-C3	4.51	115.20	109.67
19	a	3	GAL	C1-O5-C5	4.03	117.66	112.19
19	a	2	NGA	C2-N2-C7	-3.71	117.62	122.90
18	W	3	NGA	C1-C2-N2	3.71	116.82	110.49

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	a	2	NGA	C1
21	r	1	NAG	C1
21	r	11	MAN	C1

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	W	3	NGA	C8-C7-N2-C2
18	W	3	NGA	O7-C7-N2-C2
19	a	4	SIA	C5-C6-C7-C8
19	a	4	SIA	C5-C6-C7-O7
19	a	4	SIA	O6-C6-C7-C8

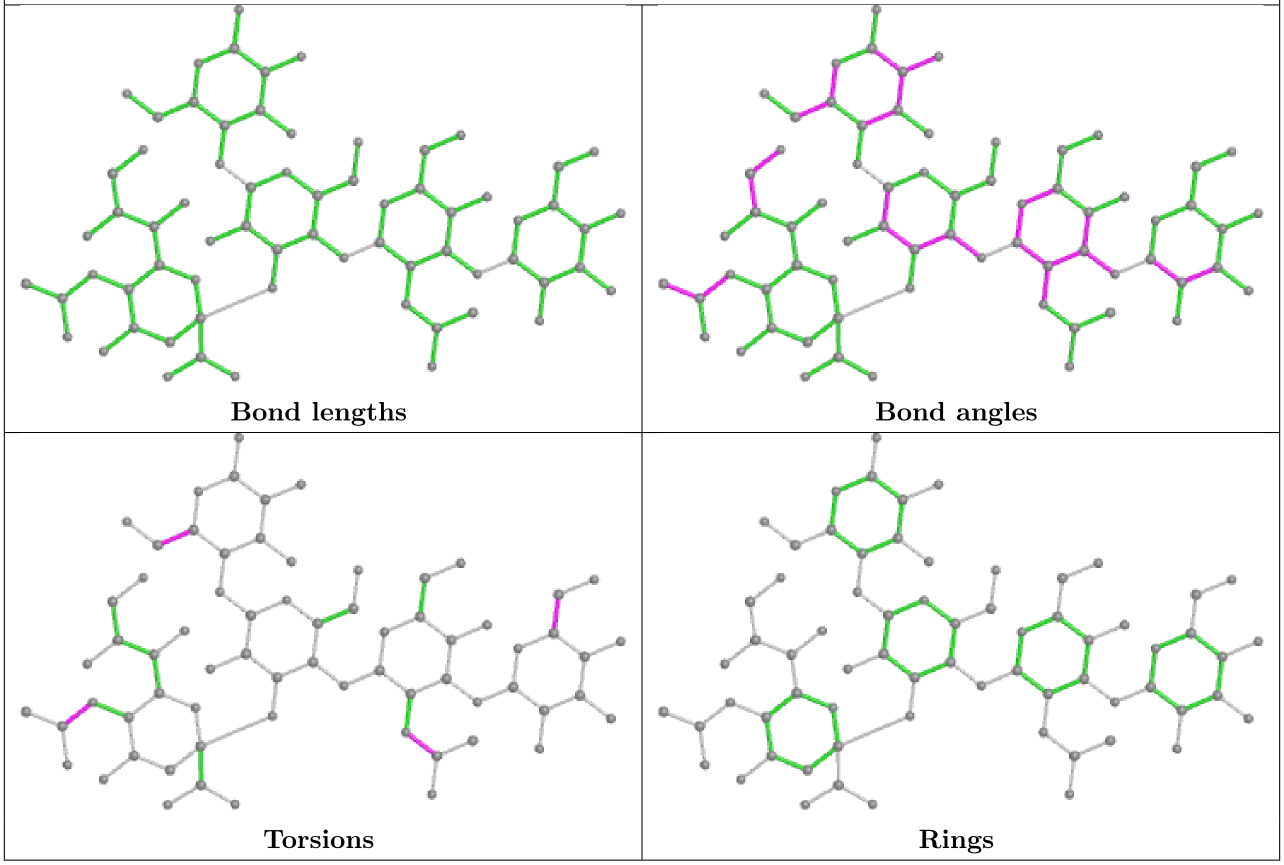
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	W	5	SIA	2	0
18	W	1	BGC	1	0

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

Oligosaccharide Chain W



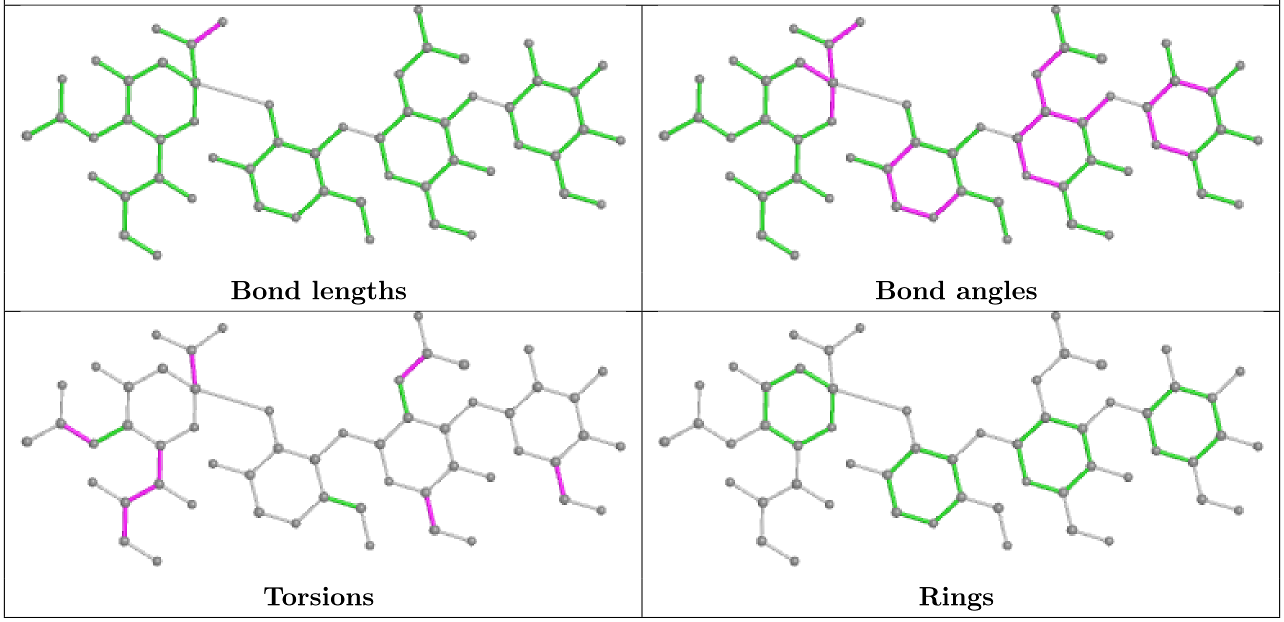
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain a



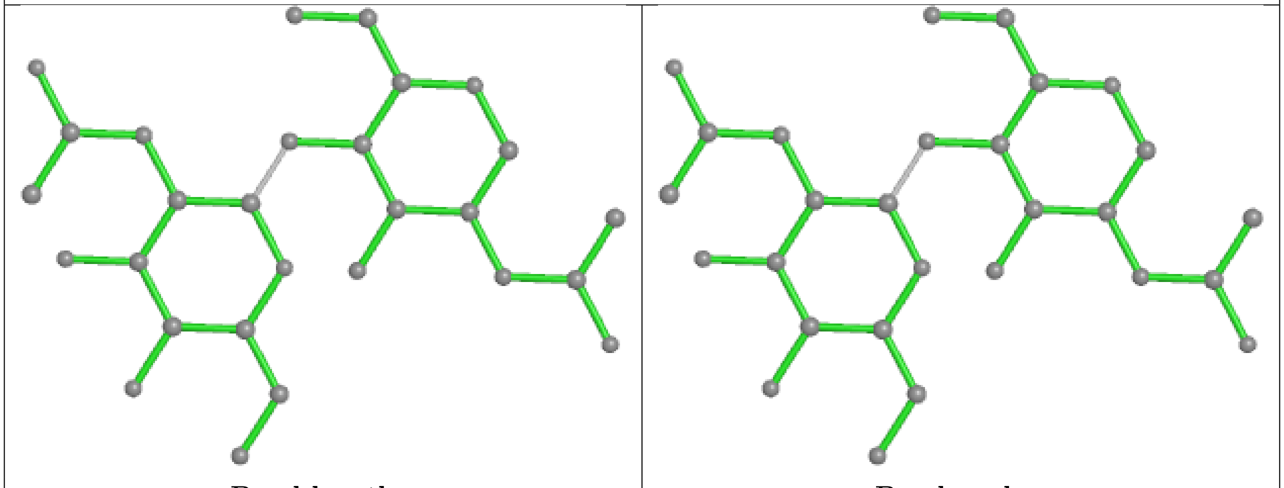
Bond lengths

Bond angles

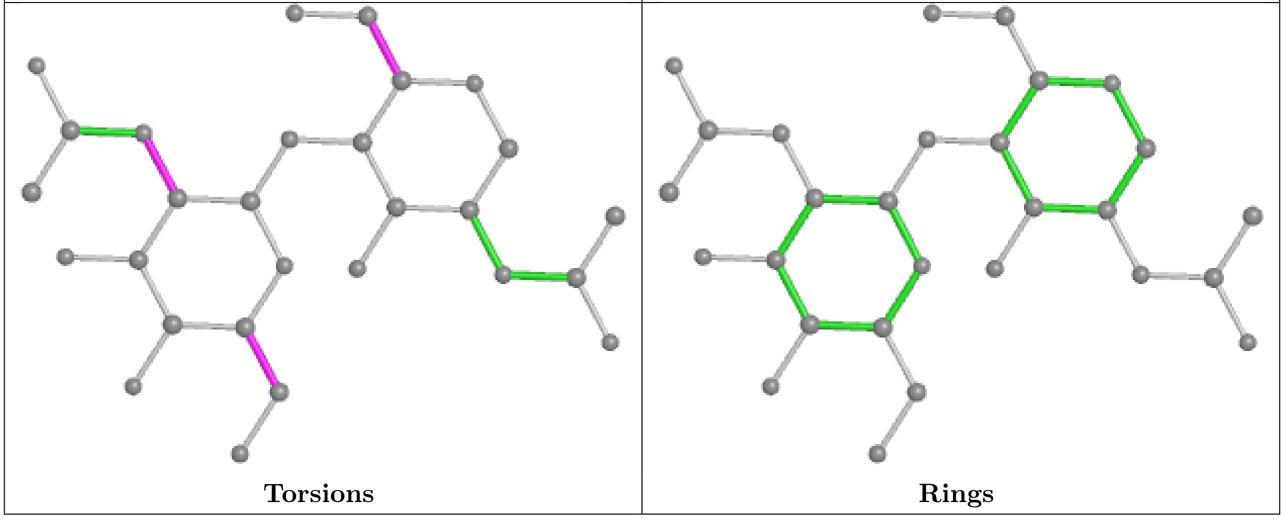
Torsions

Rings

Oligosaccharide Chain u

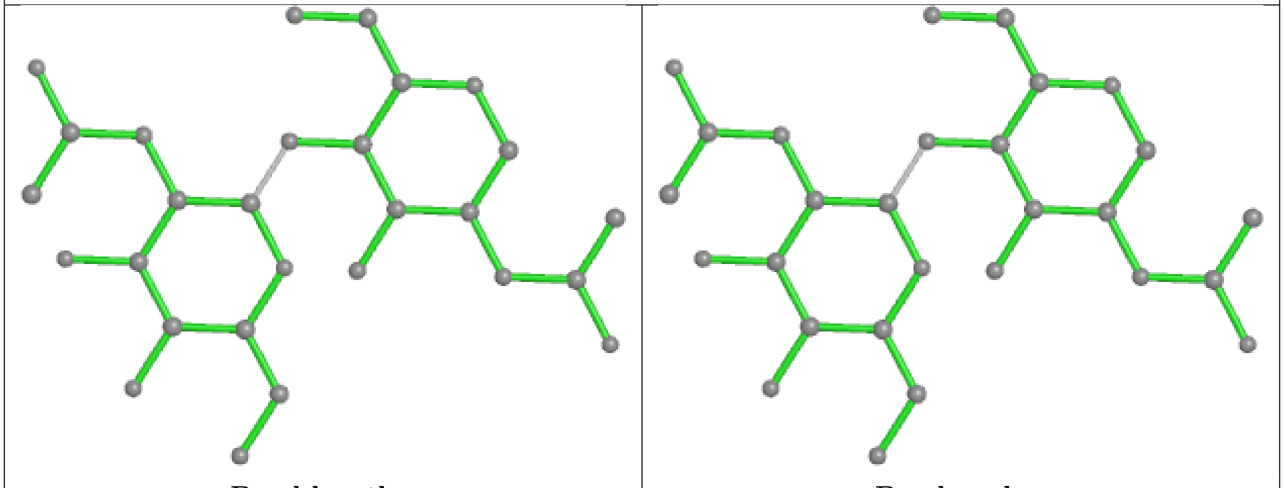


Bond lengths **Bond angles**



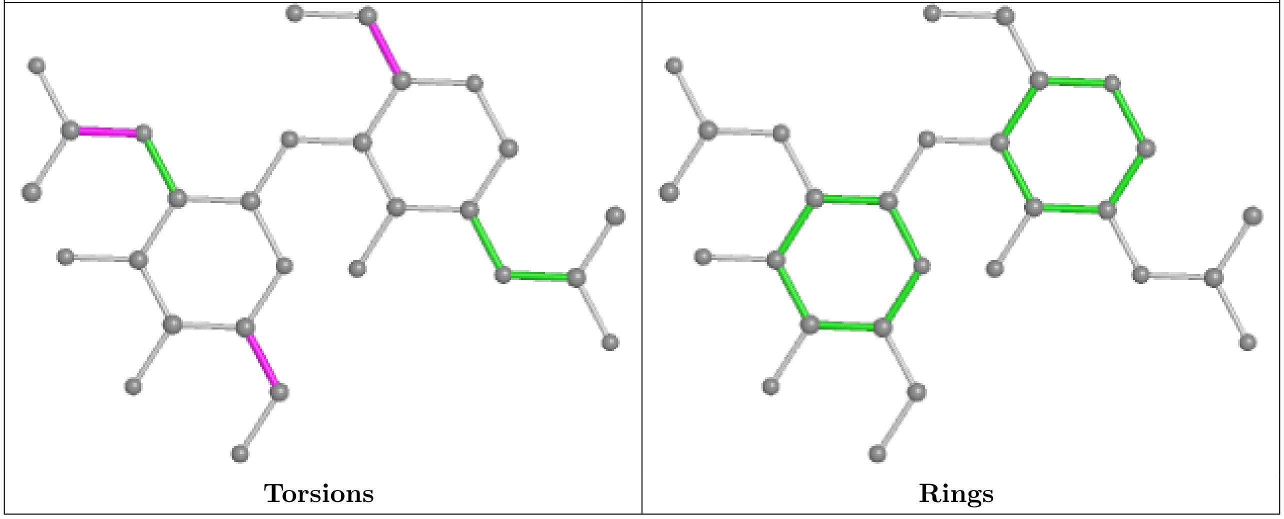
Torsions **Rings**

Oligosaccharide Chain b



Bond lengths

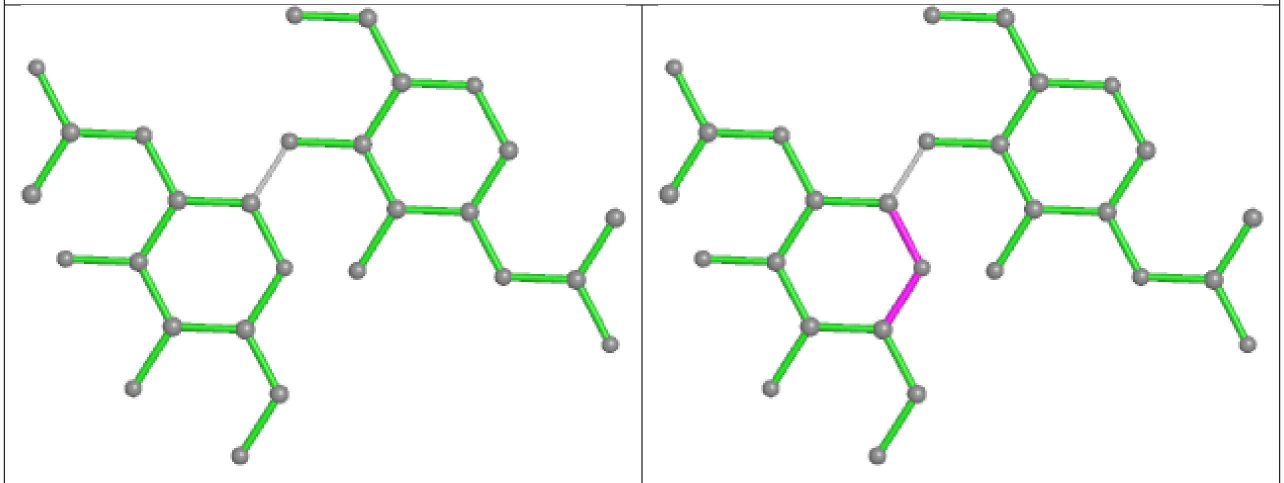
Bond angles



Torsions

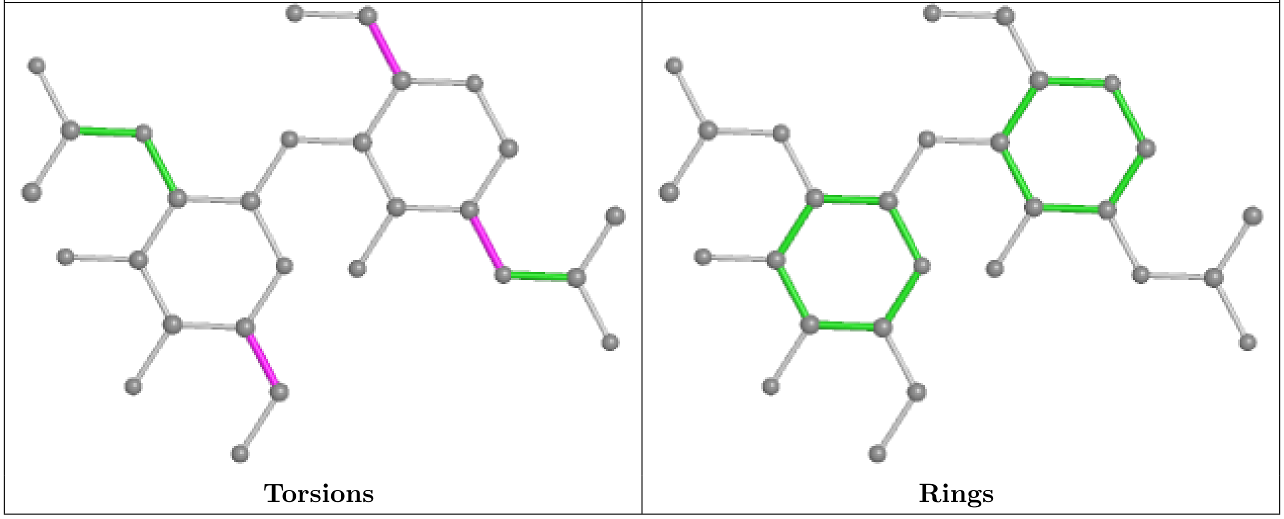
Rings

Oligosaccharide Chain c



Bond lengths

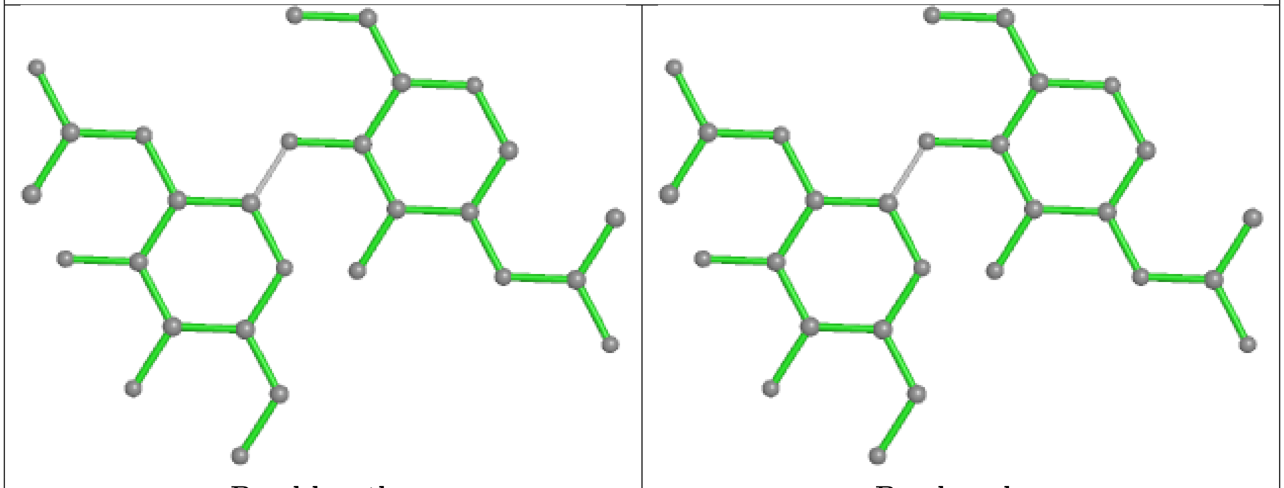
Bond angles



Torsions

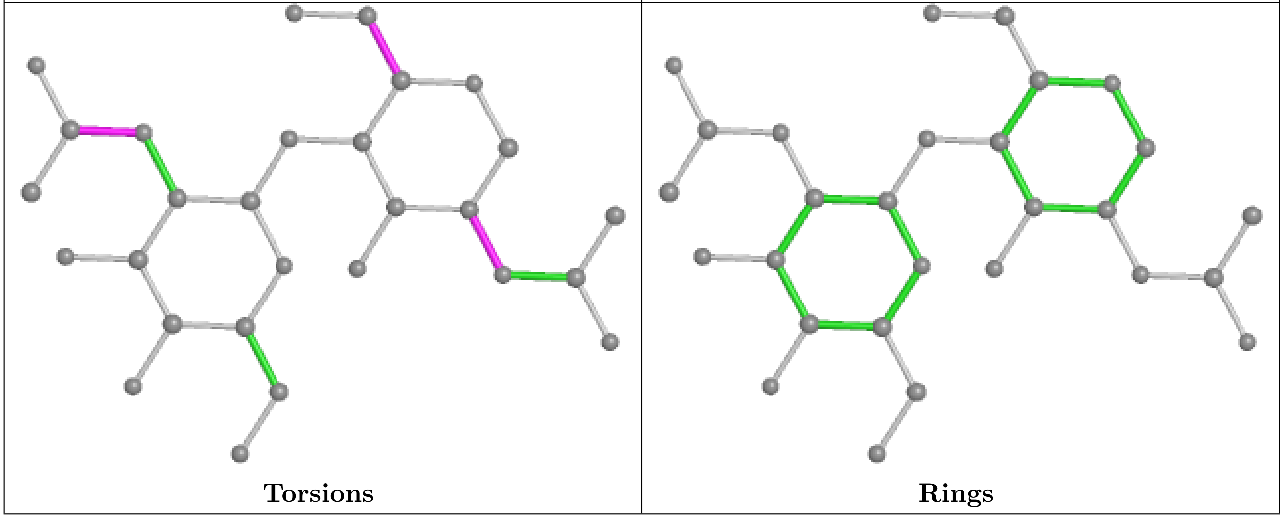
Rings

Oligosaccharide Chain d



Bond lengths

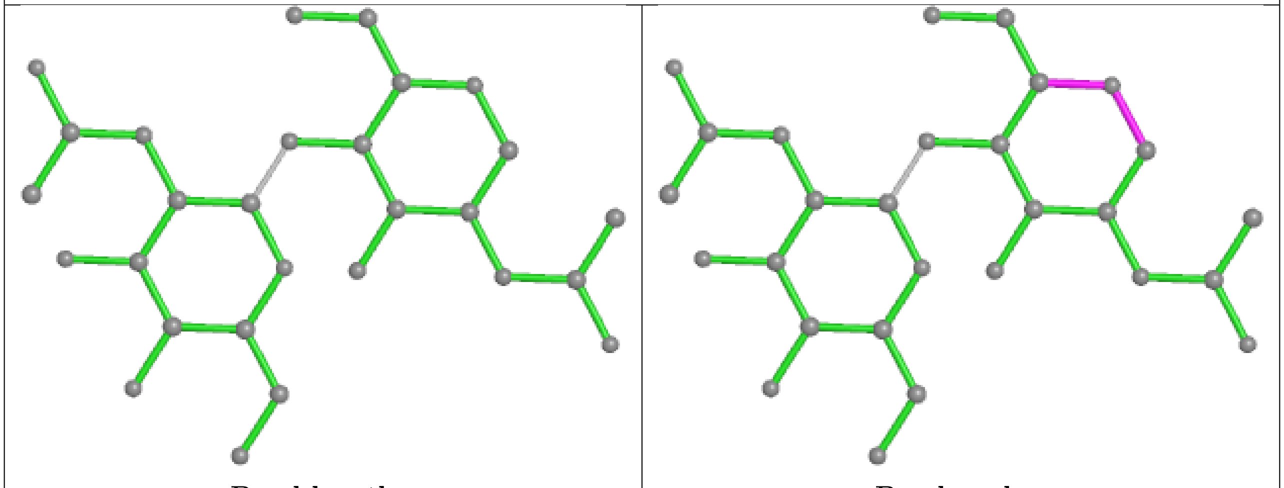
Bond angles



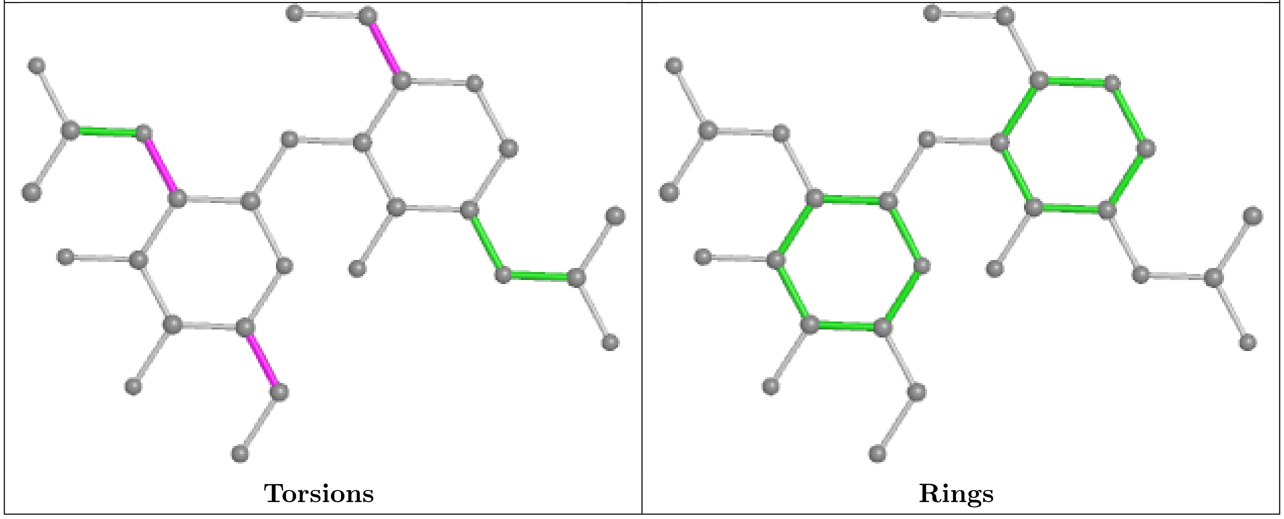
Torsions

Rings

Oligosaccharide Chain s

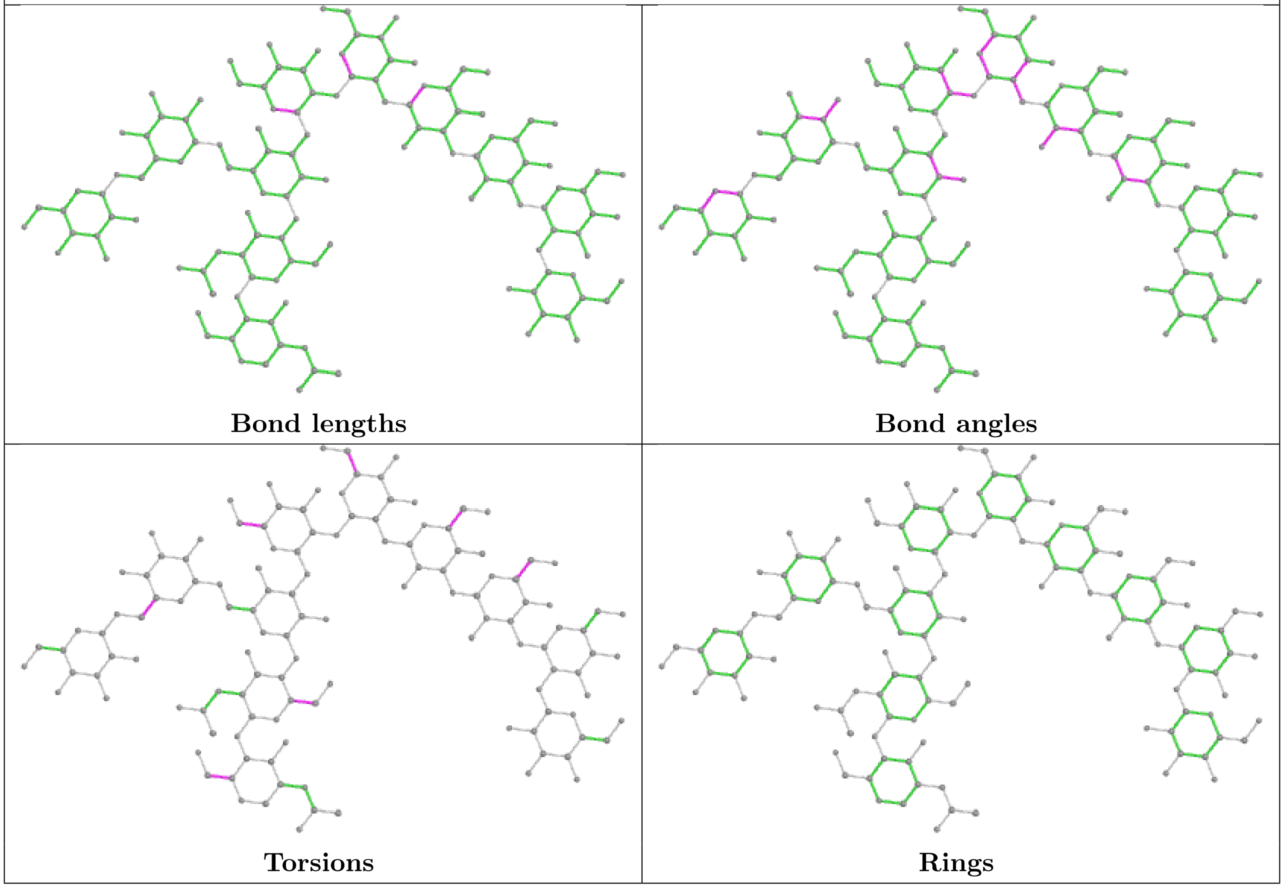


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain r



5.6 Ligand geometry ⓘ

33 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	$\#\|Z\| > 2$
23	PSF	R	902	-	28,29,29	0.51	0	32,36,36	0.57	0
25	WSS	0	302	-	40,40,53	0.34	0	45,48,61	0.41	0
24	PTY	8	201	-	49,49,49	0.29	0	52,54,54	0.31	0
22	CLR	V	402	-	31,31,31	0.52	0	48,48,48	0.61	0
24	PTY	0	306	-	16,16,49	0.58	0	19,20,54	0.72	1 (5%)
25	WSS	3	201	-	40,40,53	0.46	0	43,45,61	0.69	1 (2%)
25	WSS	V	401	-	36,36,53	0.35	0	42,44,61	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
26	NAG	U	504	16	14,14,15	0.20	0	17,19,21	0.42	0
24	PTY	0	307	-	47,47,49	0.28	0	50,52,54	0.34	0
24	PTY	2	201	-	28,28,49	0.34	0	30,32,54	0.48	0
22	CLR	R	901	-	31,31,31	0.27	0	48,48,48	0.49	0
25	WSS	R	905	-	39,39,53	0.35	0	45,47,61	0.39	0
24	PTY	5	202	-	34,34,49	0.36	0	37,39,54	0.43	0
22	CLR	5	201	-	31,31,31	0.30	0	48,48,48	0.64	1 (2%)
24	PTY	R	904	-	28,28,49	0.32	0	30,32,54	0.45	0
29	WJS	3	202	-	25,26,34	1.40	2 (8%)	28,32,40	1.54	2 (7%)
24	PTY	V	403	-	28,28,49	0.35	0	30,32,54	0.40	0
25	WSS	0	301	-	43,43,53	0.36	0	48,51,61	0.81	1 (2%)
22	CLR	0	304	-	31,31,31	0.32	0	48,48,48	0.41	0
25	WSS	U	501	-	38,38,53	0.38	0	43,46,61	0.34	0
25	WSS	0	303	-	25,25,53	0.39	0	31,33,61	0.81	1 (3%)
24	PTY	U	503	-	25,25,49	0.34	0	27,27,54	0.32	0
25	WSS	1	201	-	33,33,53	0.37	0	39,41,61	0.66	1 (2%)
24	PTY	7	201	-	41,41,49	0.30	0	44,46,54	0.38	0
25	WSS	U	502	-	36,36,53	0.39	0	42,44,61	0.54	0
25	WSS	0	305	-	30,30,53	0.47	0	33,35,61	0.63	1 (3%)
28	ADP	C	701	-	24,29,29	0.96	1 (4%)	29,45,45	1.43	4 (13%)
26	NAG	R	906	5	14,14,15	0.42	0	17,19,21	0.47	0
24	PTY	Q	401	-	29,29,49	0.36	0	32,34,54	0.46	0
24	PTY	8	202	-	32,32,49	0.28	0	34,34,54	0.44	0
27	WJP	R	907	21	31,33,34	1.53	5 (16%)	39,43,44	1.97	11 (28%)
24	PTY	R	903	-	31,31,49	0.31	0	33,33,54	0.32	0
24	PTY	6	201	-	20,20,49	0.42	0	22,24,54	0.43	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
23	PSF	R	902	-	-	18/35/35/35	-
25	WSS	0	302	-	-	12/44/44/57	-
24	PTY	8	201	-	-	29/53/53/53	-
22	CLR	V	402	-	-	0/10/68/68	0/4/4/4
24	PTY	0	306	-	-	6/16/16/53	-
25	WSS	3	201	-	-	10/44/44/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	WSS	V	401	-	-	6/40/40/57	-
26	NAG	U	504	16	-	2/6/23/26	0/1/1/1
24	PTY	0	307	-	1/1/4/4	35/51/51/53	-
24	PTY	2	201	-	-	11/30/30/53	-
22	CLR	R	901	-	-	6/10/68/68	0/4/4/4
25	WSS	R	905	-	-	18/43/43/57	-
24	PTY	5	202	-	-	23/38/38/53	-
22	CLR	5	201	-	-	0/10/68/68	0/4/4/4
24	PTY	R	904	-	1/1/3/4	20/31/31/53	-
29	WJS	3	202	-	-	13/30/30/38	-
24	PTY	V	403	-	-	18/30/30/53	-
25	WSS	0	301	-	-	15/47/47/57	-
22	CLR	0	304	-	-	0/10/68/68	0/4/4/4
25	WSS	U	501	-	-	4/42/42/57	-
25	WSS	0	303	-	-	7/29/29/57	-
24	PTY	U	503	-	-	10/27/27/53	-
25	WSS	1	201	-	-	5/37/37/57	-
24	PTY	7	201	-	-	22/45/45/53	-
25	WSS	U	502	-	-	4/40/40/57	-
25	WSS	0	305	-	-	9/32/32/57	-
28	ADP	C	701	-	-	1/12/32/32	0/3/3/3
26	NAG	R	906	5	-	4/6/23/26	0/1/1/1
24	PTY	Q	401	-	-	15/33/33/53	-
24	PTY	8	202	-	-	18/34/34/53	-
27	WJP	R	907	21	-	10/37/37/40	-
24	PTY	R	903	-	-	20/33/33/53	-
24	PTY	6	201	-	-	11/22/22/53	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	907	WJP	P31-O34	4.69	1.72	1.54
29	3	202	WJS	P25-O24	4.29	1.76	1.59
27	R	907	WJP	P27-O26	3.00	1.71	1.59
27	R	907	WJP	C15-C16	2.98	1.40	1.33
27	R	907	WJP	C10-C11	2.87	1.39	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	3	202	WJS	O28-C29-C30	6.21	113.47	108.06
27	R	907	WJP	C12-C11-C13	5.49	124.50	115.27
27	R	907	WJP	C04-C05-C06	-4.97	115.68	127.66
27	R	907	WJP	C17-C16-C18	4.39	122.65	115.27
25	0	301	WSS	O2-C31-C32	4.05	120.22	111.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	R	904	PTY	C6
24	0	307	PTY	C6

5 of 382 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	R	902	PSF	C2-O2-P-O4
23	R	902	PSF	C2-O2-P-O3
23	R	902	PSF	C13-C1-O11-C3
24	R	903	PTY	C11-C8-O7-C6
24	R	904	PTY	C11-C8-O7-C6

There are no ring outliers.

20 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	8	201	PTY	6	0
22	V	402	CLR	11	0
24	0	306	PTY	1	0
24	0	307	PTY	3	0
24	2	201	PTY	1	0
22	R	901	CLR	1	0
25	R	905	WSS	5	0
24	5	202	PTY	6	0
22	5	201	CLR	16	0
24	R	904	PTY	2	0
29	3	202	WJS	5	0
24	V	403	PTY	9	0
22	0	304	CLR	1	0
24	U	503	PTY	21	0
24	7	201	PTY	7	0
25	0	305	WSS	1	0

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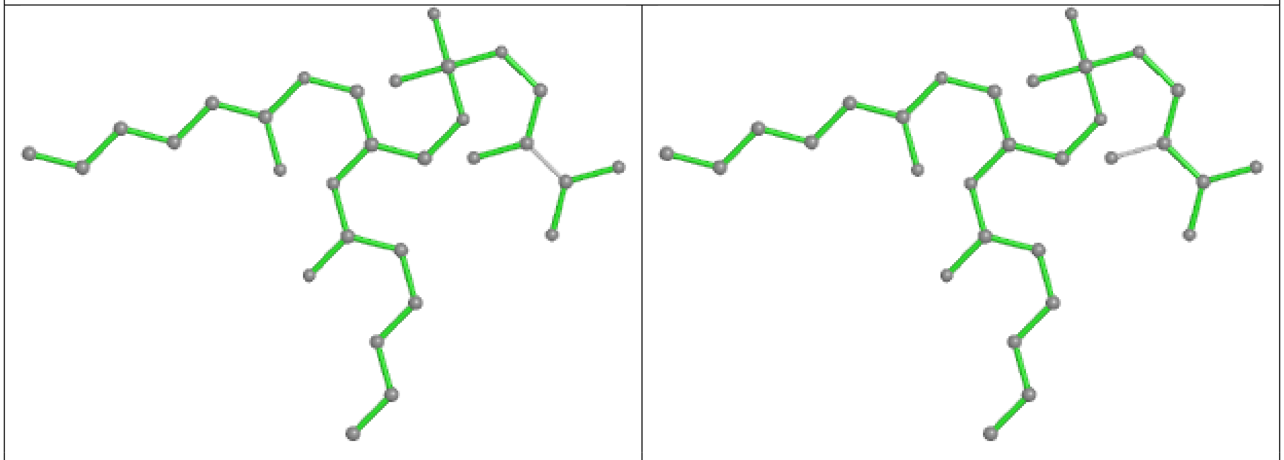
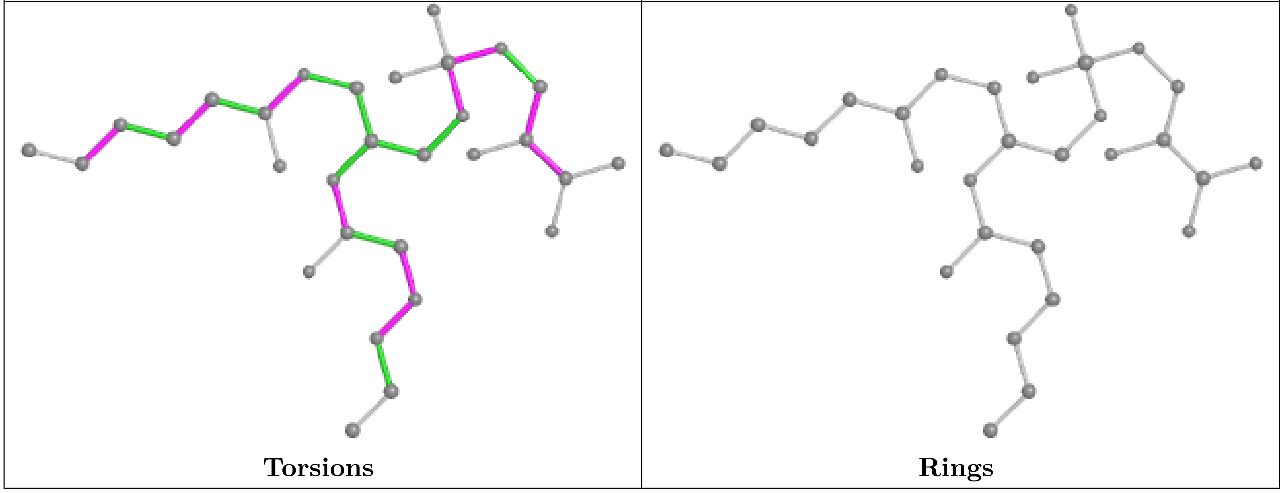
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	701	ADP	1	0
24	Q	401	PTY	6	0
24	8	202	PTY	4	0
24	6	201	PTY	7	0

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 PSF R 902

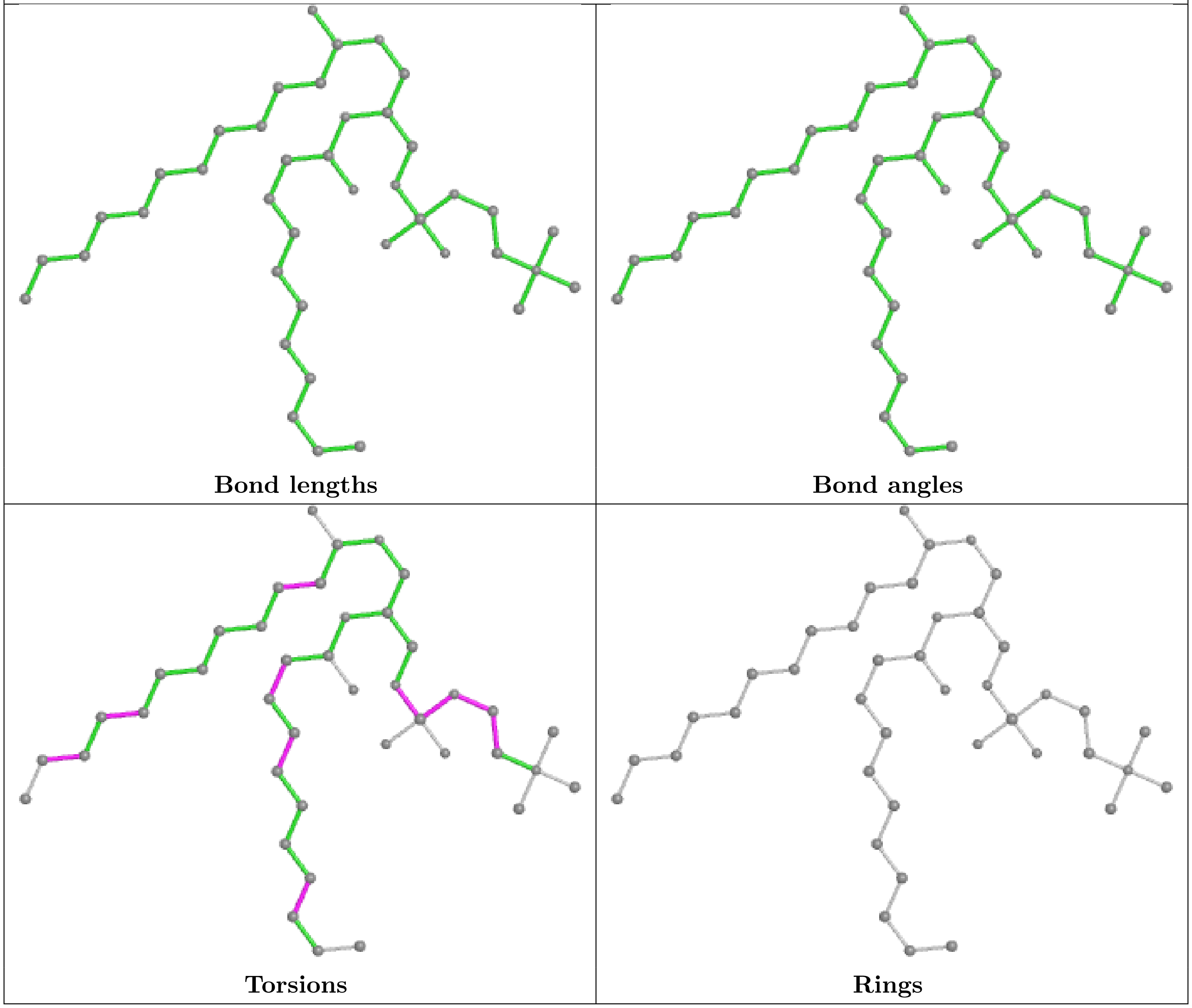


Bond lengths **Bond angles**

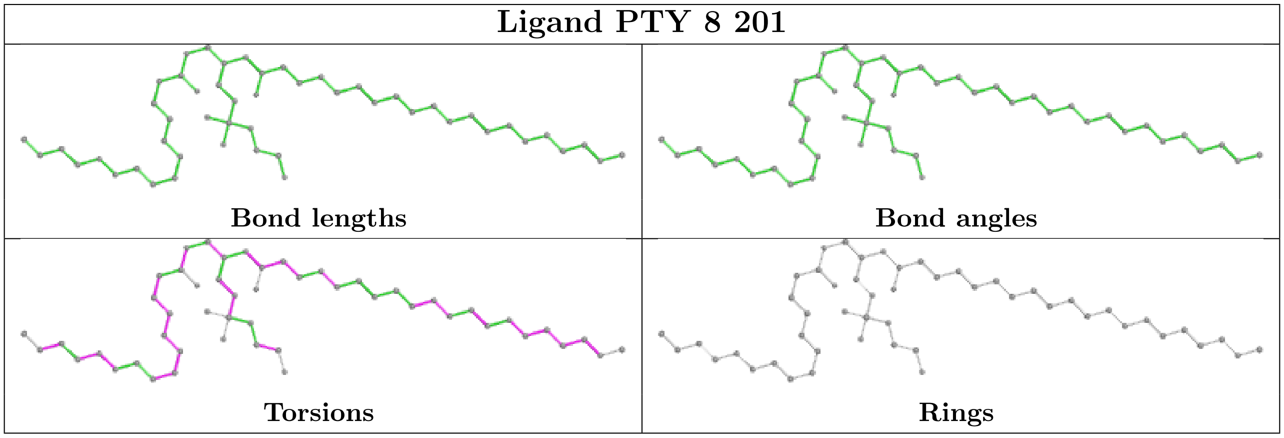


Torsions **Rings**

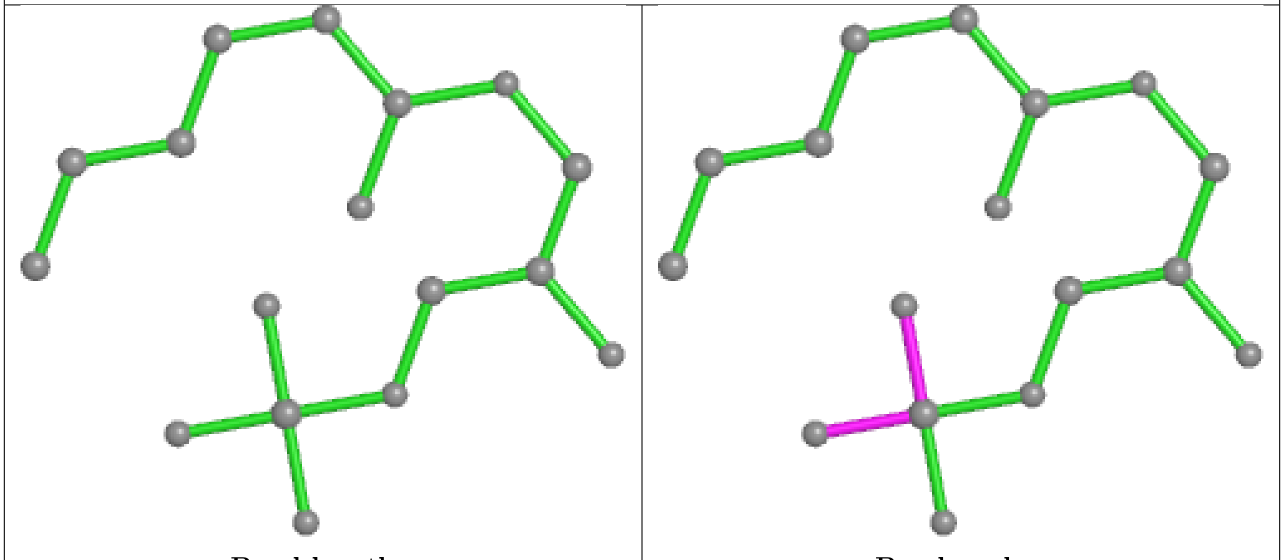
Ligand WSS 0 302



Ligand PTY 8 201

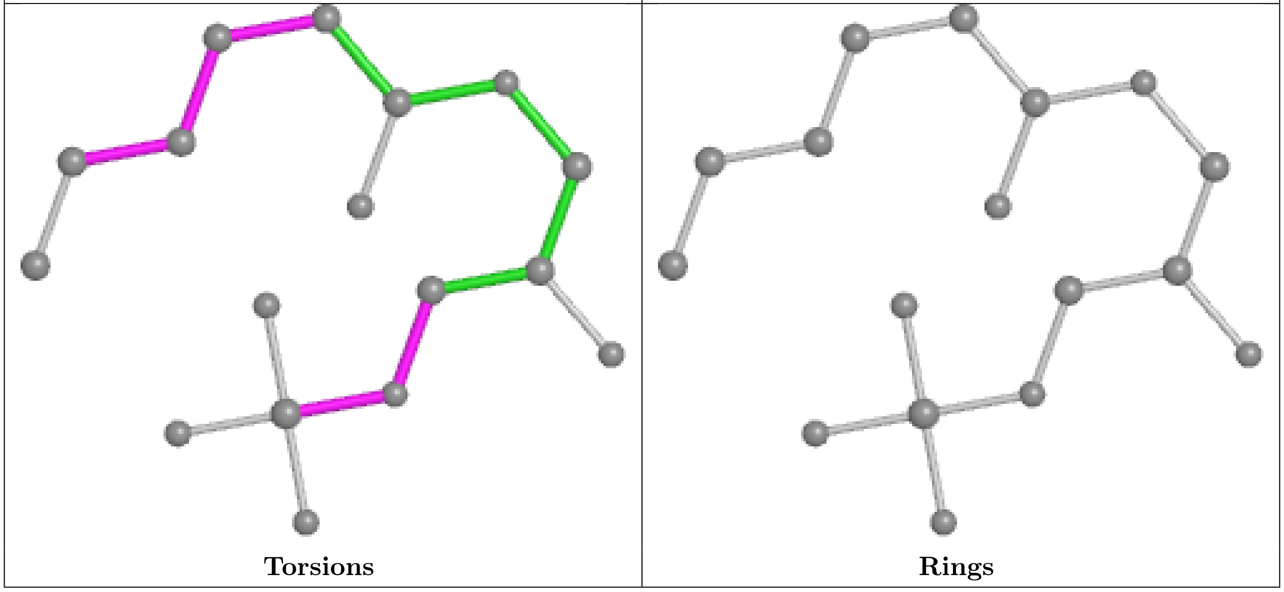


Ligand PTY 0 306



Bond lengths

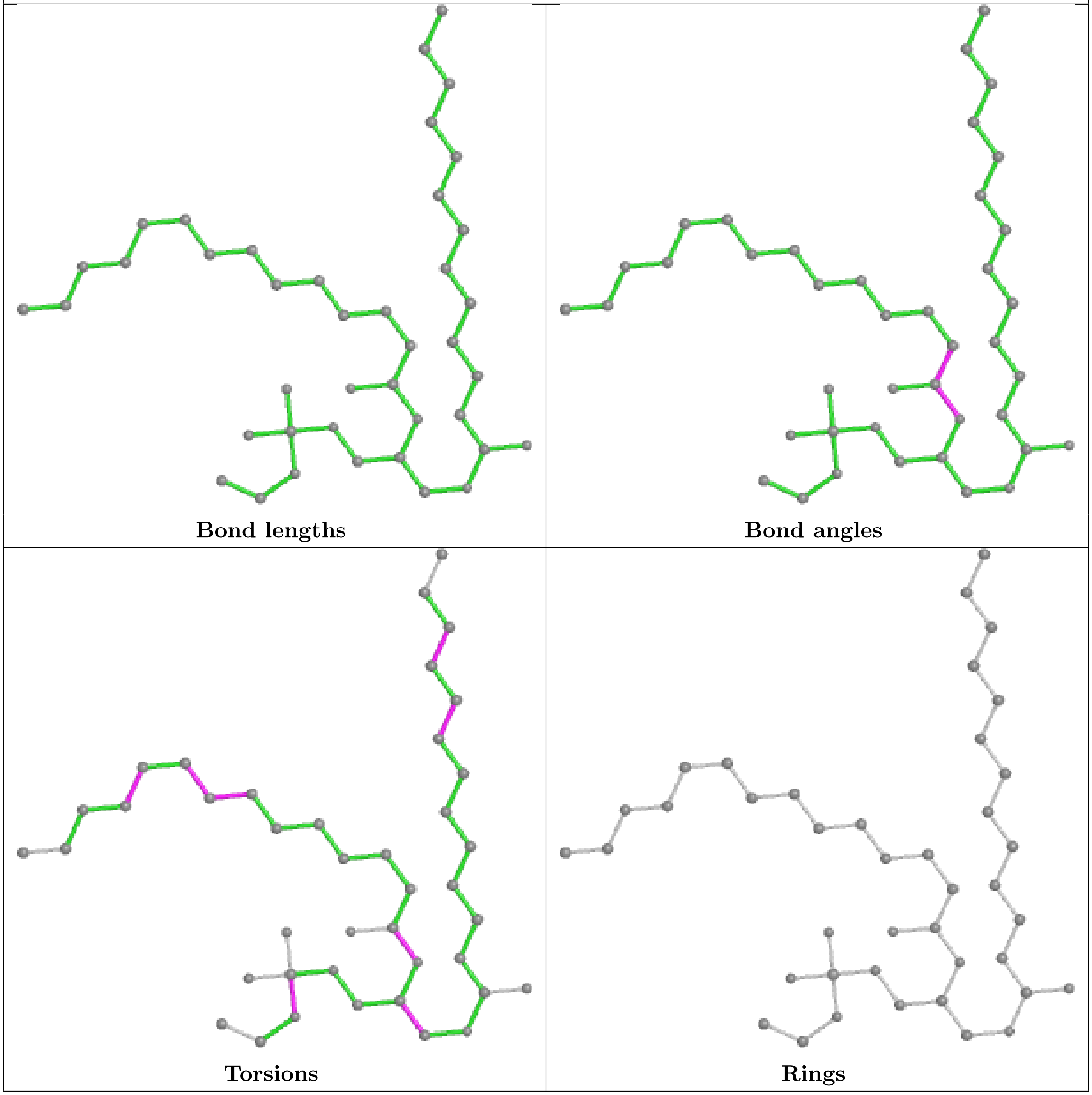
Bond angles



Torsions

Rings

Ligand WSS 3 201



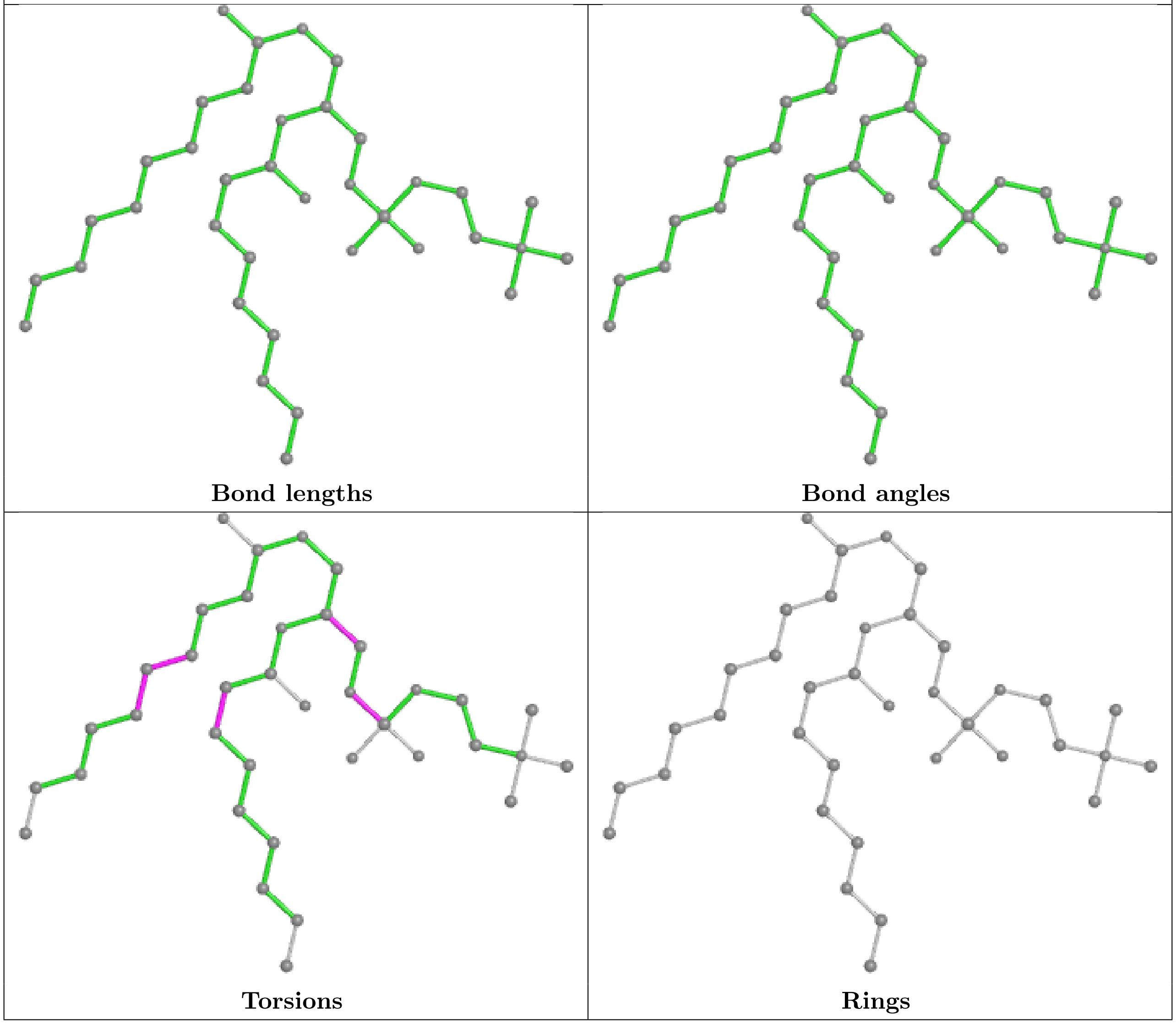
Bond lengths

Bond angles

Torsions

Rings

Ligand WSS V 401



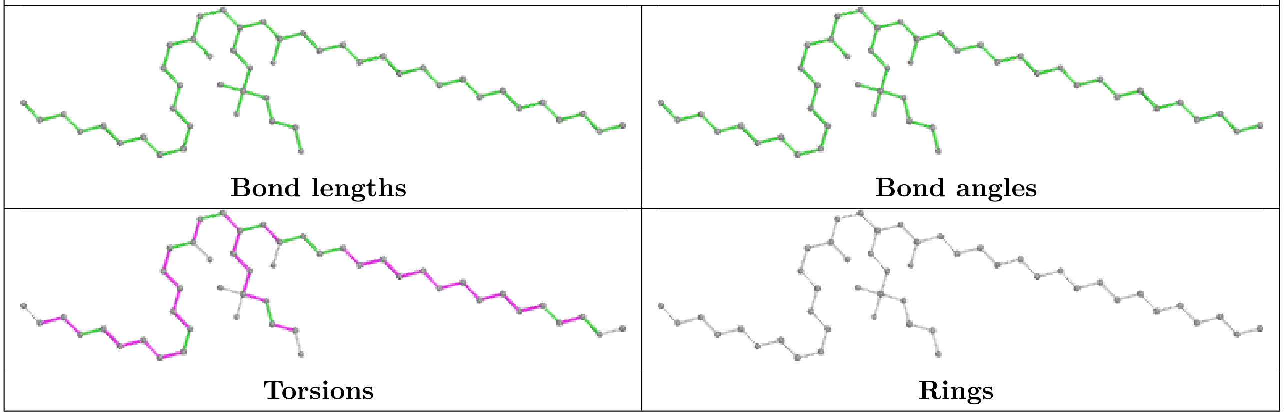
Bond lengths

Bond angles

Torsions

Rings

Ligand PTY 0 307



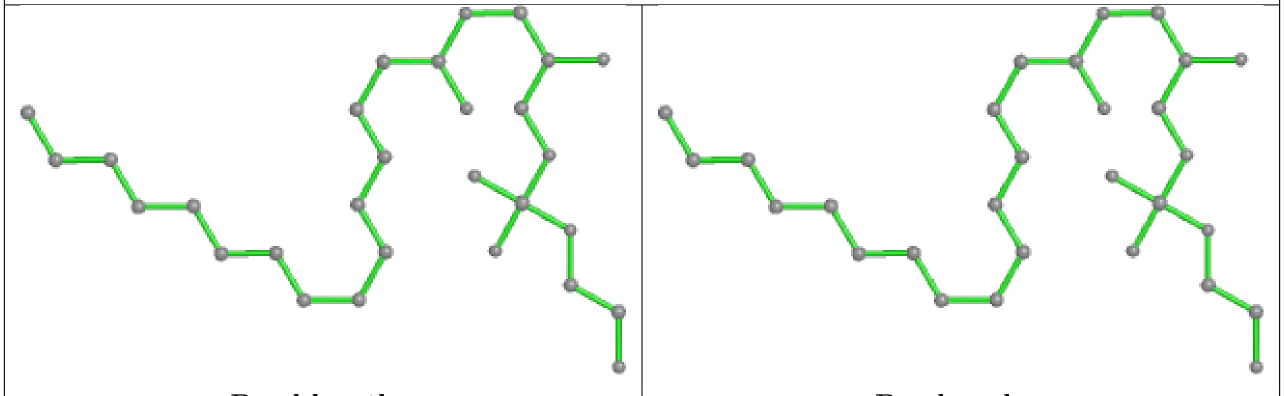
Bond lengths

Bond angles

Torsions

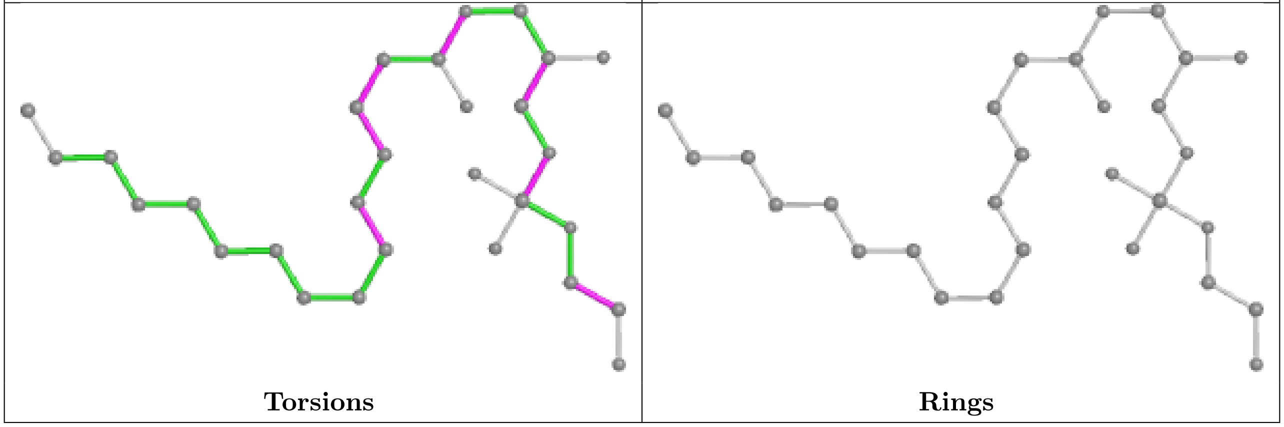
Rings

Ligand PTY 2 201



Bond lengths

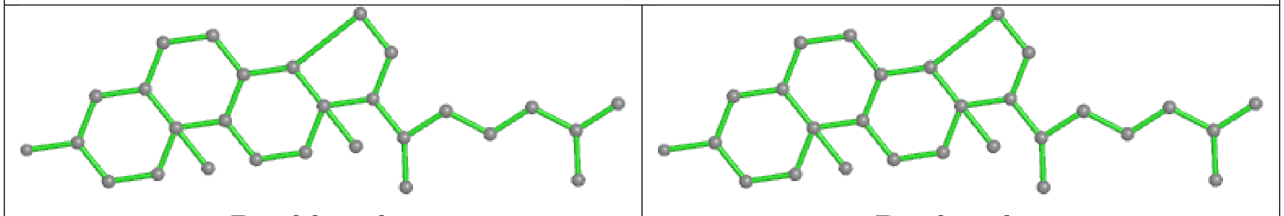
Bond angles



Torsions

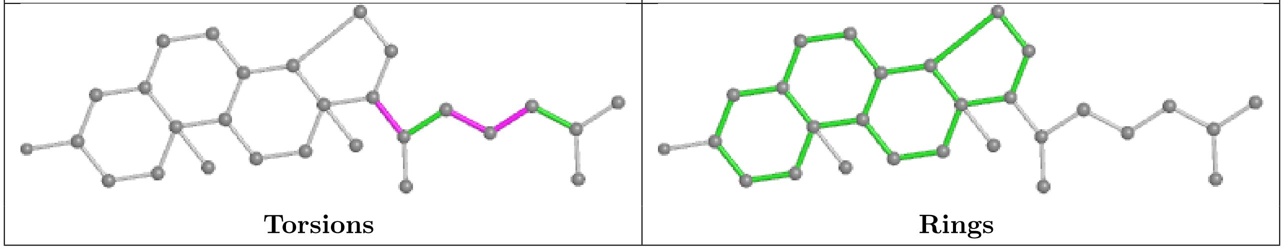
Rings

Ligand CLR R 901



Bond lengths

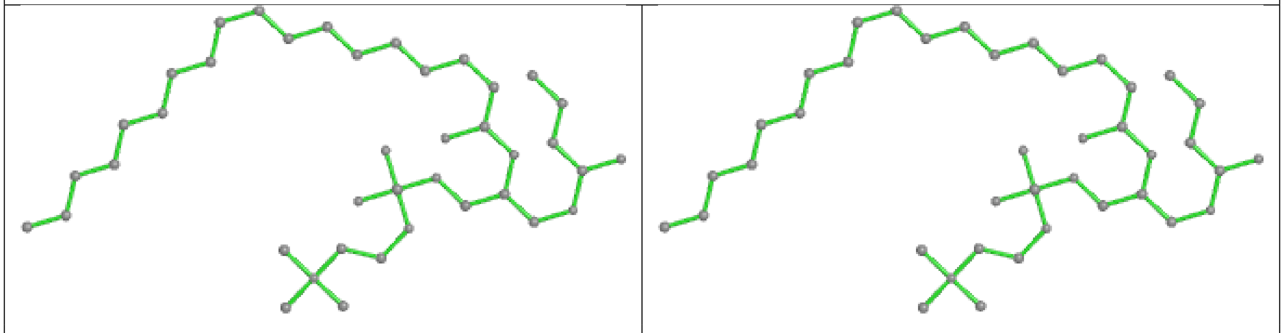
Bond angles



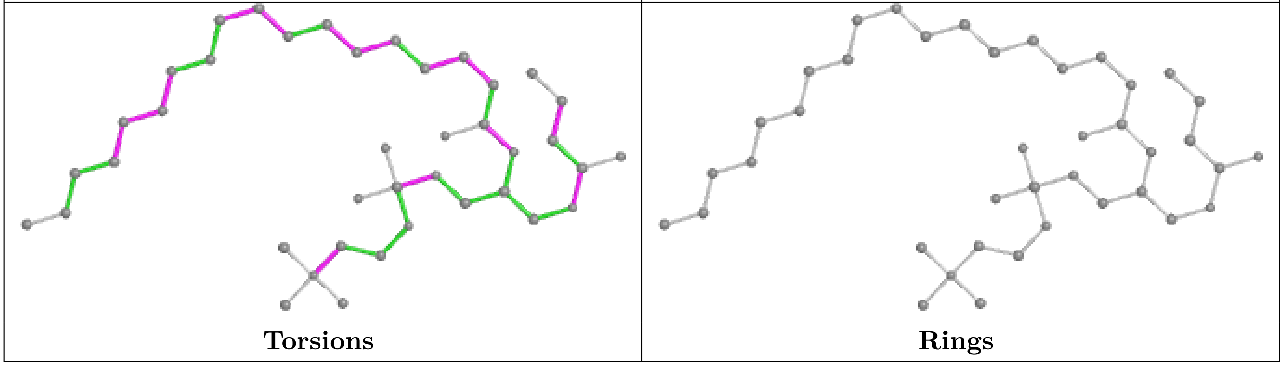
Torsions

Rings

Ligand WSS R 905

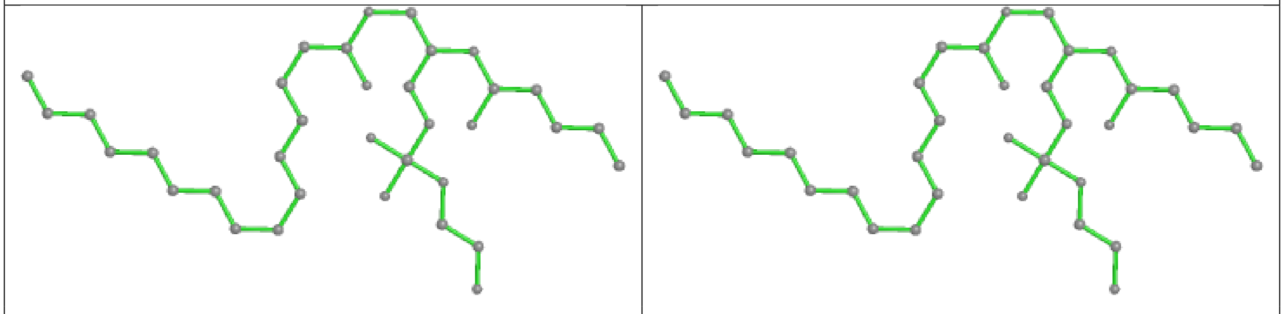


Bond lengths Bond angles

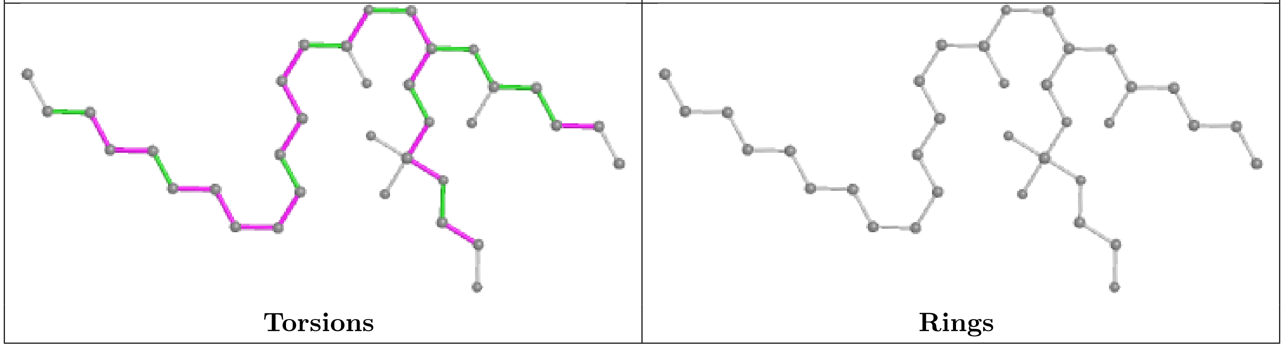


Torsions Rings

Ligand PTY 5 202

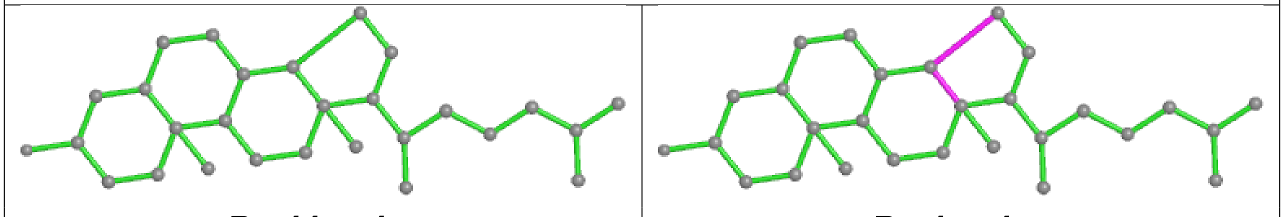


Bond lengths Bond angles



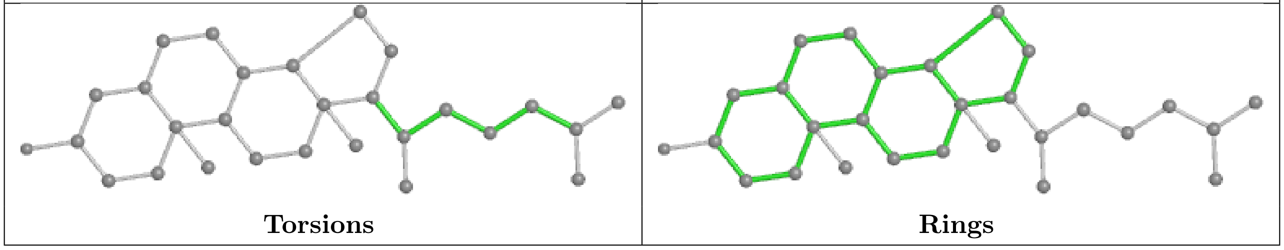
Torsions Rings

Ligand CLR 5 201



Bond lengths

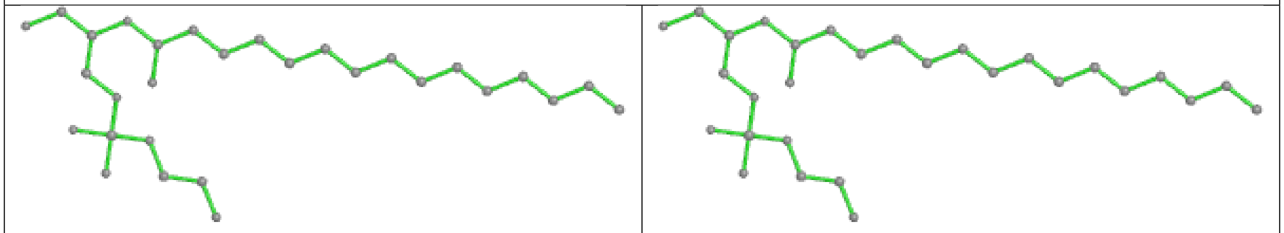
Bond angles



Torsions

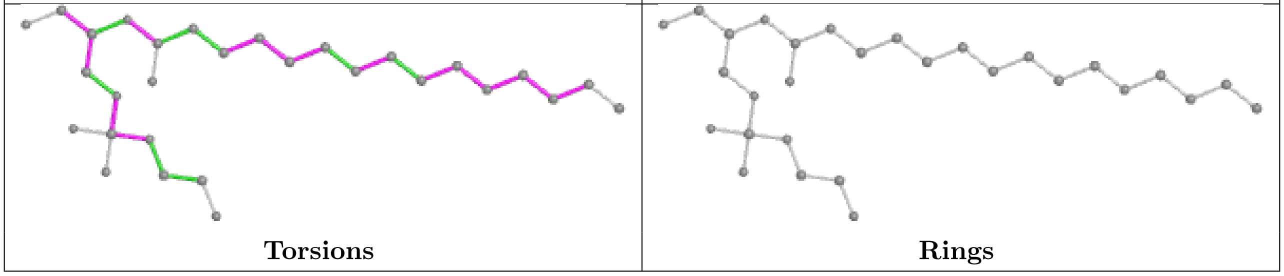
Rings

Ligand PTY R 904



Bond lengths

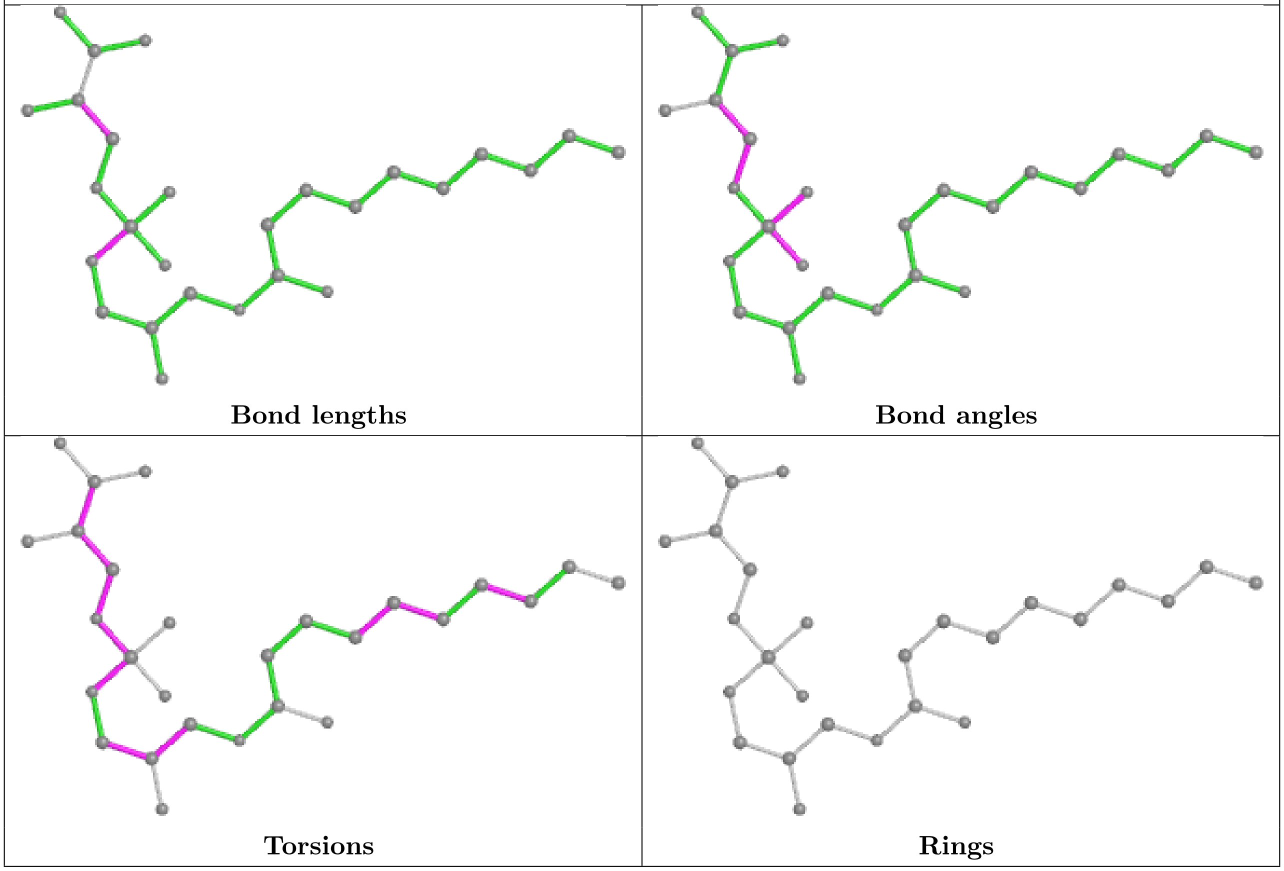
Bond angles



Torsions

Rings

Ligand WJS 3 202



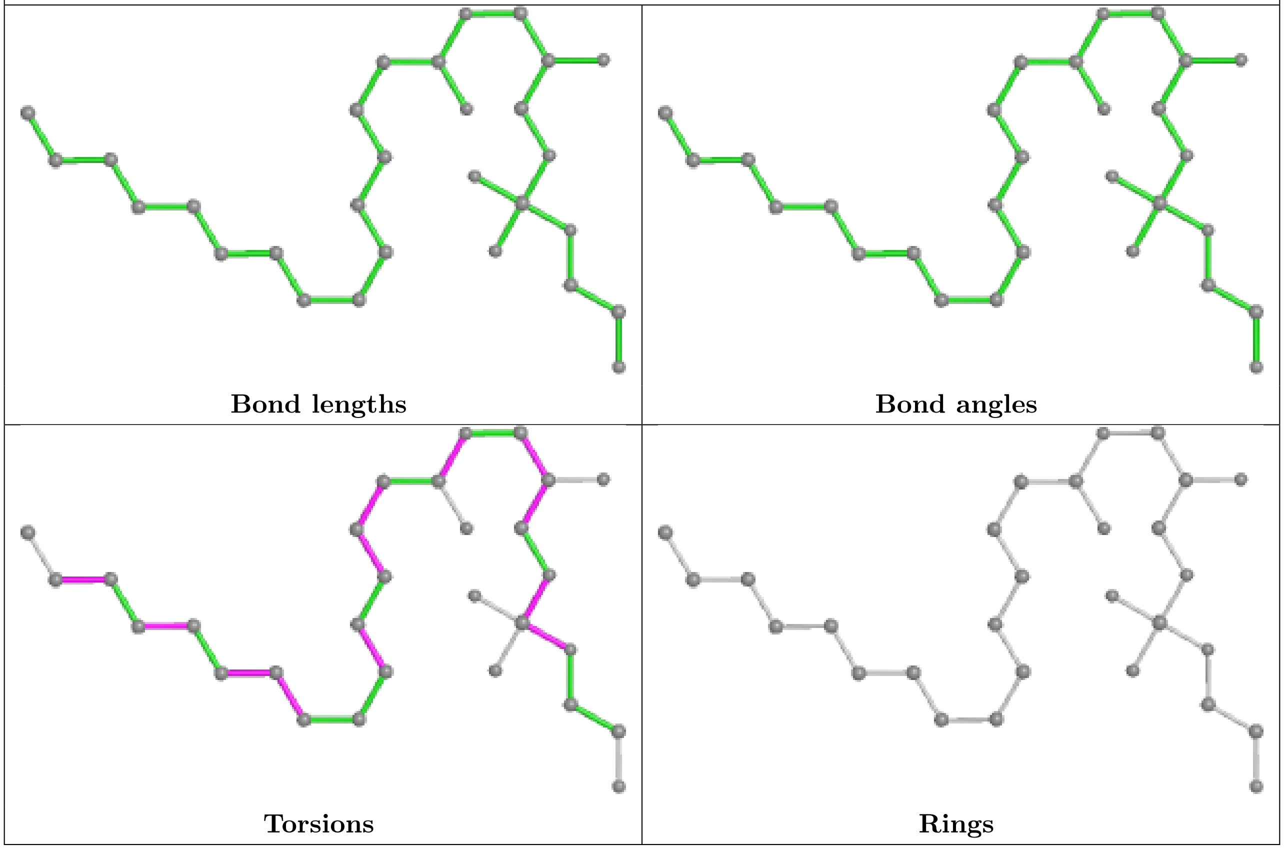
Bond lengths

Bond angles

Torsions

Rings

Ligand PTY V 403



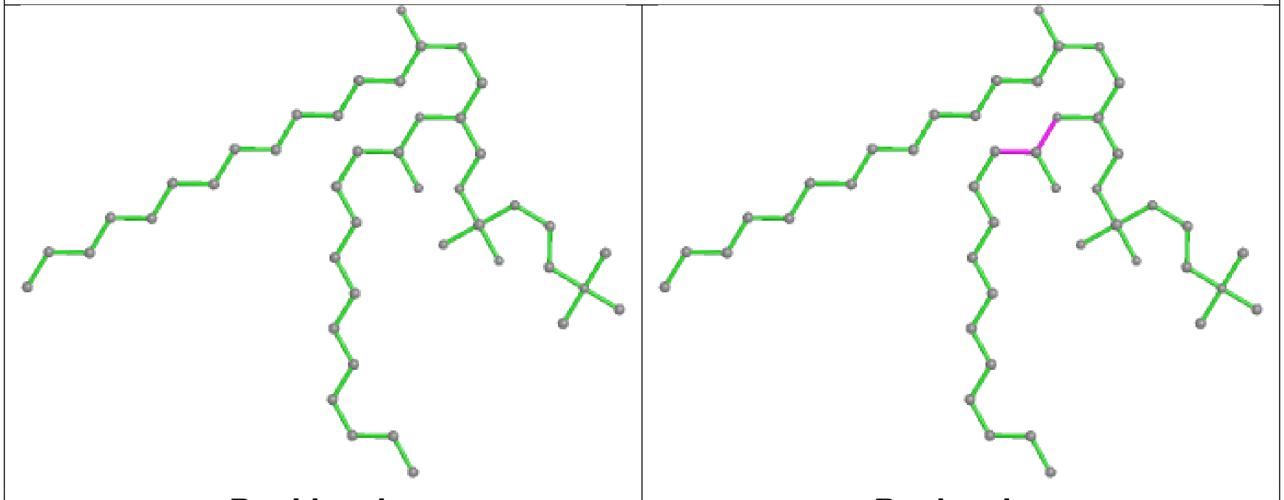
Bond lengths

Bond angles

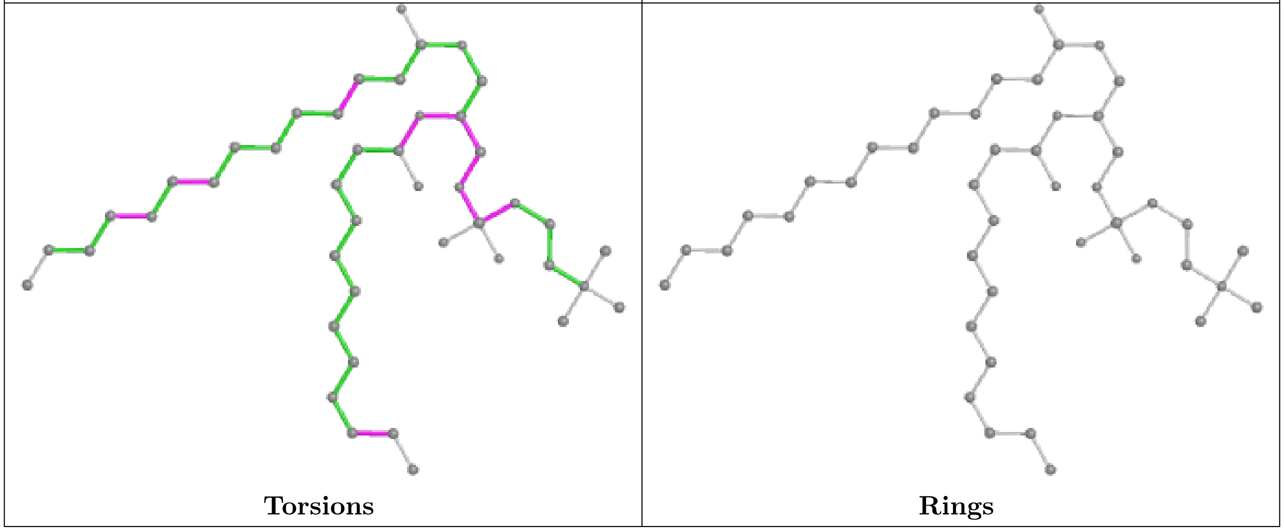
Torsions

Rings

Ligand WSS 0 301

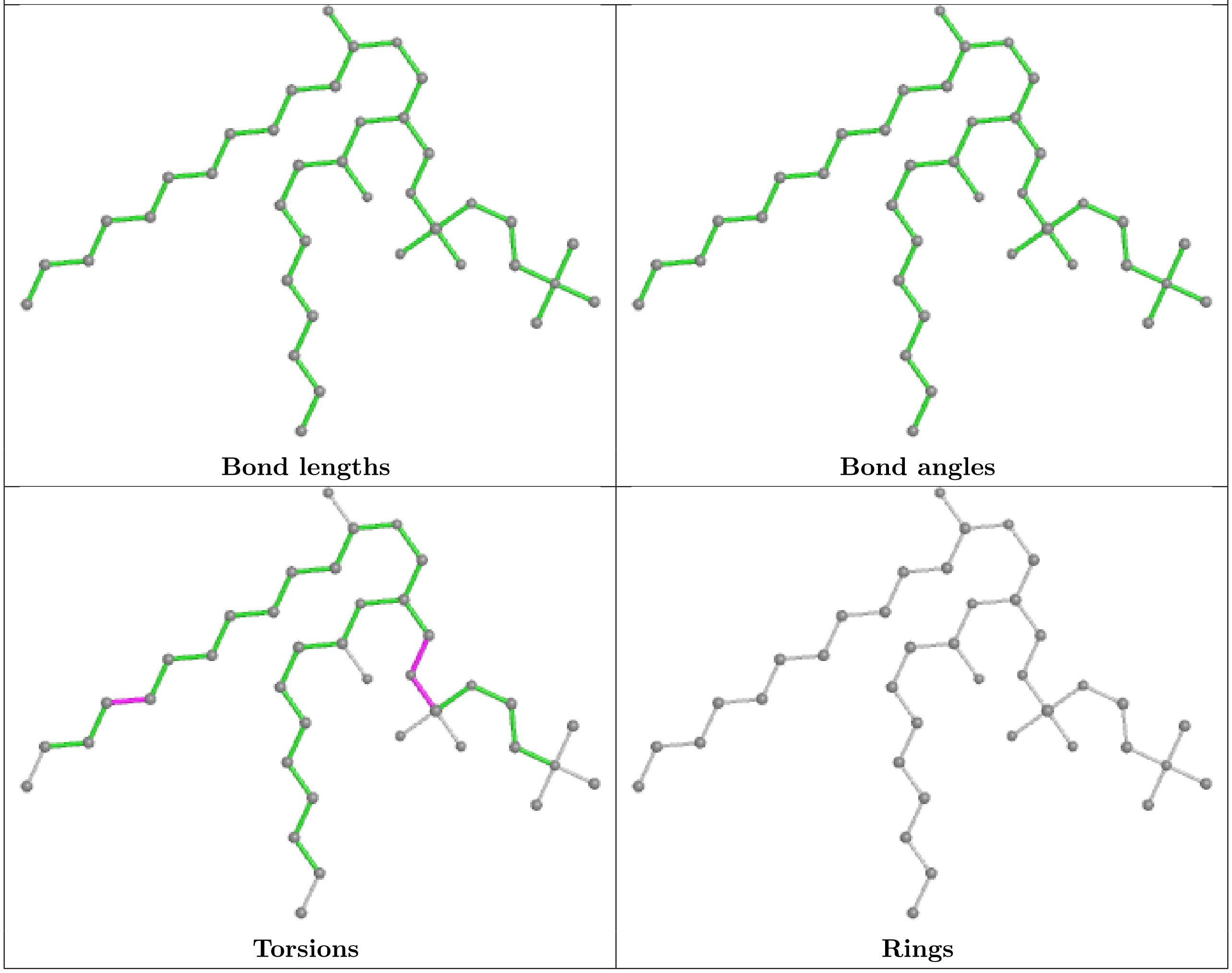


Bond lengths **Bond angles**



Torsions **Rings**

Ligand WSS U 501



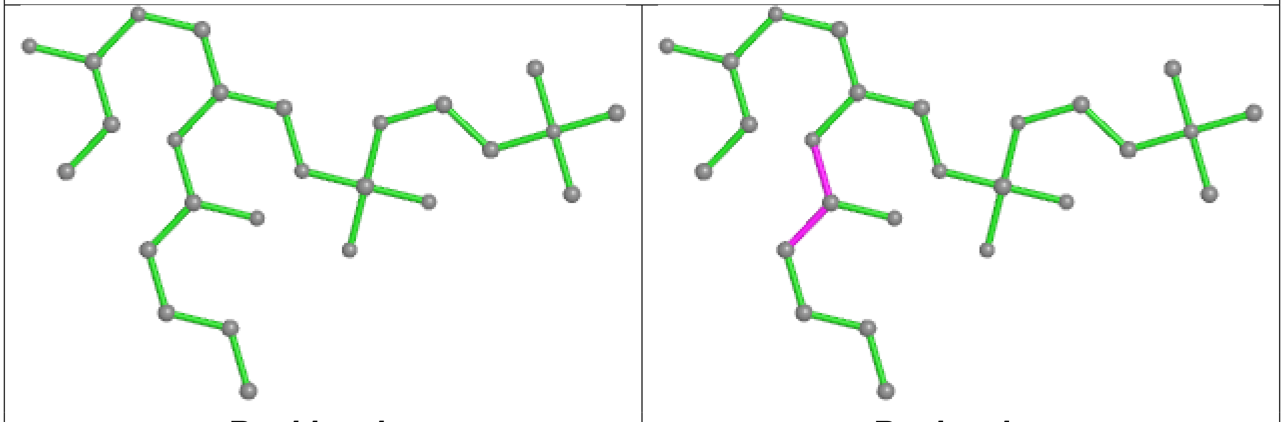
Bond lengths

Bond angles

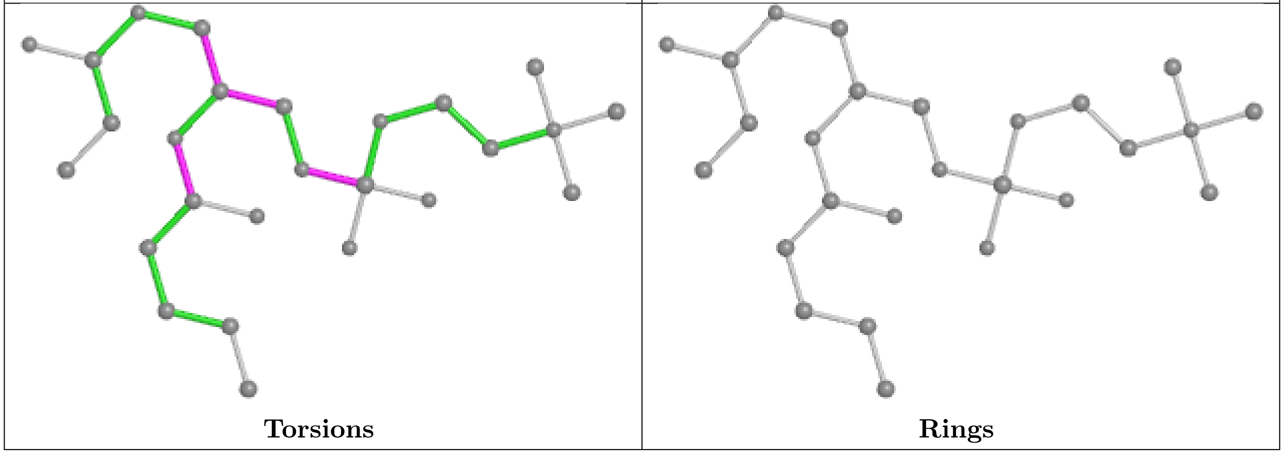
Torsions

Rings

Ligand WSS 0 303

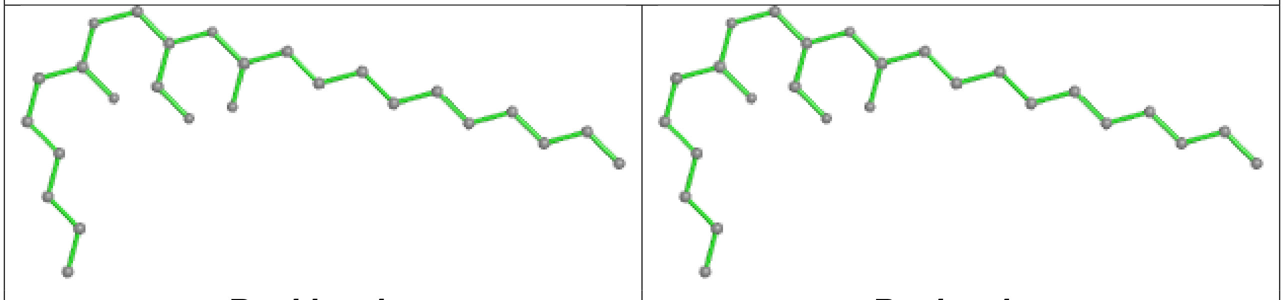


Bond lengths Bond angles

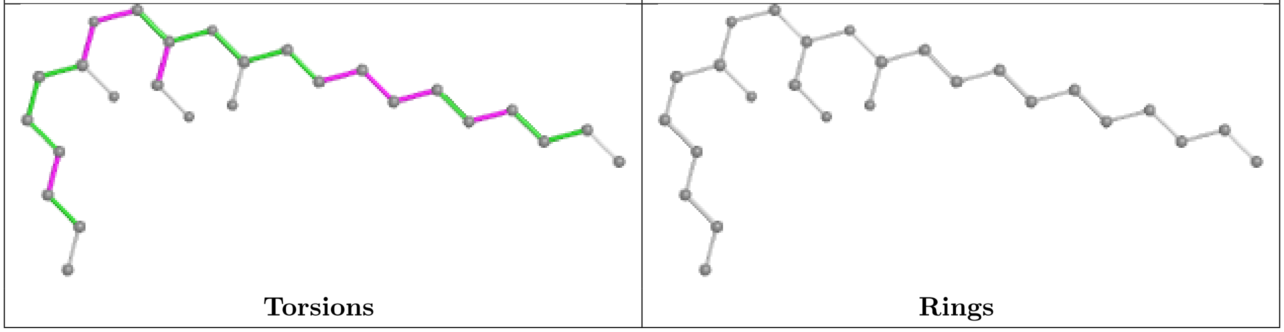


Torsions Rings

Ligand PTY U 503

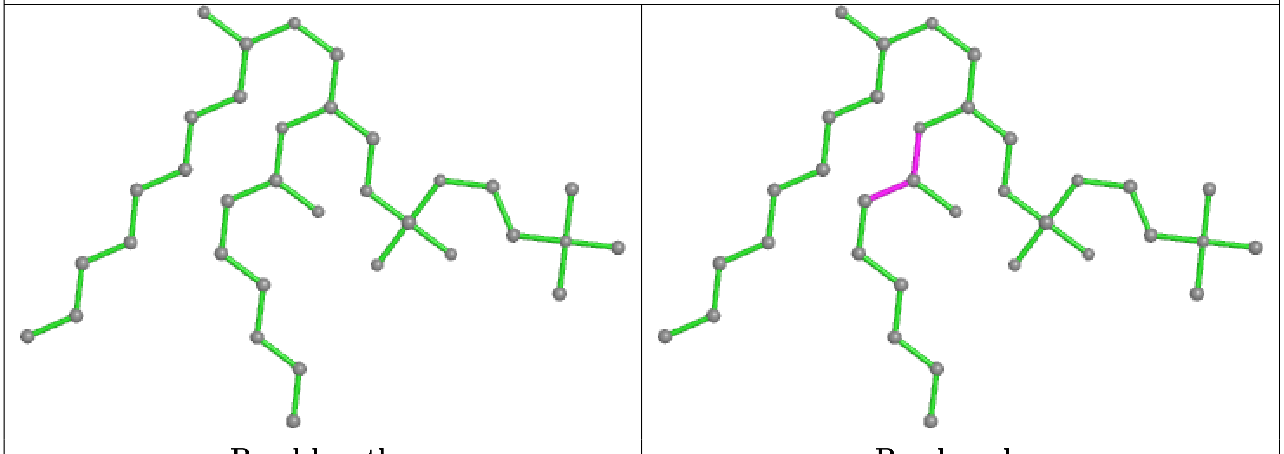


Bond lengths Bond angles



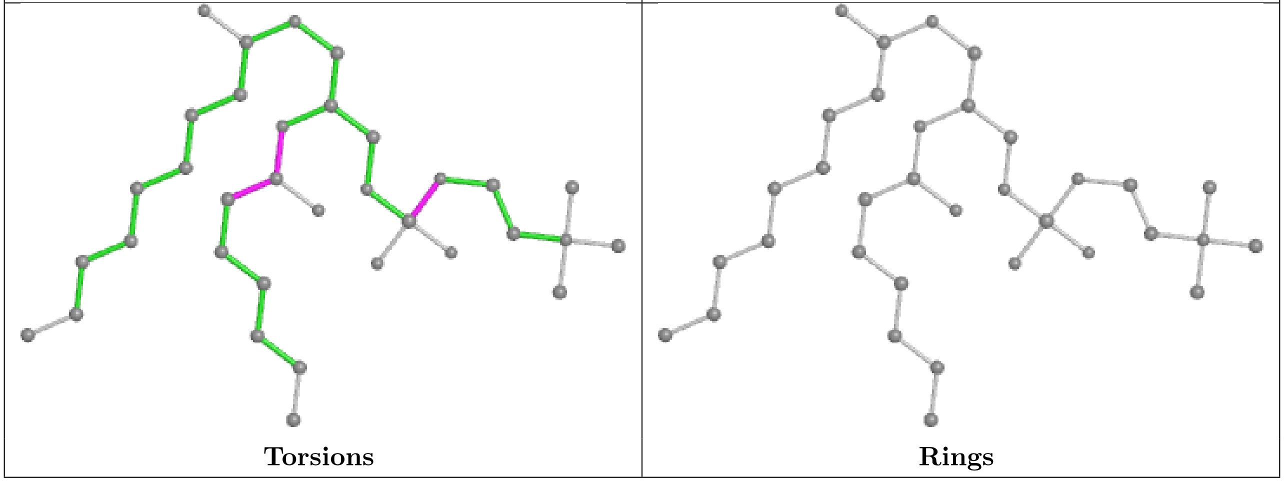
Torsions Rings

Ligand WSS 1 201



Bond lengths

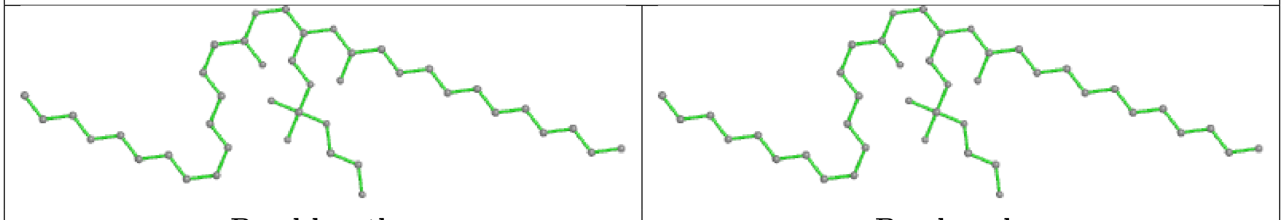
Bond angles



Torsions

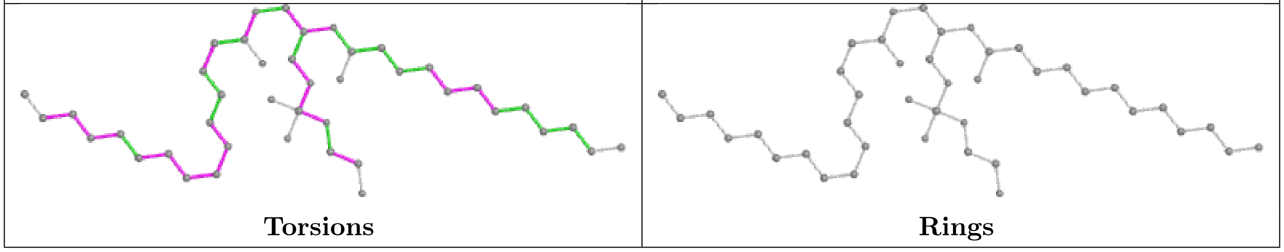
Rings

Ligand PTY 7 201



Bond lengths

Bond angles



Torsions

Rings

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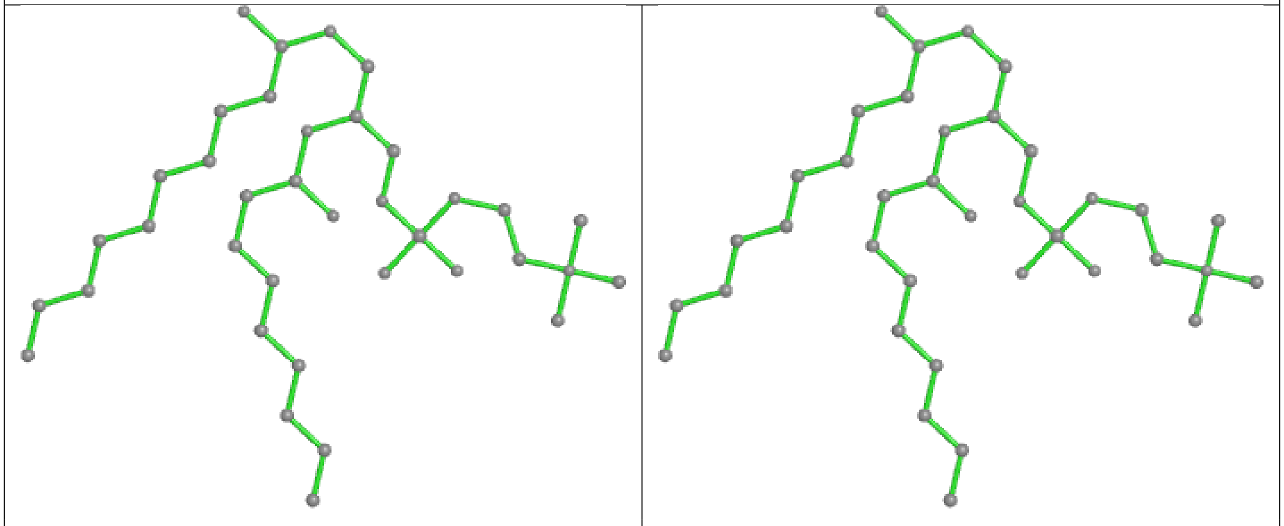
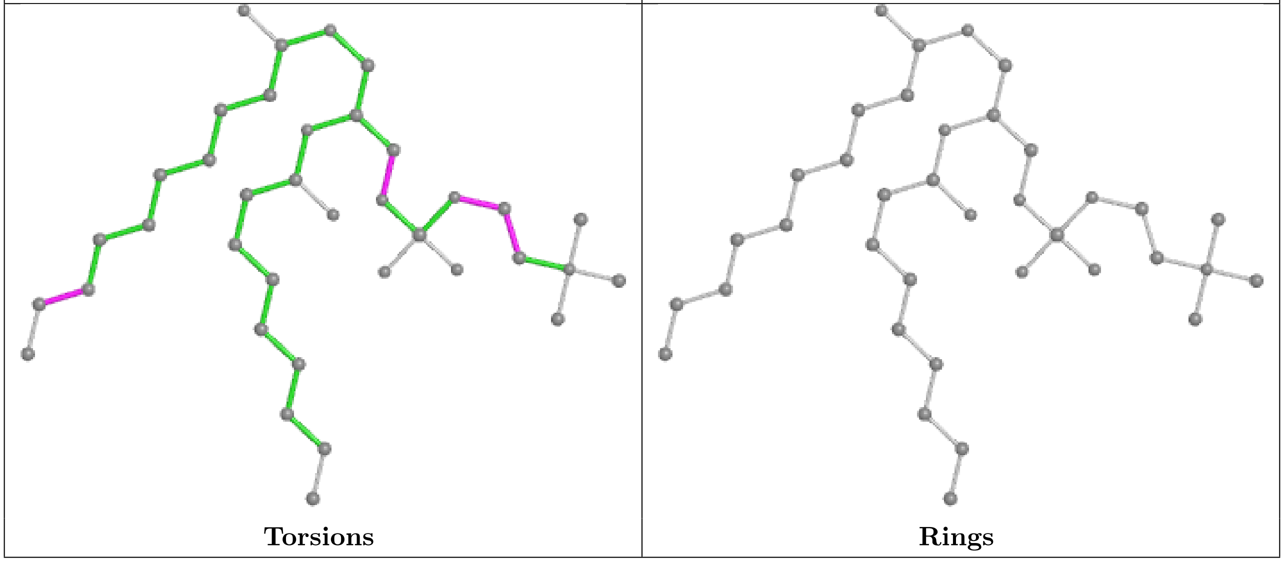


Bond lengths

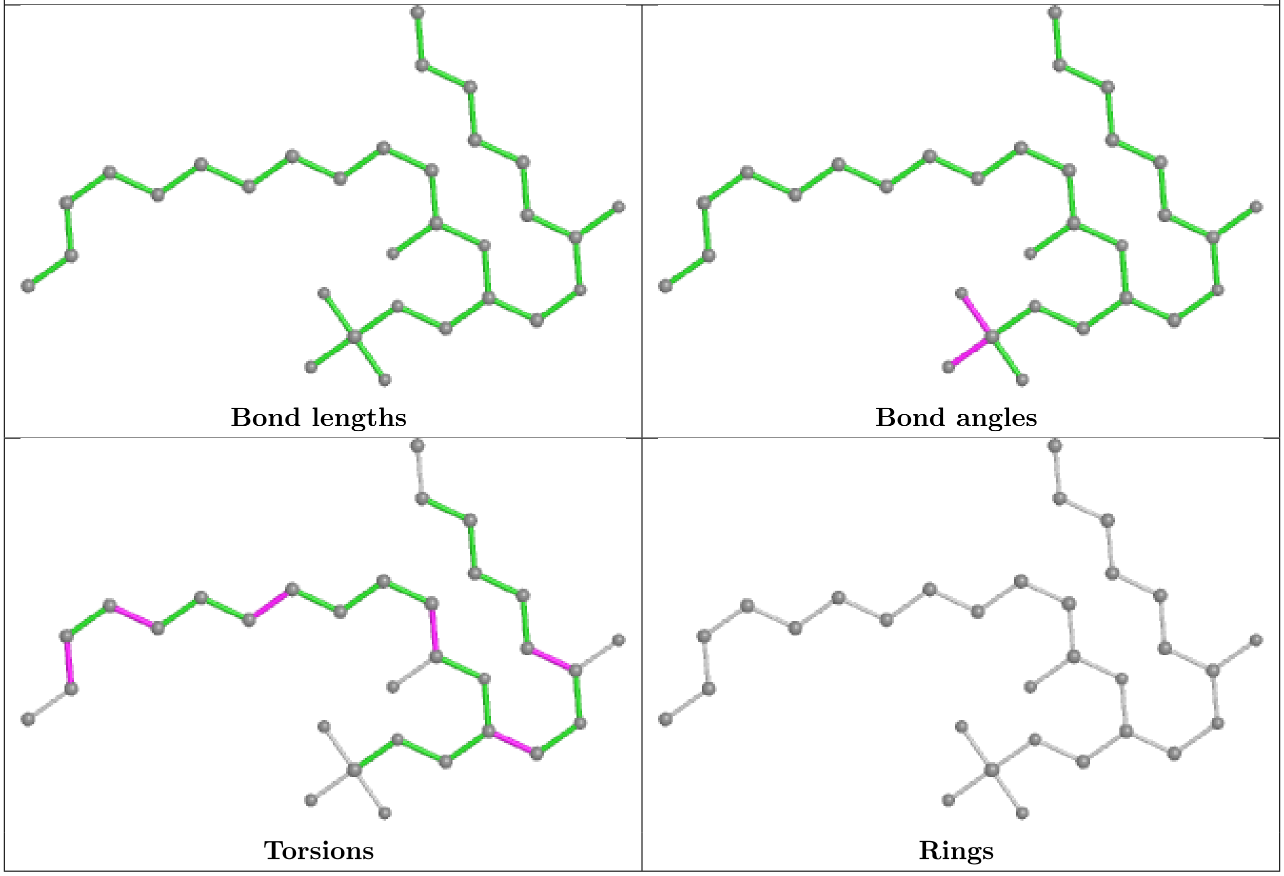
Bond angles



Torsions

Rings

Ligand WSS 0 305



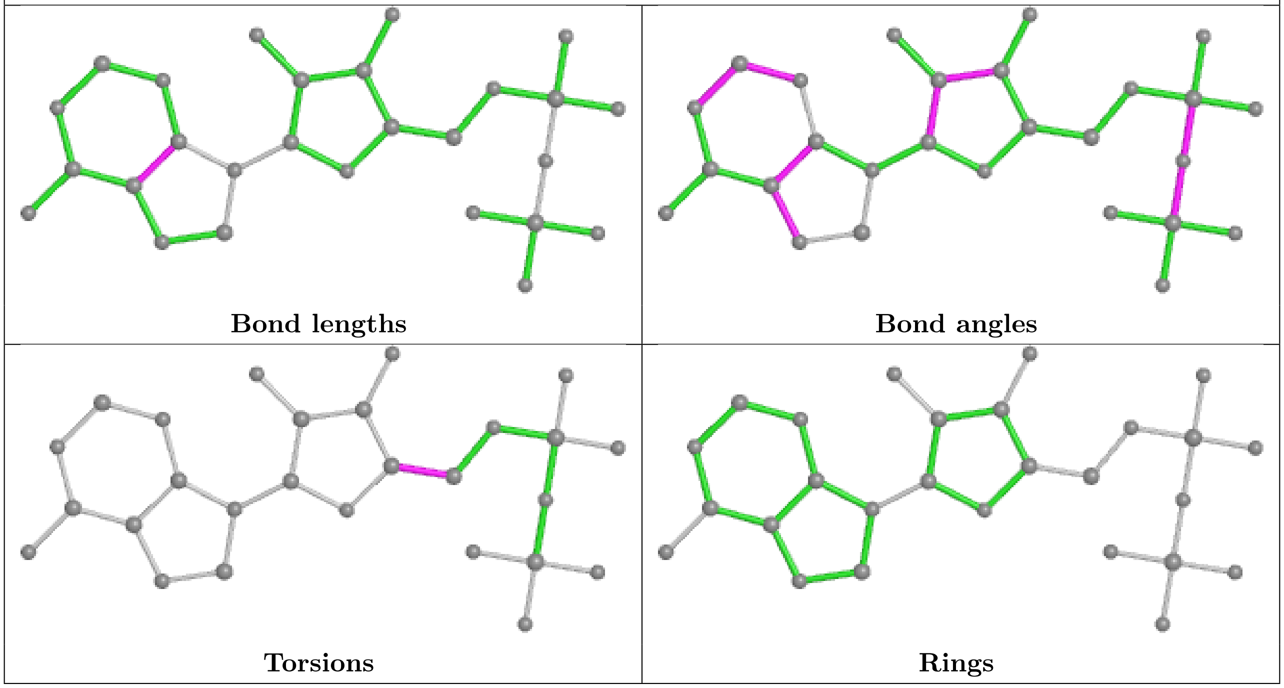
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 701



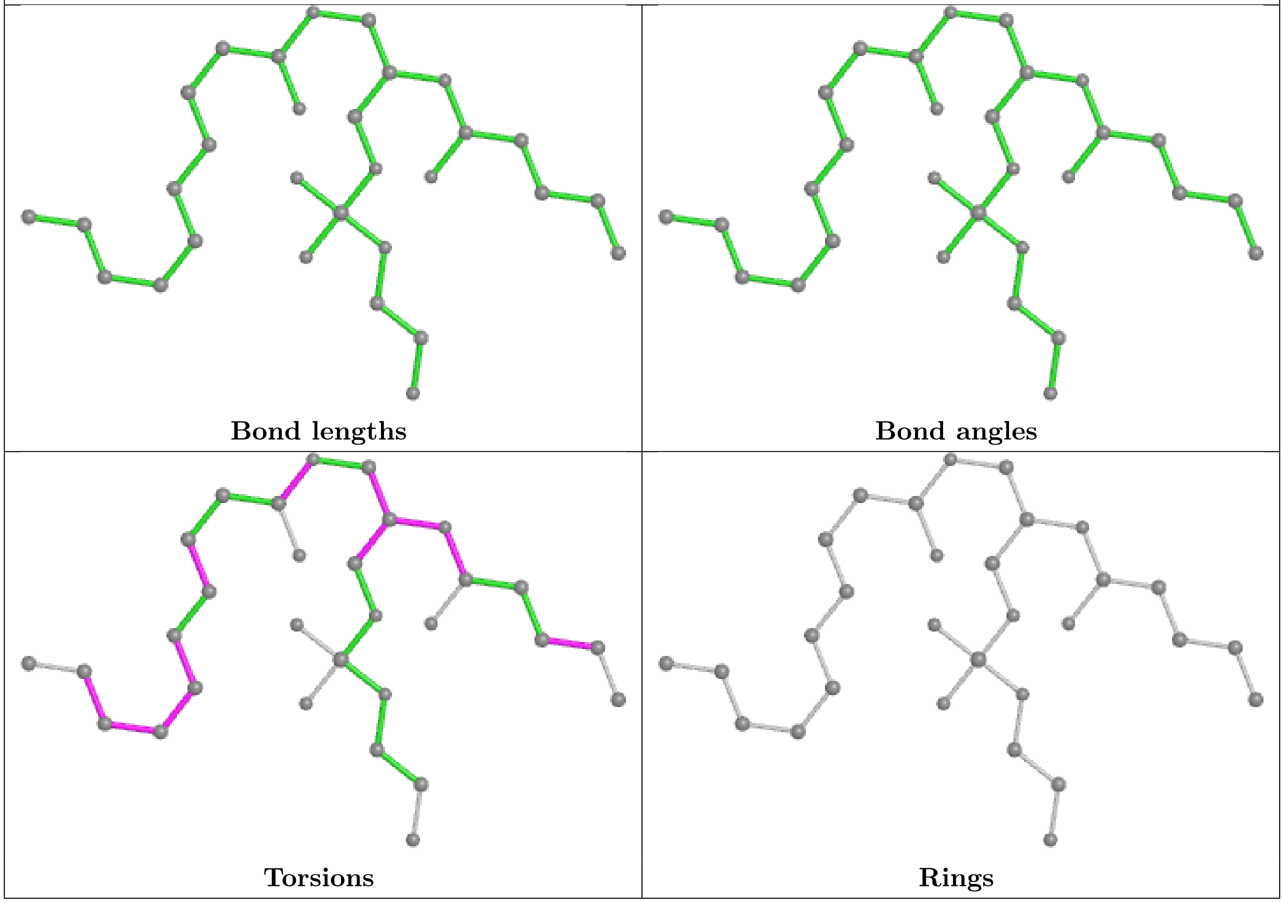
Bond lengths

Bond angles

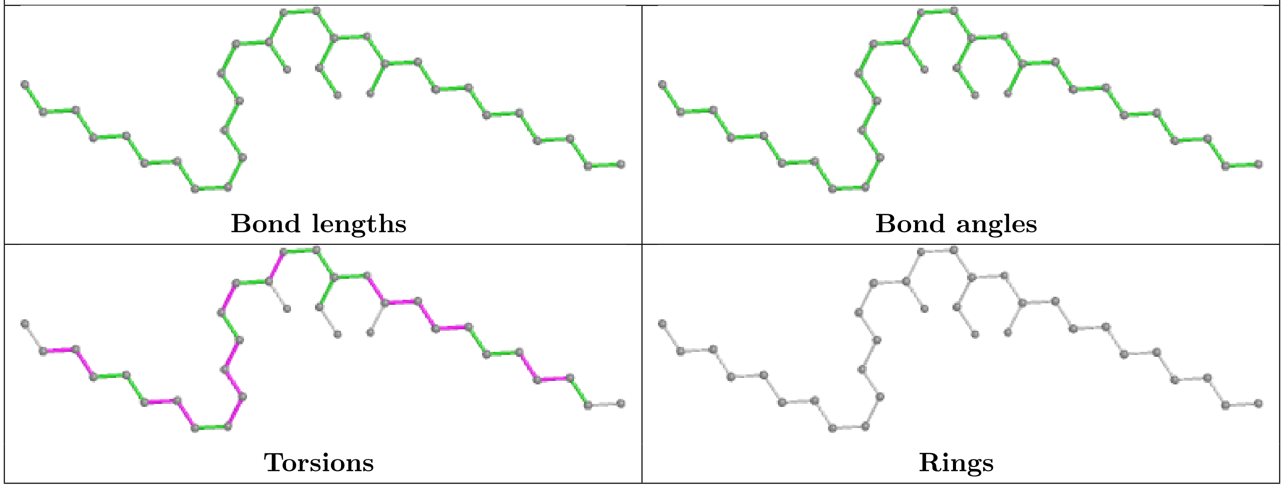
Torsions

Rings

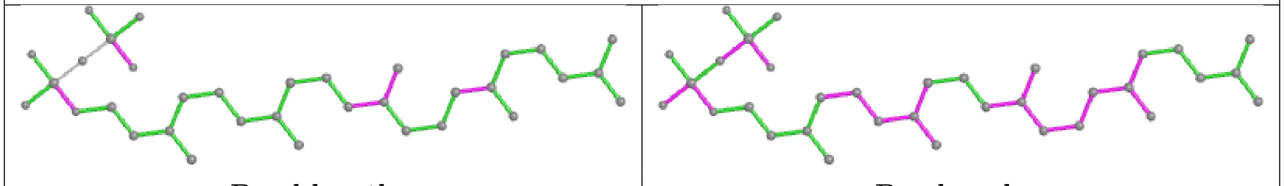
Ligand PTY Q 401



Ligand PTY 8 202

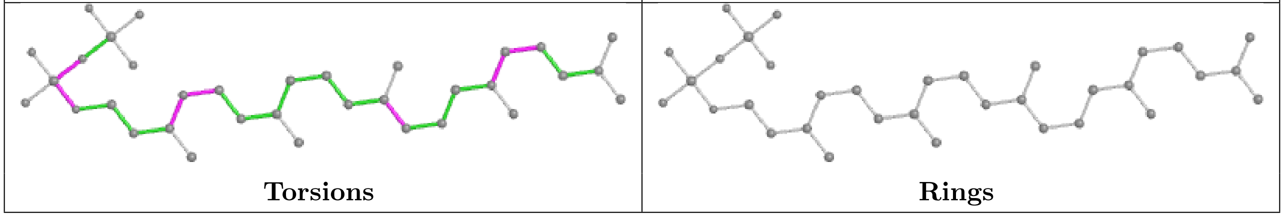


Ligand WJP R 907



Bond lengths

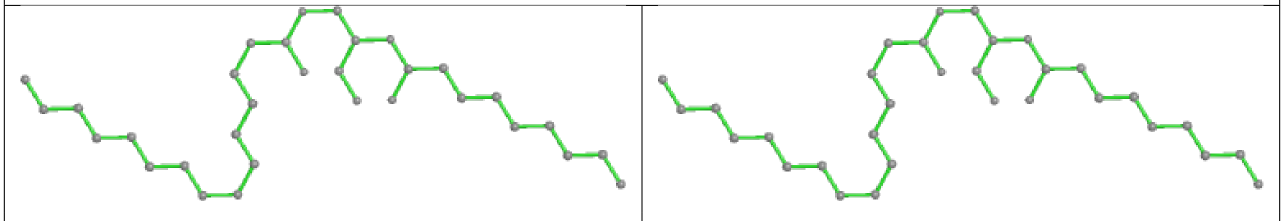
Bond angles



Torsions

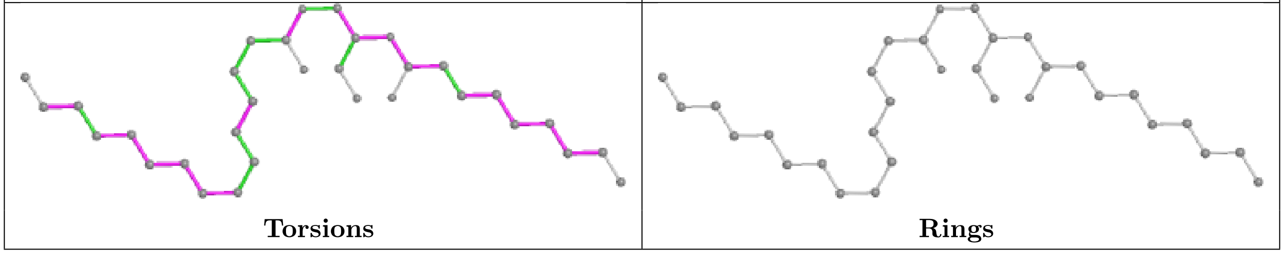
Rings

Ligand PTY R 903



Bond lengths

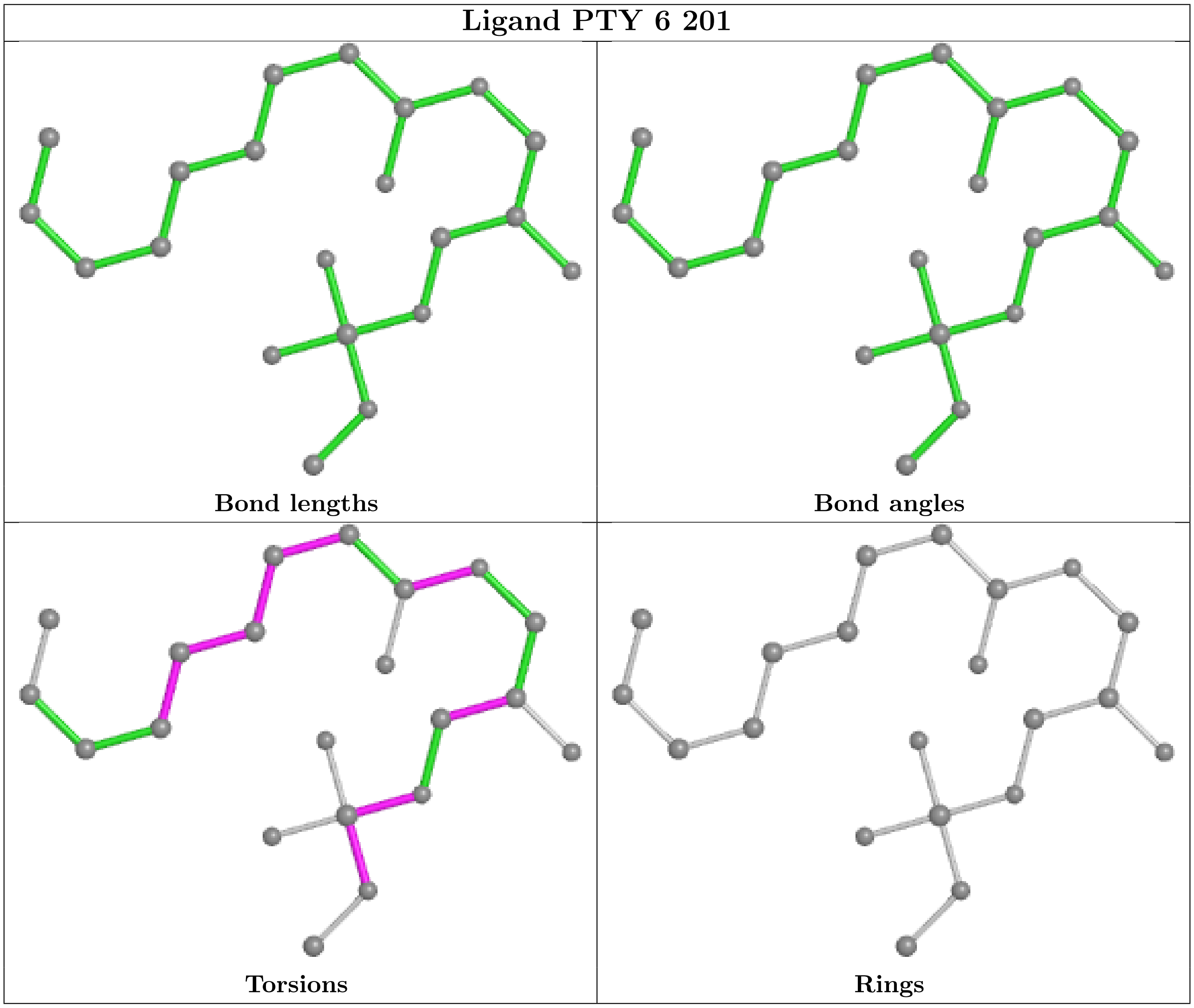
Bond angles



Torsions

Rings

Ligand PTY 6 201



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	360:THR	C	361:PRO	N	5.02

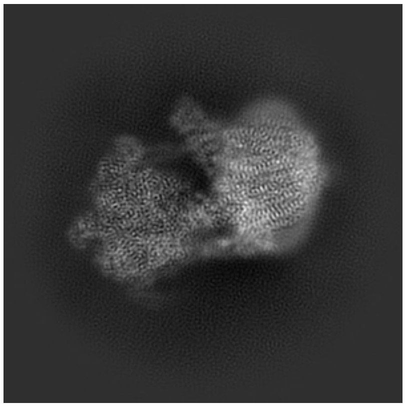
6 Map visualisation

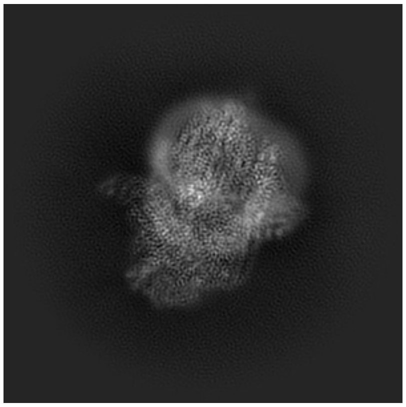
This section contains visualisations of the EMDB entry EMD-21847. These allow visual inspection of the internal detail of the map and identification of artifacts.

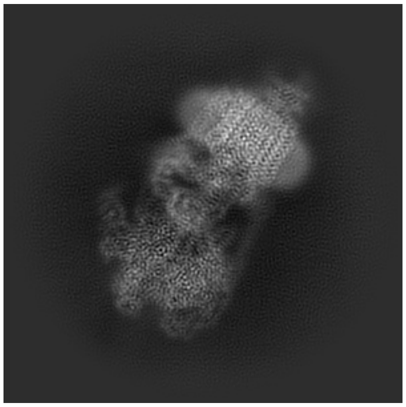
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

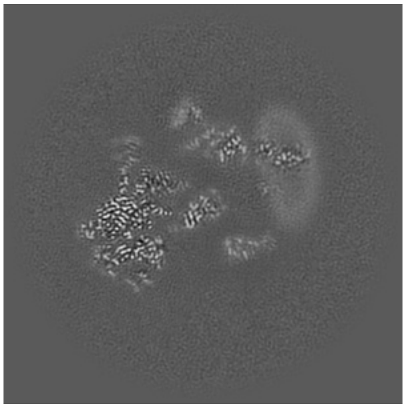

Y

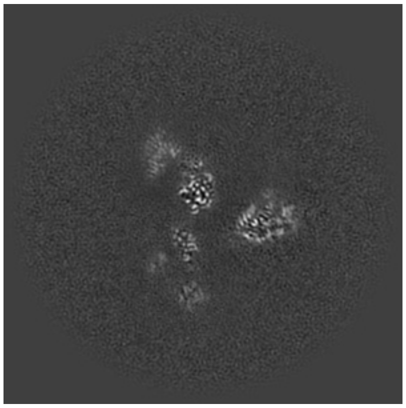

Z

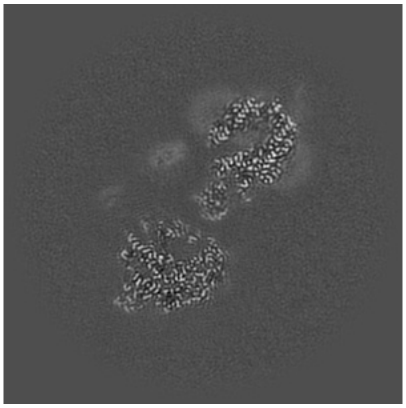
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 180

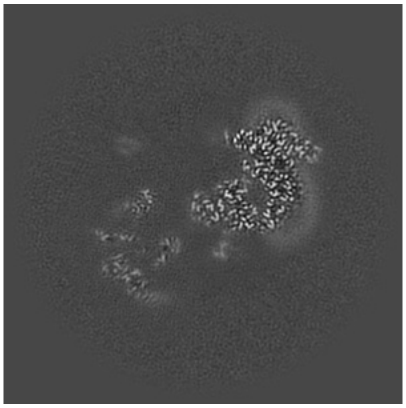

Y Index: 180


Z Index: 180

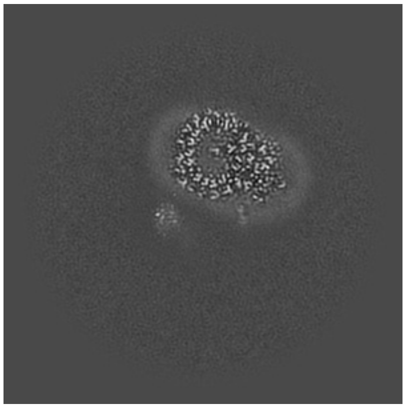
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

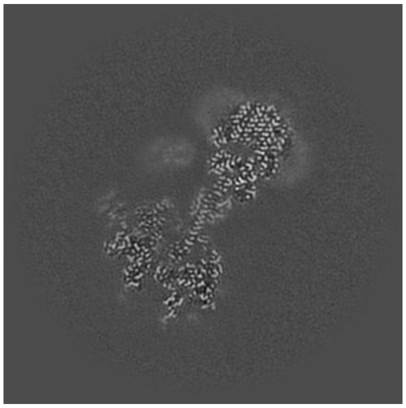
6.3.1 Primary map



X Index: 199



Y Index: 242

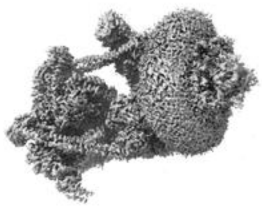


Z Index: 170

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

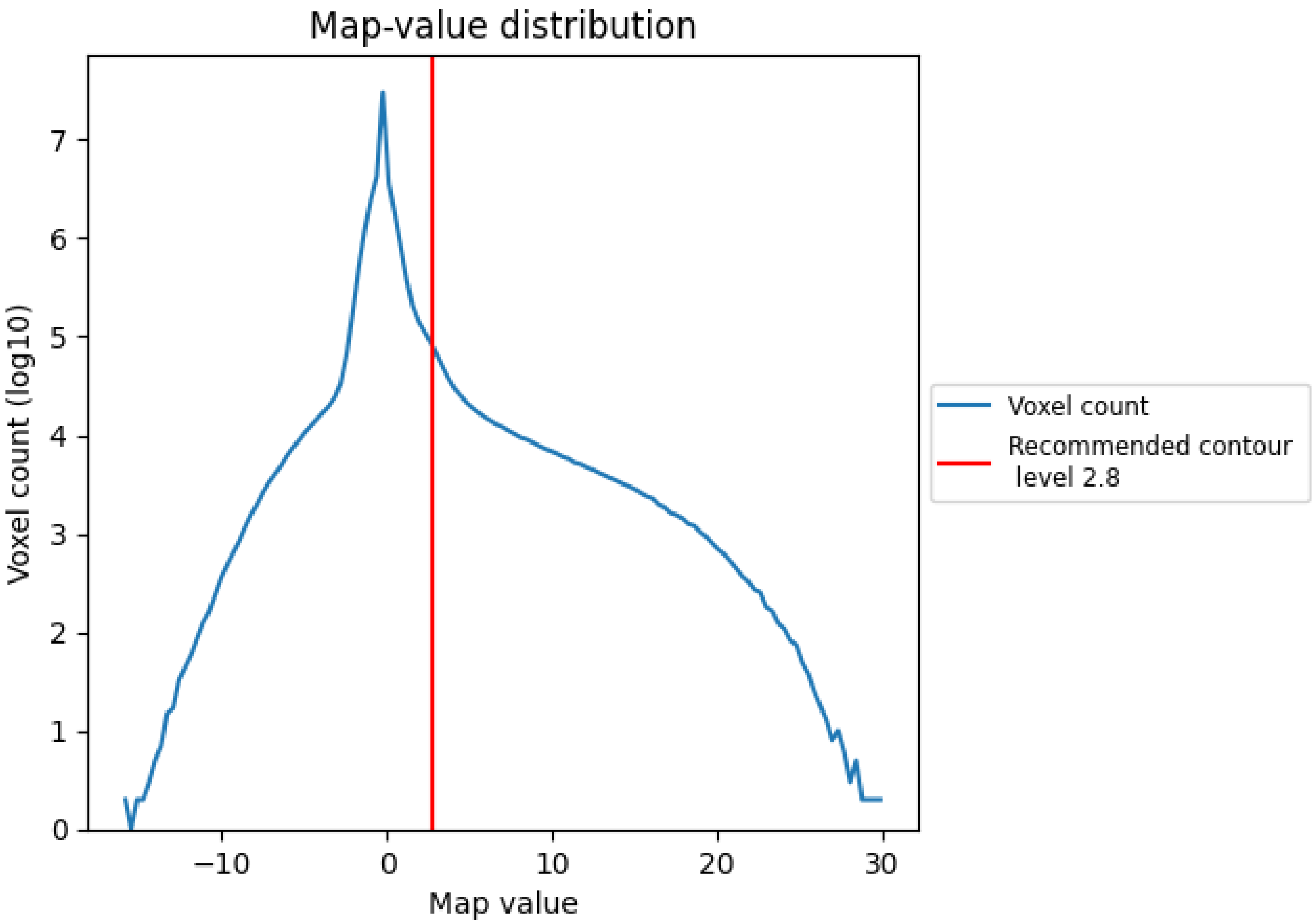
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

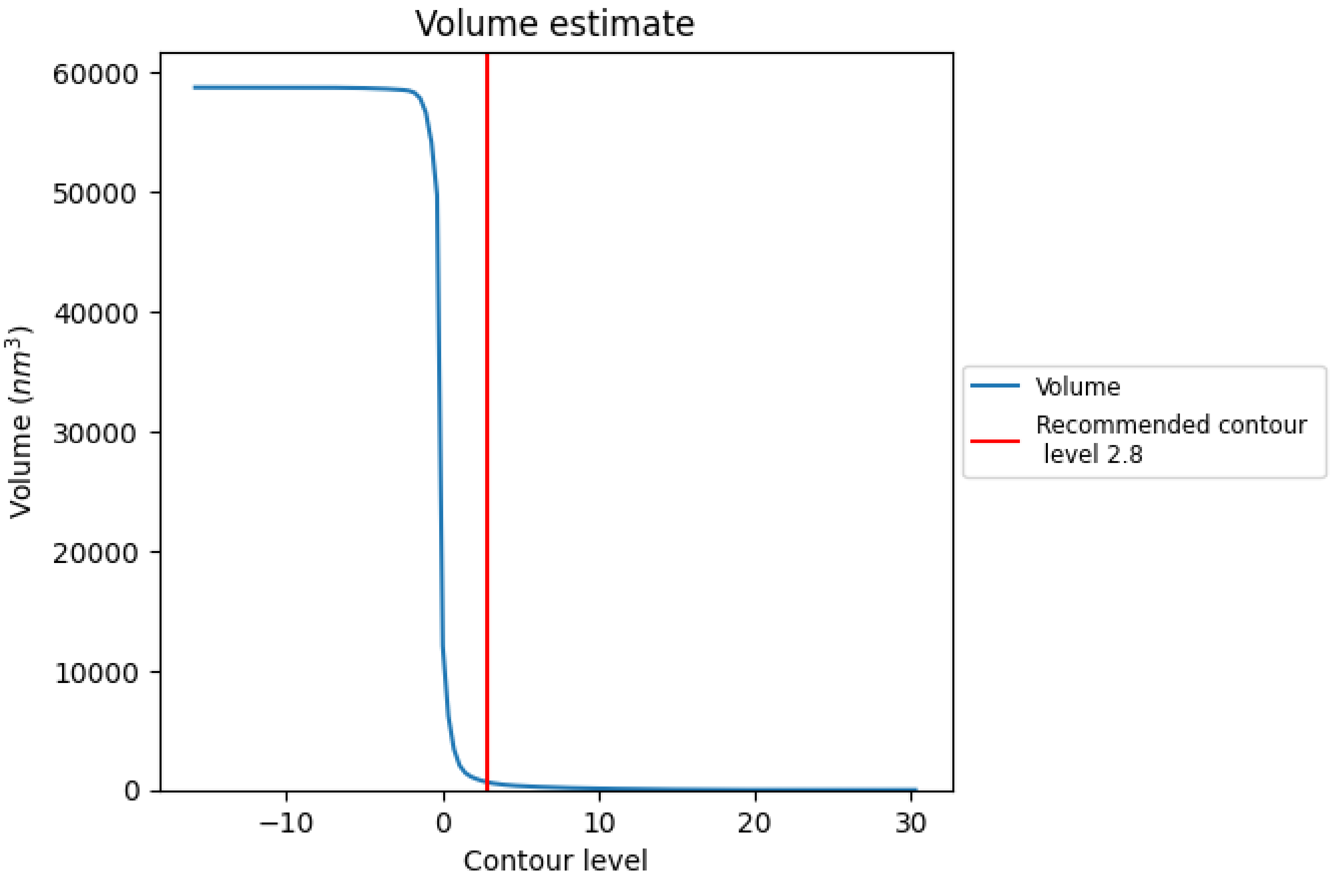
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

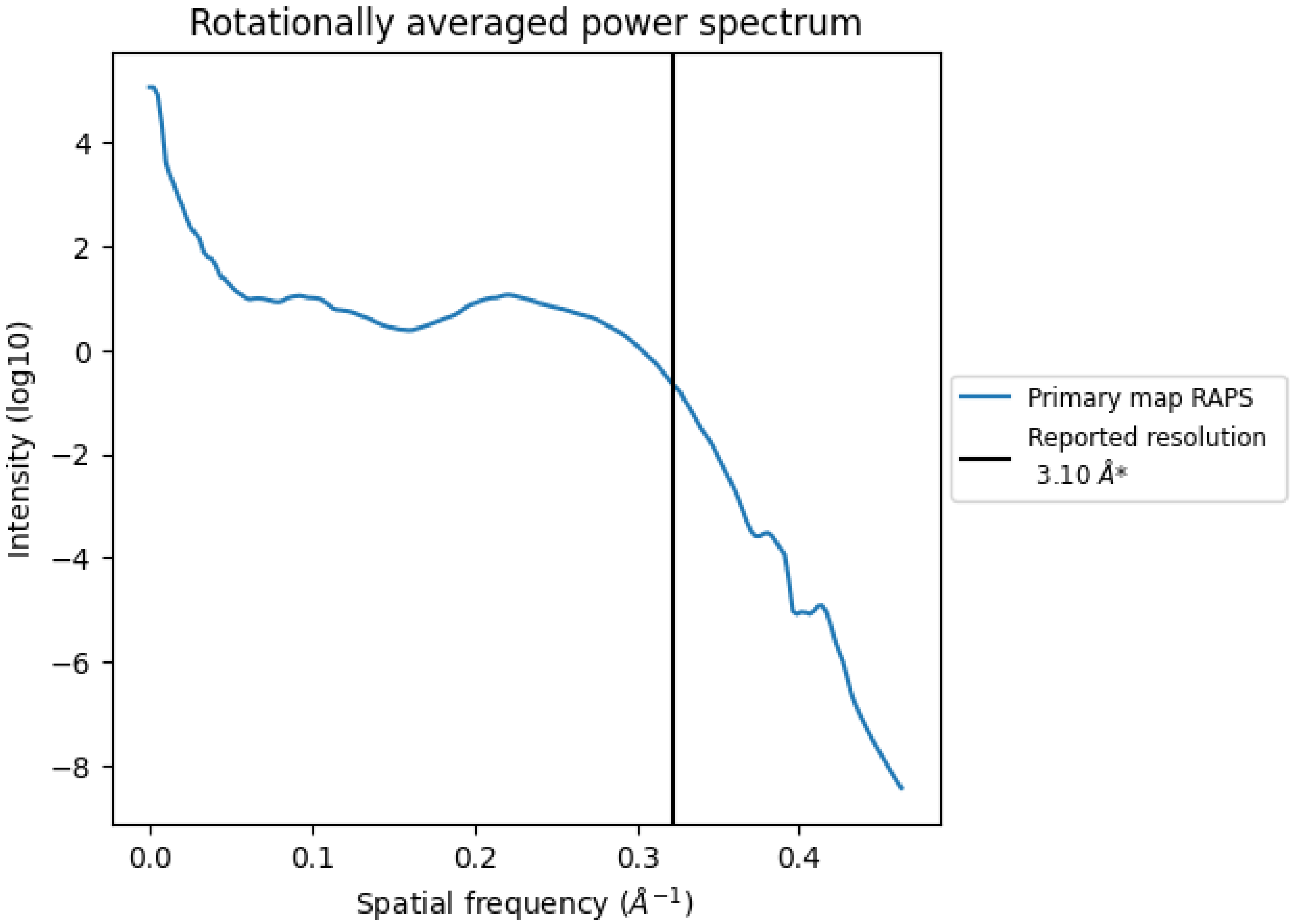
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 675 nm^3; this corresponds to an approximate mass of 610 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

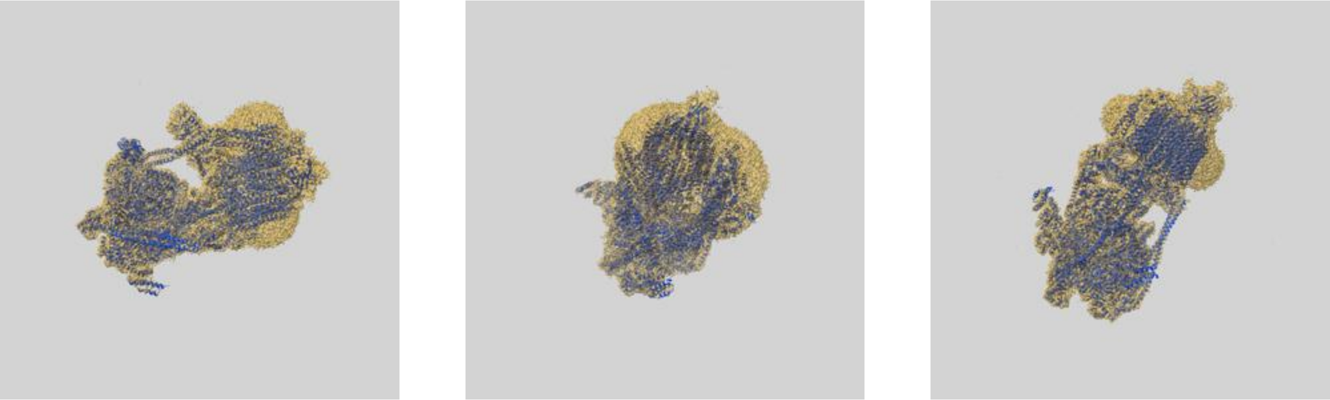
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-21847 and PDB model 6WM2. Per-residue inclusion information can be found in section 3 on page 16.

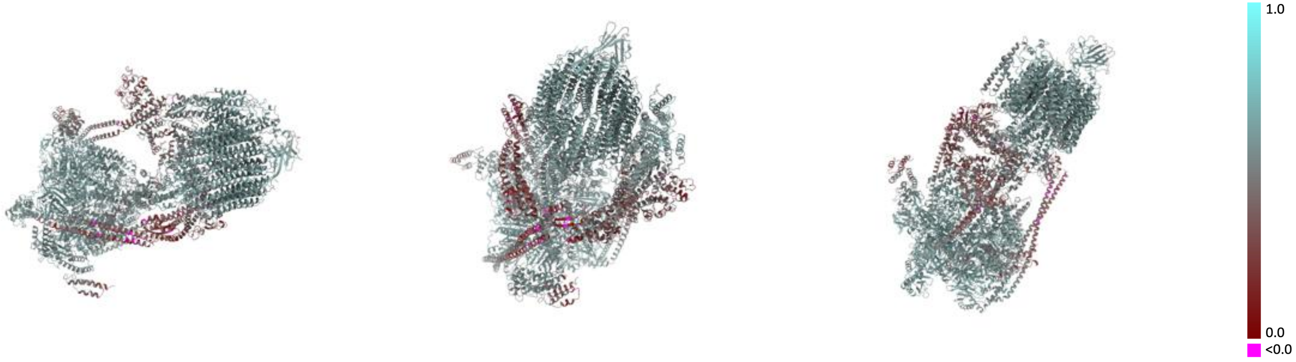
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.8 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.

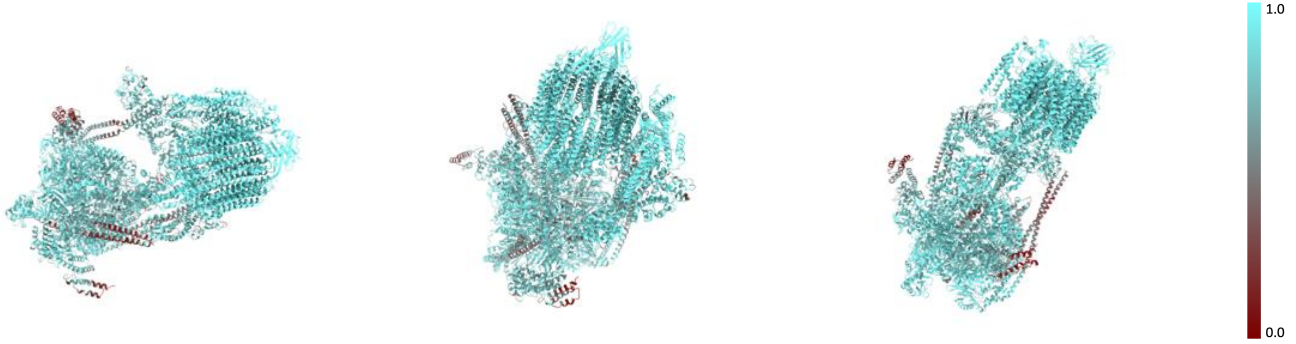
9.2 Q-score mapped to coordinate model ⓘ



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.

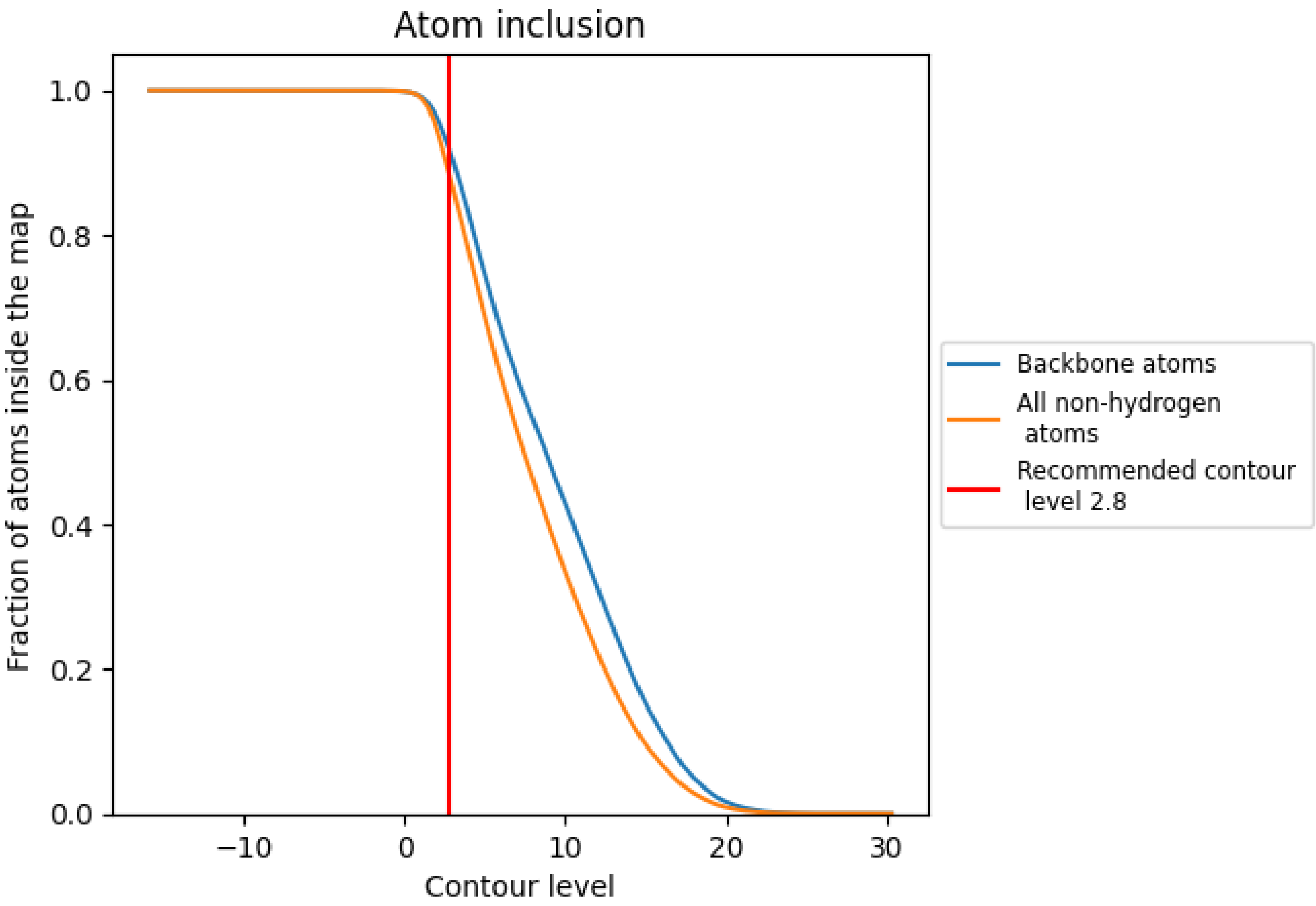
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (2.8).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 88% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8841	0.5350
0	0.9819	0.5860
1	0.9881	0.5870
2	0.9778	0.5800
3	0.9786	0.5880
4	0.9801	0.5790
5	0.9722	0.5780
6	0.9674	0.5770
7	0.9753	0.5750
8	0.9719	0.5750
9	0.9820	0.5840
A	0.9164	0.5980
B	0.9005	0.5860
C	0.9372	0.6080
D	0.9441	0.6150
E	0.9539	0.6120
F	0.9486	0.6160
G	0.8913	0.5490
H	0.8265	0.5230
I	0.8097	0.4800
J	0.7493	0.4990
K	0.6959	0.4500
L	0.6740	0.3890
M	0.5587	0.3840
N	0.9078	0.5140
O	0.7844	0.2890
P	0.8723	0.3600
Q	0.9637	0.5850
R	0.8992	0.4760
S	0.9646	0.5650
T	0.9567	0.5230
U	0.9869	0.5750
V	0.9741	0.5780
W	0.8088	0.3900
X	0.6599	0.4920

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Chain	Atom inclusion	Q-score
Y	0.7309	0.5200
Z	0.5665	0.4900
a	0.8571	0.4310
b	0.8929	0.4270
c	0.9286	0.4260
d	0.8571	0.4170
r	0.9843	0.5560
s	1.0000	0.5130
u	0.9286	0.4320