



Full wwPDB EM Validation Report ⓘ

Aug 31, 2025 – 06:14 PM JST

PDB ID : 9J99 / pdb_00009j99
EMDB ID : EMD-61256
Title : Substrate-engaged TOM complex from yeast
Authors : Yang, Y.Q.; Wang, G.P.
Deposited on : 2024-08-22
Resolution : 2.94 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

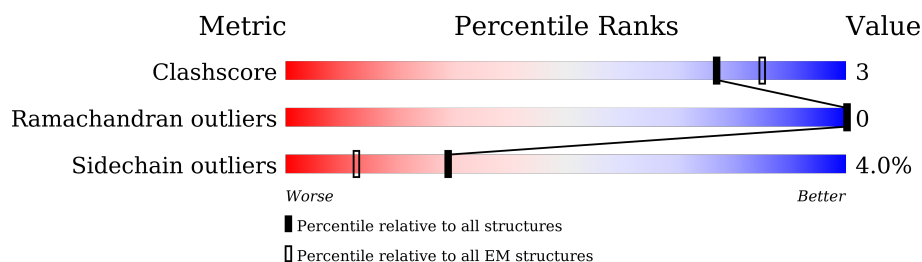
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	387	
1	I	387	
2	B	152	
2	J	152	
3	C	50	
3	K	50	
4	D	61	
4	L	61	

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Mol	Chain	Length	Quality of chain
5	E	60	<div><div>5%</div><div><div></div><div>63%</div><div></div></div><div>33%</div></div>
5	M	60	<div><div>8%</div><div><div></div><div>68%</div><div></div></div><div>28%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8859 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 Mitochondrial import receptor subunit TOM40.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2466	1552	419	487	8		
1	I	322	Total	C	N	O	S	0	0
			2469	1554	420	487	8		

- Molecule 2 is a protein called Mitochondrial import receptor subunit TOM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	49	Total	C	N	O	S	0	0
			381	246	60	74	1		
2	J	49	Total	C	N	O	S	0	0
			381	246	60	74	1		

- Molecule 3 is a protein called Mitochondrial import receptor subunit TOM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	40	Total	C	N	O	S	0	0
			341	222	59	59	1		
3	K	40	Total	C	N	O	S	0	0
			341	222	59	59	1		

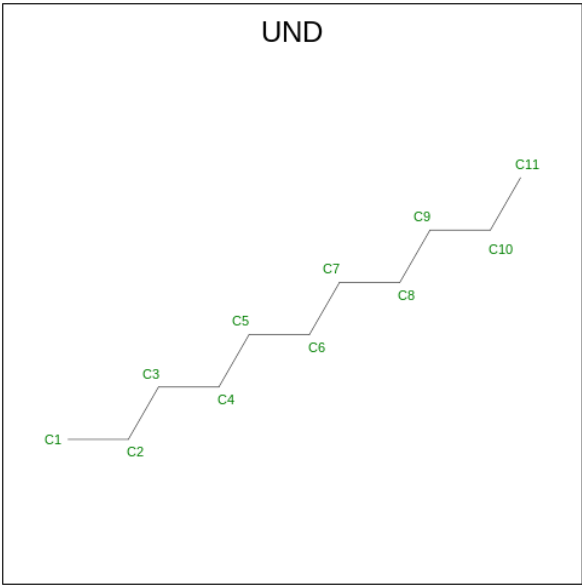
- Molecule 4 is a protein called Mitochondrial import receptor subunit TOM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	38	Total	C	N	O	S	0	0
			292	197	43	50	2		
4	L	38	Total	C	N	O	S	0	0
			292	197	43	50	2		

- Molecule 5 is a protein called Mitochondrial import receptor subunit TOM7.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	40	Total	C	N	O	0	0
			325	218	55	52		
5	M	43	Total	C	N	O	0	0
			348	233	59	56		

- Molecule 6 is UNDECANE (CCD ID: UND) (formula: C₁₁H₂₄) (labeled as "Ligand of Interest" by depositor).



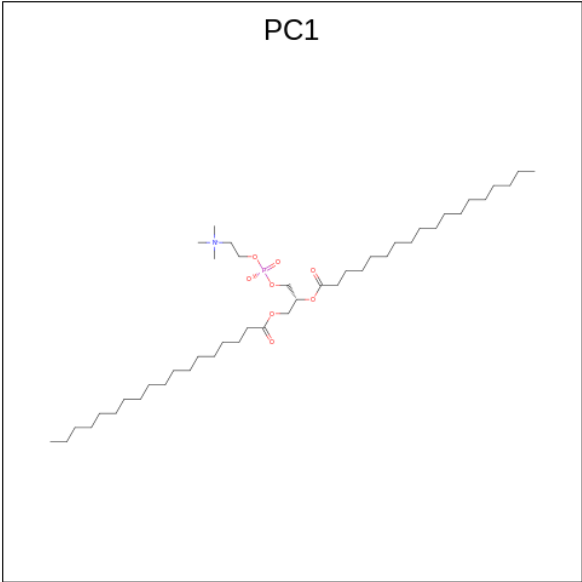
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C	0
			11	11	
6	A	1	Total	C	0
			11	11	
6	A	1	Total	C	0
			11	11	
6	A	1	Total	C	0
			11	11	
6	A	1	Total	C	0
			9	9	
6	B	1	Total	C	0
			11	11	
6	C	1	Total	C	0
			10	10	
6	C	1	Total	C	0
			11	11	
6	D	1	Total	C	0
			11	11	

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Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total C 9 9	0
6	D	1	Total C 11 11	0
6	E	1	Total C 11 11	0
6	E	1	Total C 11 11	0
6	E	1	Total C 11 11	0
6	I	1	Total C 11 11	0
6	I	1	Total C 8 8	0
6	I	1	Total C 11 11	0
6	I	1	Total C 11 11	0
6	I	1	Total C 11 11	0
6	L	1	Total C 9 9	0
6	L	1	Total C 11 11	0
6	L	1	Total C 11 11	0
6	M	1	Total C 11 11	0
6	M	1	Total C 11 11	0
6	M	1	Total C 11 11	0
6	M	1	Total C 11 11	0

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
7	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	A	1	Total	C	N	O	P	0
			30	20	1	8	1	
7	A	1	Total	C	N	O	P	0
			35	26	1	7	1	
7	A	1	Total	C	N	O	P	0
			24	16	1	6	1	
7	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
7	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
7	B	1	Total	C	N	O	P	0
			28	18	1	8	1	
7	B	1	Total	C	N	O	P	0
			32	24	1	6	1	
7	D	1	Total	C	N	O	P	0
			31	21	1	8	1	
7	D	1	Total	C	N	O	P	0
			29	20	1	7	1	
7	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	I	1	Total	C	N	O	P	0
			33	23	1	8	1	

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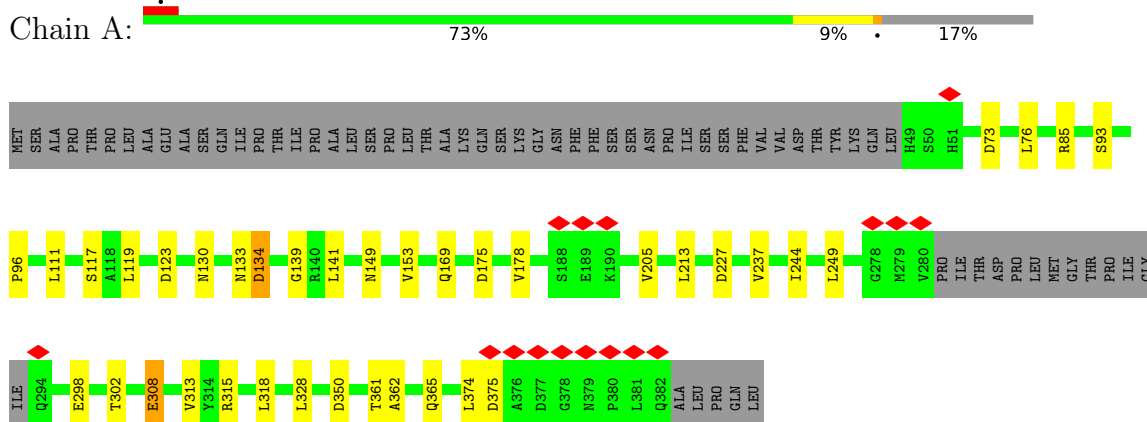
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Mol	Chain	Residues	Atoms					AltConf
7	I	1	Total	C	N	O	P	0
			38	28	1	8	1	
7	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
7	I	1	Total	C	N	O	P	0
			46	36	1	8	1	
7	I	1	Total	C	N	O	P	0
			43	33	1	8	1	
7	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	I	1	Total	C	N	O	P	0
			39	29	1	8	1	
7	I	1	Total	C	N	O	P	0
			37	27	1	8	1	
7	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
7	J	1	Total	C	N	O	P	0
			31	21	1	8	1	
7	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
7	M	1	Total	C	N	O	P	0
			27	17	1	8	1	

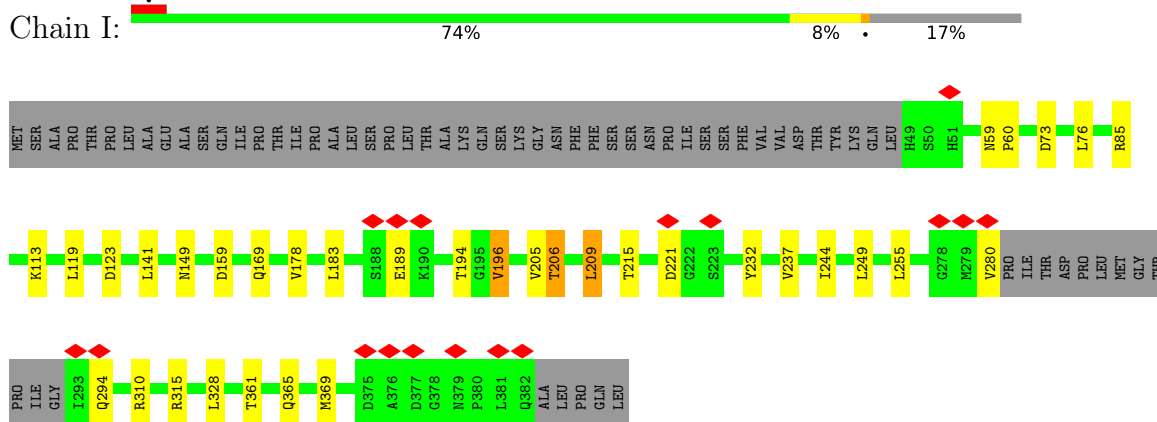
3 Residue-property plots

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.

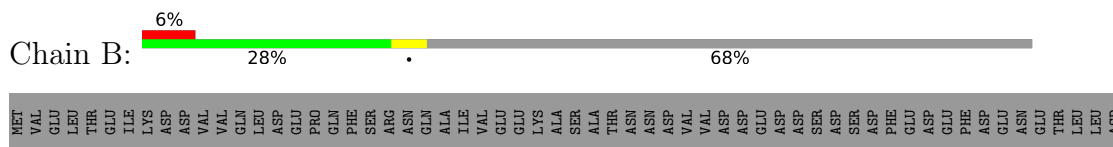
- Molecule 1: Mitochondrial import receptor subunit TOM40



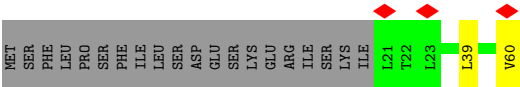
- Molecule 1: Mitochondrial import receptor subunit TOM40



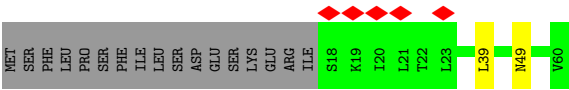
- Molecule 2: Mitochondrial import receptor subunit TOM22







• Molecule 5: Mitochondrial import receptor subunit TOM7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1028127	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0082	Depositor
Map size (Å)	285.0, 285.0, 285.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, UND

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/2510	0.49	2/3397 (0.1%)
1	I	0.32	0/2514	0.46	0/3401
2	B	0.25	0/386	0.41	0/524
2	J	0.25	0/386	0.42	0/524
3	C	0.24	0/351	0.42	0/474
3	K	0.24	0/351	0.46	1/474 (0.2%)
4	D	0.16	0/300	0.30	0/407
4	L	0.18	0/300	0.38	0/407
5	E	0.41	0/339	0.54	0/469
5	M	0.21	0/362	0.41	0/499
All	All	0.29	0/7799	0.46	3/10576 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	38	SER	N-CA-C	5.87	122.77	109.81
1	A	134	ASP	CB-CA-C	5.13	120.15	110.35
1	A	133	ASN	N-CA-C	-5.01	103.07	110.48

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	A	2466	0	2400	16	0
1	I	2469	0	2394	17	0
2	B	381	0	391	4	0
2	J	381	0	391	2	0
3	C	341	0	337	2	0
3	K	341	0	337	2	0
4	D	292	0	293	2	0
4	L	292	0	293	0	0
5	E	325	0	319	1	0
5	M	348	0	348	1	0
6	A	53	0	113	1	0
6	B	11	0	24	1	0
6	C	21	0	43	1	0
6	D	31	0	65	1	0
6	E	33	0	72	1	0
6	I	52	0	111	0	0
6	L	31	0	65	0	0
6	M	44	0	96	0	0
7	A	266	0	372	2	0
7	B	60	0	74	0	0
7	D	104	0	134	2	0
7	E	32	0	38	1	0
7	I	342	0	488	8	0
7	J	77	0	102	0	0
7	L	39	0	52	0	0
7	M	27	0	28	0	0
All	All	8859	0	9380	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:73:ASP:O	1:I:315:ARG:NH1	2.36	0.58
1:I:206:THR:HG22	1:I:209:LEU:H	1.68	0.57
1:I:59:ASN:ND2	1:I:60:PRO:O	2.37	0.57
1:I:205:VAL:HA	3:K:39:PRO:HG3	1.87	0.57
1:A:73:ASP:O	1:A:315:ARG:NH1	2.38	0.56
2:B:89:ARG:HD2	6:B:201:UND:H12	1.87	0.56
1:A:350:ASP:N	1:A:350:ASP:OD1	2.39	0.55
1:A:365:GLN:HG3	5:E:60:VAL:HG11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:365:GLN:HE21	1:I:369:MET:HE3	1.72	0.54
7:A:405:PC1:H31	6:C:102:UND:H101	1.90	0.53
1:I:123:ASP:OD1	1:I:123:ASP:N	2.42	0.53
1:A:328:LEU:HD22	2:B:112:PRO:HB3	1.92	0.52
1:I:328:LEU:HD22	2:J:112:PRO:HB3	1.91	0.52
1:A:227:ASP:OD1	1:A:227:ASP:N	2.42	0.51
1:A:139:GLY:HA3	7:A:403:PC1:H2G2	1.91	0.51
1:I:149:ASN:OD1	1:I:169:GLN:NE2	2.44	0.51
3:K:22:GLU:HG2	3:K:26:LYS:HE2	1.92	0.51
1:A:205:VAL:HA	3:C:39:PRO:HG3	1.94	0.49
1:I:237:VAL:HG13	1:I:244:ILE:HG12	1.93	0.49
1:I:310:ARG:NH1	2:J:127:GLU:OE2	2.45	0.49
6:A:401:UND:H101	6:A:406:UND:H11	1.94	0.49
4:D:50:GLN:HE21	7:D:104:PC1:H262	1.79	0.47
1:I:232:TYR:HB3	7:I:409:PC1:H372	1.96	0.47
1:I:249:LEU:HD13	1:I:255:LEU:HD12	1.97	0.46
7:I:410:PC1:H2A1	7:I:410:PC1:H272	1.77	0.46
5:M:49:ASN:OD1	5:M:49:ASN:N	2.44	0.46
1:I:221:ASP:OD1	1:I:221:ASP:N	2.46	0.45
2:B:121:GLN:HE21	4:D:61:LEU:HD22	1.81	0.45
1:A:149:ASN:OD1	1:A:169:GLN:NE2	2.50	0.45
1:A:175:ASP:N	1:A:175:ASP:OD1	2.49	0.45
7:E:103:PC1:H241	7:E:103:PC1:H271	1.72	0.44
7:I:408:PC1:H2C1	7:I:408:PC1:H2F2	1.77	0.44
1:I:113:LYS:HD3	7:I:406:PC1:H122	2.00	0.43
1:A:375:ASP:N	1:A:375:ASP:OD1	2.51	0.43
2:B:131:ASP:O	2:B:134:SER:OG	2.36	0.43
3:C:46:LYS:HB3	3:C:46:LYS:HE2	1.86	0.43
1:A:361:THR:OG1	1:A:362:ALA:N	2.51	0.43
1:I:159:ASP:OD1	1:I:159:ASP:N	2.52	0.43
7:I:403:PC1:H342	7:I:403:PC1:H371	1.77	0.43
7:I:410:PC1:H2E1	7:I:410:PC1:H2B2	1.89	0.43
7:D:104:PC1:H241	6:D:106:UND:H81	2.00	0.43
1:A:93:SER:HB3	1:A:96:PRO:HD2	2.01	0.42
7:I:410:PC1:H111	7:I:410:PC1:H2	2.02	0.42
1:A:123:ASP:OD1	1:A:123:ASP:N	2.50	0.42
1:I:183:LEU:HB3	1:I:196:VAL:HG13	2.01	0.42
6:E:101:UND:H51	6:E:101:UND:H22	1.80	0.42
1:A:308:GLU:HG2	1:A:313:VAL:HG13	2.02	0.41
1:I:280:VAL:HG22	1:I:294:GLN:H	1.85	0.41
1:A:237:VAL:HG13	1:A:244:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:SER:HB2	1:A:130:ASN:HD22	1.86	0.41
7:I:401:PC1:H252	7:I:401:PC1:H282	1.86	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	317/387 (82%)	306 (96%)	11 (4%)	0	100	100
1	I	318/387 (82%)	306 (96%)	12 (4%)	0	100	100
2	B	47/152 (31%)	47 (100%)	0	0	100	100
2	J	47/152 (31%)	47 (100%)	0	0	100	100
3	C	38/50 (76%)	38 (100%)	0	0	100	100
3	K	38/50 (76%)	37 (97%)	1 (3%)	0	100	100
4	D	36/61 (59%)	36 (100%)	0	0	100	100
4	L	36/61 (59%)	36 (100%)	0	0	100	100
5	E	38/60 (63%)	36 (95%)	2 (5%)	0	100	100
5	M	41/60 (68%)	39 (95%)	2 (5%)	0	100	100
All	All	956/1420 (67%)	928 (97%)	28 (3%)	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	A	268/327 (82%)	253 (94%)	15 (6%)	17	39
1	I	266/327 (81%)	254 (96%)	12 (4%)	23	47
2	B	43/133 (32%)	42 (98%)	1 (2%)	45	69
2	J	43/133 (32%)	43 (100%)	0	100	100
3	C	35/44 (80%)	35 (100%)	0	100	100
3	K	35/44 (80%)	34 (97%)	1 (3%)	37	62
4	D	30/44 (68%)	29 (97%)	1 (3%)	33	57
4	L	30/44 (68%)	29 (97%)	1 (3%)	33	57
5	E	36/56 (64%)	35 (97%)	1 (3%)	38	63
5	M	39/56 (70%)	38 (97%)	1 (3%)	41	65
All	All	825/1208 (68%)	792 (96%)	33 (4%)	29	51

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	85	ARG
1	A	111	LEU
1	A	119	LEU
1	A	134	ASP
1	A	141	LEU
1	A	153	VAL
1	A	178	VAL
1	A	213	LEU
1	A	249	LEU
1	A	298	GLU
1	A	302	THR
1	A	308	GLU
1	A	318	LEU
1	A	374	LEU
2	B	92	PHE
4	D	61	LEU
5	E	39	LEU
1	I	76	LEU
1	I	85	ARG
1	I	119	LEU
1	I	141	LEU

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Mol	Chain	Res	Type
1	I	178	VAL
1	I	189	GLU
1	I	194	THR
1	I	196	VAL
1	I	206	THR
1	I	209	LEU
1	I	215	THR
1	I	361	THR
3	K	44	LEU
4	L	32	LEU
5	M	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	65	ASN
1	A	130	ASN
1	A	311	GLN
2	B	121	GLN
4	D	50	GLN
5	E	25	HIS
1	I	59	ASN
1	I	65	ASN
1	I	130	ASN
1	I	250	GLN
1	I	349	ASN
1	I	365	GLN
1	I	372	GLN
2	J	133	GLN
3	K	17	HIS
4	L	38	ASN
4	L	50	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

51 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	$\# Z > 2$
7	PC1	A	412	-	48,48,53	0.50	0	54,56,61	0.59	1 (1%)
6	UND	I	404	-	10,10,10	0.23	0	9,9,9	0.21	0
7	PC1	A	402	-	37,37,53	0.55	0	43,45,61	0.66	2 (4%)
6	UND	E	102	-	10,10,10	0.22	0	9,9,9	0.27	0
7	PC1	A	409	-	23,23,53	0.64	0	28,29,61	0.63	1 (3%)
7	PC1	I	406	-	42,42,53	0.54	0	48,50,61	0.51	1 (2%)
7	PC1	I	401	-	32,32,53	0.61	0	38,40,61	0.59	1 (2%)
6	UND	L	104	-	10,10,10	0.23	0	9,9,9	0.20	0
6	UND	I	413	-	10,10,10	0.22	0	9,9,9	0.23	0
6	UND	E	104	-	10,10,10	0.22	0	9,9,9	0.21	0
6	UND	A	401	-	10,10,10	0.23	0	9,9,9	0.23	0
6	UND	A	407	-	10,10,10	0.23	0	9,9,9	0.21	0
7	PC1	J	202	-	30,30,53	0.60	0	36,38,61	0.79	2 (5%)
7	PC1	I	408	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
6	UND	C	101	-	9,9,10	0.23	0	8,8,9	0.24	0
7	PC1	D	104	-	43,43,53	0.54	0	49,51,61	0.53	1 (2%)
7	PC1	L	101	-	38,38,53	0.54	0	44,46,61	0.68	2 (4%)
7	PC1	B	202	-	27,27,53	0.62	0	33,35,61	0.82	2 (6%)
6	UND	M	103	-	10,10,10	0.23	0	9,9,9	0.24	0
7	PC1	I	410	-	36,36,53	0.55	0	42,44,61	0.75	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PC1	I	409	-	38,38,53	0.54	0	44,46,61	0.69	2 (4%)
7	PC1	I	402	-	37,37,53	0.56	0	43,45,61	0.56	1 (2%)
6	UND	C	102	-	10,10,10	0.23	0	9,9,9	0.22	0
6	UND	I	407	-	7,7,10	0.21	0	6,6,9	0.25	0
6	UND	D	105	-	8,8,10	0.25	0	7,7,9	0.18	0
6	UND	I	412	-	10,10,10	0.22	0	9,9,9	0.23	0
6	UND	E	101	-	10,10,10	0.23	0	9,9,9	0.22	0
6	UND	I	411	-	10,10,10	0.22	0	9,9,9	0.25	0
6	UND	D	101	-	10,10,10	0.23	0	9,9,9	0.22	0
6	UND	M	105	-	10,10,10	0.22	0	9,9,9	0.26	0
6	UND	D	106	-	10,10,10	0.22	0	9,9,9	0.22	0
7	PC1	A	403	-	43,43,53	0.53	0	49,51,61	0.60	2 (4%)
7	PC1	D	102	-	30,30,53	0.62	0	36,38,61	0.61	1 (2%)
7	PC1	J	201	-	45,45,53	0.51	0	51,53,61	0.51	1 (1%)
7	PC1	M	102	-	26,26,53	0.68	0	32,34,61	0.62	1 (3%)
7	PC1	E	103	-	31,31,53	0.60	0	37,39,61	0.74	2 (5%)
6	UND	A	408	-	10,10,10	0.22	0	9,9,9	0.22	0
6	UND	L	103	-	10,10,10	0.22	0	9,9,9	0.20	0
7	PC1	A	404	-	29,29,53	0.66	0	35,37,61	0.64	1 (2%)
7	PC1	A	411	-	45,45,53	0.52	0	51,53,61	0.63	2 (3%)
6	UND	A	410	-	8,8,10	0.22	0	7,7,9	0.26	0
6	UND	A	406	-	10,10,10	0.21	0	9,9,9	0.26	0
7	PC1	B	203	-	31,31,53	0.65	1 (3%)	36,38,61	0.77	2 (5%)
7	PC1	I	405	-	45,45,53	0.51	0	51,53,61	0.54	1 (1%)
7	PC1	A	405	-	34,34,53	0.53	0	39,41,61	0.58	1 (2%)
6	UND	M	101	-	10,10,10	0.24	0	9,9,9	0.20	0
6	UND	M	104	-	10,10,10	0.22	0	9,9,9	0.27	0
7	PC1	I	403	-	51,51,53	0.49	0	57,59,61	0.52	1 (1%)
7	PC1	D	103	-	28,28,53	0.75	1 (3%)	33,35,61	0.74	2 (6%)
6	UND	L	102	-	8,8,10	0.24	0	7,7,9	0.21	0
6	UND	B	201	-	10,10,10	0.24	0	9,9,9	0.22	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
7	PC1	A	412	-	-	25/52/52/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UND	I	404	-	-	1/8/8/8	-
7	PC1	A	402	-	-	17/41/41/57	-
6	UND	E	102	-	-	0/8/8/8	-
7	PC1	A	409	-	-	8/24/24/57	-
7	PC1	I	406	-	-	15/46/46/57	-
7	PC1	I	401	-	-	17/36/36/57	-
6	UND	L	104	-	-	2/8/8/8	-
6	UND	I	413	-	-	2/8/8/8	-
6	UND	E	104	-	-	0/8/8/8	-
6	UND	A	401	-	-	3/8/8/8	-
6	UND	A	407	-	-	1/8/8/8	-
7	PC1	J	202	-	-	11/33/33/57	-
7	PC1	I	408	-	-	16/57/57/57	-
6	UND	C	101	-	-	0/7/7/8	-
7	PC1	D	104	-	-	15/47/47/57	-
7	PC1	L	101	-	-	14/42/42/57	-
7	PC1	B	202	-	-	19/30/30/57	-
6	UND	M	103	-	-	0/8/8/8	-
7	PC1	I	410	-	-	19/40/40/57	-
7	PC1	I	409	-	-	13/42/42/57	-
7	PC1	I	402	-	-	16/41/41/57	-
6	UND	C	102	-	-	2/8/8/8	-
6	UND	I	407	-	-	0/5/5/8	-
6	UND	D	105	-	-	0/6/6/8	-
6	UND	I	412	-	-	1/8/8/8	-
6	UND	E	101	-	-	2/8/8/8	-
6	UND	I	411	-	-	0/8/8/8	-
6	UND	D	101	-	-	0/8/8/8	-
6	UND	M	105	-	-	1/8/8/8	-
6	UND	D	106	-	-	1/8/8/8	-
7	PC1	A	403	-	-	21/47/47/57	-
7	PC1	D	102	-	-	13/34/34/57	-
7	PC1	J	201	-	-	13/49/49/57	-
7	PC1	M	102	-	-	12/29/29/57	-
7	PC1	E	103	-	-	15/34/34/57	-
6	UND	A	408	-	-	2/8/8/8	-
6	UND	L	103	-	-	1/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PC1	A	404	-	-	17/32/32/57	-
7	PC1	A	411	-	-	16/49/49/57	-
6	UND	A	410	-	-	0/6/6/8	-
6	UND	A	406	-	-	4/8/8/8	-
7	PC1	B	203	-	-	13/33/33/57	-
7	PC1	I	405	-	-	13/49/49/57	-
7	PC1	A	405	-	-	19/36/36/57	-
6	UND	M	101	-	-	2/8/8/8	-
6	UND	M	104	-	-	2/8/8/8	-
7	PC1	I	403	-	-	17/55/55/57	-
7	PC1	D	103	-	-	11/31/31/57	-
6	UND	L	102	-	-	0/6/6/8	-
6	UND	B	201	-	-	1/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	103	PC1	O21-C21	-2.44	1.33	1.42
7	B	203	PC1	O21-C2	-2.00	1.43	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	202	PC1	C2-O21-C21	2.92	124.97	117.79
7	I	410	PC1	C2-O21-C21	2.81	124.70	117.79
7	L	101	PC1	C2-O21-C21	2.79	124.65	117.79
7	B	203	PC1	O21-C2-C1	2.75	112.50	106.13
7	B	202	PC1	C2-O21-C21	2.72	124.48	117.79
7	E	103	PC1	C2-O21-C21	2.68	124.38	117.79
7	I	409	PC1	C2-O21-C21	2.68	124.38	117.79
7	A	411	PC1	C2-O21-C21	2.58	124.15	117.79
7	A	402	PC1	C2-O21-C21	2.50	123.94	117.79
7	I	405	PC1	O12-P-O14	2.50	124.60	112.24
7	D	103	PC1	C21-O21-C2	2.49	119.95	113.87
7	A	412	PC1	O12-P-O14	2.43	124.24	112.24
7	M	102	PC1	O12-P-O14	2.41	124.13	112.24
7	A	403	PC1	O12-P-O14	2.40	124.11	112.24
7	A	405	PC1	O12-P-O14	2.38	124.02	112.24
7	A	402	PC1	O12-P-O14	2.38	124.00	112.24
7	A	404	PC1	O12-P-O14	2.35	123.85	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	401	PC1	O12-P-O14	2.35	123.85	112.24
7	B	202	PC1	O12-P-O14	2.34	123.82	112.24
7	I	402	PC1	O12-P-O14	2.34	123.80	112.24
7	E	103	PC1	O12-P-O14	2.34	123.79	112.24
7	D	102	PC1	O12-P-O14	2.33	123.78	112.24
7	I	408	PC1	O12-P-O14	2.32	123.69	112.24
7	A	403	PC1	C2-O21-C21	2.31	123.49	117.79
7	I	409	PC1	O12-P-O14	2.31	123.68	112.24
7	D	104	PC1	O12-P-O14	2.31	123.67	112.24
7	I	410	PC1	O12-P-O14	2.31	123.67	112.24
7	J	201	PC1	O12-P-O14	2.31	123.64	112.24
7	I	406	PC1	O12-P-O14	2.29	123.54	112.24
7	B	203	PC1	O12-P-O14	2.29	123.54	112.24
7	A	409	PC1	O12-P-O14	2.28	123.52	112.24
7	L	101	PC1	O12-P-O14	2.28	123.51	112.24
7	I	403	PC1	O12-P-O14	2.28	123.49	112.24
7	D	103	PC1	O12-P-O14	2.27	123.46	112.24
7	J	202	PC1	O12-P-O14	2.26	123.41	112.24
7	A	411	PC1	O12-P-O14	2.18	123.02	112.24

There are no chirality outliers.

All (413) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	403	PC1	C11-O13-P-O12
7	A	403	PC1	C11-O13-P-O14
7	A	403	PC1	C11-O13-P-O11
7	A	403	PC1	C1-O11-P-O14
7	A	403	PC1	O22-C21-O21-C2
7	A	403	PC1	C22-C21-O21-C2
7	A	404	PC1	C11-O13-P-O12
7	A	404	PC1	C11-O13-P-O14
7	A	404	PC1	C1-O11-P-O14
7	A	404	PC1	O22-C21-O21-C2
7	A	404	PC1	C22-C21-O21-C2
7	A	405	PC1	C11-O13-P-O12
7	A	405	PC1	C1-O11-P-O12
7	A	405	PC1	C1-O11-P-O13
7	A	405	PC1	O13-C11-C12-N
7	A	409	PC1	C11-O13-P-O14
7	A	409	PC1	C11-O13-P-O11
7	A	409	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
7	A	412	PC1	C11-O13-P-O14
7	A	412	PC1	C22-C21-O21-C2
7	B	202	PC1	C11-O13-P-O14
7	B	203	PC1	C11-O13-P-O12
7	B	203	PC1	C11-O13-P-O14
7	B	203	PC1	O11-C1-C2-O21
7	B	203	PC1	O11-C1-C2-C3
7	B	203	PC1	O22-C21-O21-C2
7	D	102	PC1	C11-O13-P-O12
7	D	102	PC1	C11-O13-P-O14
7	D	102	PC1	O13-C11-C12-N
7	D	102	PC1	O22-C21-O21-C2
7	D	103	PC1	C11-O13-P-O12
7	D	103	PC1	C3-C2-O21-C21
7	D	104	PC1	C11-O13-P-O12
7	D	104	PC1	C11-O13-P-O11
7	D	104	PC1	C1-O11-P-O12
7	D	104	PC1	O13-C11-C12-N
7	E	103	PC1	O13-C11-C12-N
7	I	401	PC1	C11-O13-P-O14
7	I	402	PC1	C11-O13-P-O14
7	I	402	PC1	C11-O13-P-O11
7	I	402	PC1	O22-C21-O21-C2
7	I	402	PC1	C22-C21-O21-C2
7	I	403	PC1	C11-O13-P-O12
7	I	405	PC1	C1-O11-P-O13
7	I	405	PC1	O13-C11-C12-N
7	I	406	PC1	C11-O13-P-O12
7	I	408	PC1	C11-O13-P-O14
7	I	408	PC1	C22-C21-O21-C2
7	I	409	PC1	C11-O13-P-O12
7	I	409	PC1	O13-C11-C12-N
7	I	410	PC1	C1-O11-P-O12
7	I	410	PC1	C1-O11-P-O13
7	I	410	PC1	O21-C2-C3-O31
7	I	410	PC1	C22-C21-O21-C2
7	J	201	PC1	O13-C11-C12-N
7	J	202	PC1	C11-O13-P-O12
7	J	202	PC1	C11-O13-P-O14
7	J	202	PC1	C11-O13-P-O11
7	J	202	PC1	O13-C11-C12-N
7	L	101	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
7	L	101	PC1	C1-O11-P-O12
7	L	101	PC1	O13-C11-C12-N
7	M	102	PC1	C22-C21-O21-C2
7	M	102	PC1	O22-C21-O21-C2
7	A	403	PC1	O32-C31-O31-C3
7	A	411	PC1	O32-C31-O31-C3
7	A	403	PC1	C32-C31-O31-C3
7	A	411	PC1	C32-C31-O31-C3
7	A	402	PC1	O32-C31-O31-C3
7	A	412	PC1	O32-C31-O31-C3
7	M	102	PC1	O32-C31-O31-C3
7	I	408	PC1	O22-C21-O21-C2
7	A	412	PC1	C32-C31-O31-C3
7	M	102	PC1	C32-C31-O31-C3
7	B	202	PC1	C32-C31-O31-C3
7	B	203	PC1	C22-C21-O21-C2
7	D	102	PC1	C22-C21-O21-C2
7	I	410	PC1	O32-C31-O31-C3
7	A	402	PC1	C32-C31-O31-C3
7	A	405	PC1	C32-C31-O31-C3
7	D	102	PC1	C32-C31-O31-C3
7	A	412	PC1	O22-C21-O21-C2
7	I	410	PC1	O22-C21-O21-C2
7	E	103	PC1	O32-C31-O31-C3
7	J	202	PC1	O32-C31-O31-C3
7	E	103	PC1	C32-C31-O31-C3
7	J	202	PC1	C32-C31-O31-C3
7	D	102	PC1	O32-C31-O31-C3
7	B	202	PC1	C22-C21-O21-C2
7	I	410	PC1	C32-C31-O31-C3
7	L	101	PC1	C2-C1-O11-P
7	A	405	PC1	O32-C31-O31-C3
7	A	402	PC1	C22-C21-O21-C2
7	A	411	PC1	C22-C21-O21-C2
7	B	202	PC1	O22-C21-O21-C2
7	B	203	PC1	C3-C2-O21-C21
7	E	103	PC1	O11-C1-C2-O21
7	B	202	PC1	O32-C31-O31-C3
7	A	412	PC1	C21-C22-C23-C24
7	A	402	PC1	C31-C32-C33-C34
7	A	402	PC1	O22-C21-O21-C2
7	A	411	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
7	I	408	PC1	C31-C32-C33-C34
7	I	409	PC1	C22-C21-O21-C2
7	J	201	PC1	C21-C22-C23-C24
7	B	203	PC1	C1-C2-O21-C21
7	E	103	PC1	C22-C21-O21-C2
7	A	402	PC1	C1-O11-P-O13
7	A	404	PC1	C11-O13-P-O11
7	A	405	PC1	C11-O13-P-O11
7	B	202	PC1	C11-O13-P-O11
7	B	203	PC1	C11-O13-P-O11
7	D	102	PC1	C11-O13-P-O11
7	D	104	PC1	C1-O11-P-O13
7	E	103	PC1	C11-O13-P-O11
7	I	401	PC1	C11-O13-P-O11
7	I	403	PC1	C11-O13-P-O11
7	I	406	PC1	C11-O13-P-O11
7	I	409	PC1	C11-O13-P-O11
7	J	201	PC1	C11-O13-P-O11
7	L	101	PC1	C1-O11-P-O13
7	M	102	PC1	C11-O13-P-O11
7	E	103	PC1	O22-C21-O21-C2
7	I	409	PC1	O22-C21-O21-C2
7	A	404	PC1	C11-C12-N-C13
7	B	202	PC1	C11-C12-N-C13
7	A	404	PC1	C31-C32-C33-C34
7	I	408	PC1	C36-C37-C38-C39
7	I	410	PC1	C1-C2-O21-C21
7	I	403	PC1	C21-C22-C23-C24
6	A	408	UND	C4-C5-C6-C7
7	A	412	PC1	C3D-C3E-C3F-C3G
7	B	203	PC1	C26-C27-C28-C29
7	I	409	PC1	C22-C23-C24-C25
6	D	106	UND	C4-C5-C6-C7
7	J	201	PC1	C23-C24-C25-C26
6	A	406	UND	C6-C7-C8-C9
7	L	101	PC1	C2C-C2D-C2E-C2F
7	A	403	PC1	C24-C25-C26-C27
7	I	410	PC1	C26-C27-C28-C29
7	L	101	PC1	O22-C21-O21-C2
7	L	101	PC1	C22-C21-O21-C2
7	A	412	PC1	C39-C3A-C3B-C3C
7	D	103	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
7	D	103	PC1	C37-C38-C39-C3A
7	A	404	PC1	C11-C12-N-C15
7	B	202	PC1	C11-C12-N-C15
7	I	401	PC1	C27-C28-C29-C2A
7	I	408	PC1	C23-C24-C25-C26
7	D	104	PC1	C21-C22-C23-C24
7	A	403	PC1	C33-C34-C35-C36
7	A	405	PC1	C39-C3A-C3B-C3C
6	M	101	UND	C5-C6-C7-C8
7	A	403	PC1	C2C-C2D-C2E-C2F
7	A	412	PC1	C27-C28-C29-C2A
7	A	412	PC1	C29-C2A-C2B-C2C
7	B	203	PC1	C29-C2A-C2B-C2C
7	I	405	PC1	C22-C21-O21-C2
6	I	412	UND	C5-C6-C7-C8
7	D	104	PC1	C26-C27-C28-C29
7	I	402	PC1	C31-C32-C33-C34
7	A	409	PC1	C25-C26-C27-C28
7	L	101	PC1	C29-C2A-C2B-C2C
7	A	404	PC1	C11-C12-N-C14
7	B	202	PC1	C11-C12-N-C14
7	I	401	PC1	C24-C25-C26-C27
7	J	201	PC1	C32-C31-O31-C3
7	D	104	PC1	C22-C21-O21-C2
6	A	406	UND	C3-C4-C5-C6
7	A	402	PC1	C25-C26-C27-C28
6	M	104	UND	C6-C7-C8-C9
6	M	105	UND	C3-C4-C5-C6
7	E	103	PC1	C26-C27-C28-C29
7	J	202	PC1	O22-C21-O21-C2
7	A	404	PC1	C32-C31-O31-C3
7	A	411	PC1	C38-C39-C3A-C3B
7	I	401	PC1	C26-C27-C28-C29
7	J	202	PC1	C22-C21-O21-C2
6	E	101	UND	C4-C5-C6-C7
7	A	412	PC1	C26-C27-C28-C29
7	A	403	PC1	C2A-C2B-C2C-C2D
7	D	104	PC1	O22-C21-O21-C2
7	I	405	PC1	O22-C21-O21-C2
7	I	403	PC1	C31-C32-C33-C34
7	I	402	PC1	O21-C2-C3-O31
7	J	201	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
7	I	402	PC1	C21-C22-C23-C24
7	I	410	PC1	C2B-C2C-C2D-C2E
7	I	410	PC1	C27-C28-C29-C2A
7	A	412	PC1	C23-C24-C25-C26
7	I	403	PC1	C2B-C2C-C2D-C2E
7	I	401	PC1	C1-O11-P-O13
7	E	103	PC1	O11-C1-C2-C3
7	A	409	PC1	C24-C25-C26-C27
7	I	405	PC1	C33-C34-C35-C36
6	I	413	UND	C5-C6-C7-C8
7	I	403	PC1	C1-C2-C3-O31
7	I	410	PC1	C1-C2-C3-O31
7	A	412	PC1	C24-C25-C26-C27
7	A	412	PC1	C33-C34-C35-C36
7	A	404	PC1	O32-C31-O31-C3
7	I	401	PC1	C32-C31-O31-C3
7	I	401	PC1	O11-C1-C2-O21
7	I	403	PC1	C34-C35-C36-C37
7	I	408	PC1	O21-C2-C3-O31
6	L	104	UND	C6-C7-C8-C9
7	A	405	PC1	C3A-C3B-C3C-C3D
7	A	411	PC1	C32-C33-C34-C35
7	I	410	PC1	C29-C2A-C2B-C2C
7	A	404	PC1	C33-C34-C35-C36
7	A	405	PC1	C33-C34-C35-C36
7	A	404	PC1	O11-C1-C2-C3
7	A	411	PC1	O11-C1-C2-C3
7	I	402	PC1	O11-C1-C2-C3
7	I	410	PC1	O11-C1-C2-C3
7	A	409	PC1	C21-C22-C23-C24
7	E	103	PC1	C21-C22-C23-C24
7	I	402	PC1	C37-C38-C39-C3A
7	I	403	PC1	C39-C3A-C3B-C3C
7	I	403	PC1	C32-C31-O31-C3
7	I	403	PC1	C2-C1-O11-P
7	A	405	PC1	C38-C39-C3A-C3B
7	I	402	PC1	C1-C2-C3-O31
7	I	408	PC1	C1-C2-C3-O31
7	M	102	PC1	C1-C2-C3-O31
7	I	401	PC1	O32-C31-O31-C3
7	I	408	PC1	C3B-C3C-C3D-C3E
7	I	410	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
7	B	202	PC1	C23-C24-C25-C26
7	I	410	PC1	C25-C26-C27-C28
7	M	102	PC1	O21-C2-C3-O31
7	I	401	PC1	C23-C24-C25-C26
7	A	403	PC1	C2B-C2C-C2D-C2E
7	A	411	PC1	C2-C1-O11-P
7	I	402	PC1	C2-C1-O11-P
7	A	412	PC1	C28-C29-C2A-C2B
7	D	103	PC1	C38-C39-C3A-C3B
7	D	103	PC1	C1-C2-O21-C21
7	B	202	PC1	O11-C1-C2-C3
7	M	102	PC1	C32-C33-C34-C35
6	B	201	UND	C6-C7-C8-C9
7	J	201	PC1	C28-C29-C2A-C2B
7	A	411	PC1	C3-C2-O21-C21
7	J	202	PC1	C3-C2-O21-C21
7	L	101	PC1	C3-C2-O21-C21
7	I	406	PC1	C35-C36-C37-C38
7	A	405	PC1	C2-C1-O11-P
7	D	104	PC1	C2-C1-O11-P
7	L	101	PC1	C1-C2-C3-O31
7	M	102	PC1	C2-C3-O31-C31
7	A	404	PC1	O11-C1-C2-O21
7	A	411	PC1	O11-C1-C2-O21
7	A	402	PC1	O21-C2-C3-O31
7	I	405	PC1	O21-C2-C3-O31
7	I	403	PC1	O32-C31-O31-C3
7	D	104	PC1	C33-C34-C35-C36
7	A	411	PC1	C36-C37-C38-C39
7	A	403	PC1	C1-O11-P-O13
7	A	412	PC1	C11-O13-P-O11
7	B	202	PC1	C1-O11-P-O13
7	D	103	PC1	C11-O13-P-O11
7	D	103	PC1	C1-O11-P-O13
7	I	403	PC1	C1-O11-P-O13
7	A	403	PC1	C2-C1-O11-P
7	B	202	PC1	C2-C1-O11-P
7	I	405	PC1	C2-C1-O11-P
7	B	202	PC1	C22-C23-C24-C25
7	I	405	PC1	C23-C24-C25-C26
7	A	402	PC1	C1-O11-P-O14
7	A	405	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
7	A	409	PC1	C1-O11-P-O14
7	B	202	PC1	C11-O13-P-O12
7	D	104	PC1	C1-O11-P-O14
7	E	103	PC1	C11-O13-P-O14
7	I	401	PC1	C11-O13-P-O12
7	I	401	PC1	C1-O11-P-O14
7	I	403	PC1	C11-O13-P-O14
7	I	405	PC1	C1-O11-P-O12
7	J	201	PC1	C11-O13-P-O14
7	M	102	PC1	C11-O13-P-O14
7	D	103	PC1	C12-C11-O13-P
7	I	409	PC1	C12-C11-O13-P
7	M	102	PC1	C12-C11-O13-P
7	M	102	PC1	C31-C32-C33-C34
7	I	410	PC1	C22-C23-C24-C25
7	E	103	PC1	C24-C25-C26-C27
7	A	402	PC1	C21-C22-C23-C24
7	A	403	PC1	C31-C32-C33-C34
7	A	405	PC1	C35-C36-C37-C38
7	A	402	PC1	O11-C1-C2-O21
7	B	202	PC1	O11-C1-C2-O21
7	I	402	PC1	O11-C1-C2-O21
7	I	405	PC1	C21-C22-C23-C24
7	I	410	PC1	O11-C1-C2-O21
7	A	412	PC1	C3E-C3F-C3G-C3H
7	I	408	PC1	C2D-C2E-C2F-C2G
7	J	201	PC1	C22-C21-O21-C2
7	A	402	PC1	C22-C23-C24-C25
7	A	402	PC1	O13-C11-C12-N
7	A	403	PC1	O13-C11-C12-N
7	A	403	PC1	C27-C28-C29-C2A
7	A	409	PC1	O13-C11-C12-N
7	A	411	PC1	O13-C11-C12-N
7	A	412	PC1	O13-C11-C12-N
7	D	103	PC1	O13-C11-C12-N
7	I	401	PC1	O13-C11-C12-N
7	I	402	PC1	O13-C11-C12-N
7	I	403	PC1	O13-C11-C12-N
7	I	405	PC1	C1-C2-C3-O31
7	I	406	PC1	C1-C2-C3-O31
7	I	408	PC1	O13-C11-C12-N
7	A	411	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
7	I	403	PC1	O21-C2-C3-O31
6	C	102	UND	C6-C7-C8-C9
7	A	403	PC1	C35-C36-C37-C38
7	B	203	PC1	C25-C26-C27-C28
7	D	104	PC1	C32-C33-C34-C35
7	L	101	PC1	C28-C29-C2A-C2B
6	L	104	UND	C7-C8-C9-C10
6	A	406	UND	C4-C5-C6-C7
7	A	402	PC1	C3-C2-O21-C21
7	A	403	PC1	C3-C2-O21-C21
7	B	202	PC1	C3-C2-O21-C21
7	D	102	PC1	C1-C2-O21-C21
7	E	103	PC1	C3-C2-O21-C21
7	I	409	PC1	C3-C2-O21-C21
7	J	201	PC1	O22-C21-O21-C2
7	A	412	PC1	C32-C33-C34-C35
6	A	408	UND	C7-C8-C9-C10
7	I	408	PC1	C22-C23-C24-C25
7	I	403	PC1	C35-C36-C37-C38
7	I	402	PC1	C1-O11-P-O13
7	I	406	PC1	C1-O11-P-O13
7	L	101	PC1	C11-O13-P-O11
6	I	404	UND	C4-C5-C6-C7
7	E	103	PC1	C23-C24-C25-C26
6	A	401	UND	C2-C3-C4-C5
6	A	406	UND	C11-C10-C9-C8
7	I	408	PC1	C32-C33-C34-C35
7	I	409	PC1	C32-C31-O31-C3
7	I	409	PC1	O11-C1-C2-O21
7	L	101	PC1	C2B-C2C-C2D-C2E
7	I	409	PC1	O32-C31-O31-C3
7	A	404	PC1	C2-C1-O11-P
7	I	409	PC1	C36-C37-C38-C39
7	A	412	PC1	C3A-C3B-C3C-C3D
7	I	405	PC1	C25-C26-C27-C28
7	I	409	PC1	C38-C39-C3A-C3B
6	I	413	UND	C3-C4-C5-C6
7	I	401	PC1	C25-C26-C27-C28
7	D	102	PC1	C3-C2-O21-C21
7	A	412	PC1	C1-O11-P-O13
6	M	104	UND	C11-C10-C9-C8
7	I	401	PC1	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	J	202	PC1	C22-C23-C24-C25
7	I	406	PC1	C32-C31-O31-C3
7	A	405	PC1	O21-C2-C3-O31
7	J	201	PC1	C2A-C2B-C2C-C2D
7	A	404	PC1	C37-C38-C39-C3A
7	A	405	PC1	C3F-C3G-C3H-C3I
7	I	401	PC1	O31-C31-C32-C33
7	I	408	PC1	C2C-C2D-C2E-C2F
7	I	406	PC1	O22-C21-O21-C2
7	E	103	PC1	C29-C2A-C2B-C2C
7	I	406	PC1	O32-C31-O31-C3
7	A	405	PC1	C32-C33-C34-C35
7	I	408	PC1	C2A-C2B-C2C-C2D
7	A	402	PC1	O11-C1-C2-C3
7	B	203	PC1	C2B-C2C-C2D-C2E
7	A	402	PC1	C35-C36-C37-C38
7	A	402	PC1	C27-C28-C29-C2A
7	I	405	PC1	C11-O13-P-O11
6	L	103	UND	C1-C2-C3-C4
7	J	202	PC1	C23-C24-C25-C26
7	A	405	PC1	O31-C31-C32-C33
7	D	102	PC1	O31-C31-C32-C33
7	D	104	PC1	C22-C23-C24-C25
7	I	406	PC1	C23-C24-C25-C26
7	A	412	PC1	C2A-C2B-C2C-C2D
7	I	402	PC1	C27-C28-C29-C2A
6	A	401	UND	C6-C7-C8-C9
6	E	101	UND	C2-C3-C4-C5
7	I	401	PC1	C21-C22-C23-C24
6	A	401	UND	C1-C2-C3-C4
7	I	408	PC1	C26-C27-C28-C29
7	I	406	PC1	C22-C21-O21-C2
7	A	405	PC1	O32-C31-C32-C33
7	A	412	PC1	C38-C39-C3A-C3B
6	C	102	UND	C3-C4-C5-C6
7	A	412	PC1	C3B-C3C-C3D-C3E
7	I	406	PC1	C25-C26-C27-C28
7	A	411	PC1	C37-C38-C39-C3A
7	I	406	PC1	C34-C35-C36-C37
7	D	102	PC1	O32-C31-C32-C33
7	A	411	PC1	C1-C2-C3-O31
7	A	411	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
7	I	410	PC1	C2-C1-O11-P
7	B	202	PC1	C24-C25-C26-C27
7	A	412	PC1	C1-O11-P-O14
7	D	103	PC1	C11-O13-P-O14
7	I	402	PC1	C1-O11-P-O14
7	I	406	PC1	C1-O11-P-O14
7	D	102	PC1	C12-C11-O13-P
7	I	403	PC1	C12-C11-O13-P
6	A	407	UND	C3-C4-C5-C6
7	A	403	PC1	C23-C24-C25-C26
7	I	406	PC1	O21-C21-C22-C23
7	B	202	PC1	O21-C21-C22-C23
7	J	201	PC1	O21-C21-C22-C23
7	J	201	PC1	O22-C21-C22-C23
7	D	104	PC1	O31-C31-C32-C33
7	I	406	PC1	O22-C21-C22-C23
6	M	101	UND	C2-C3-C4-C5

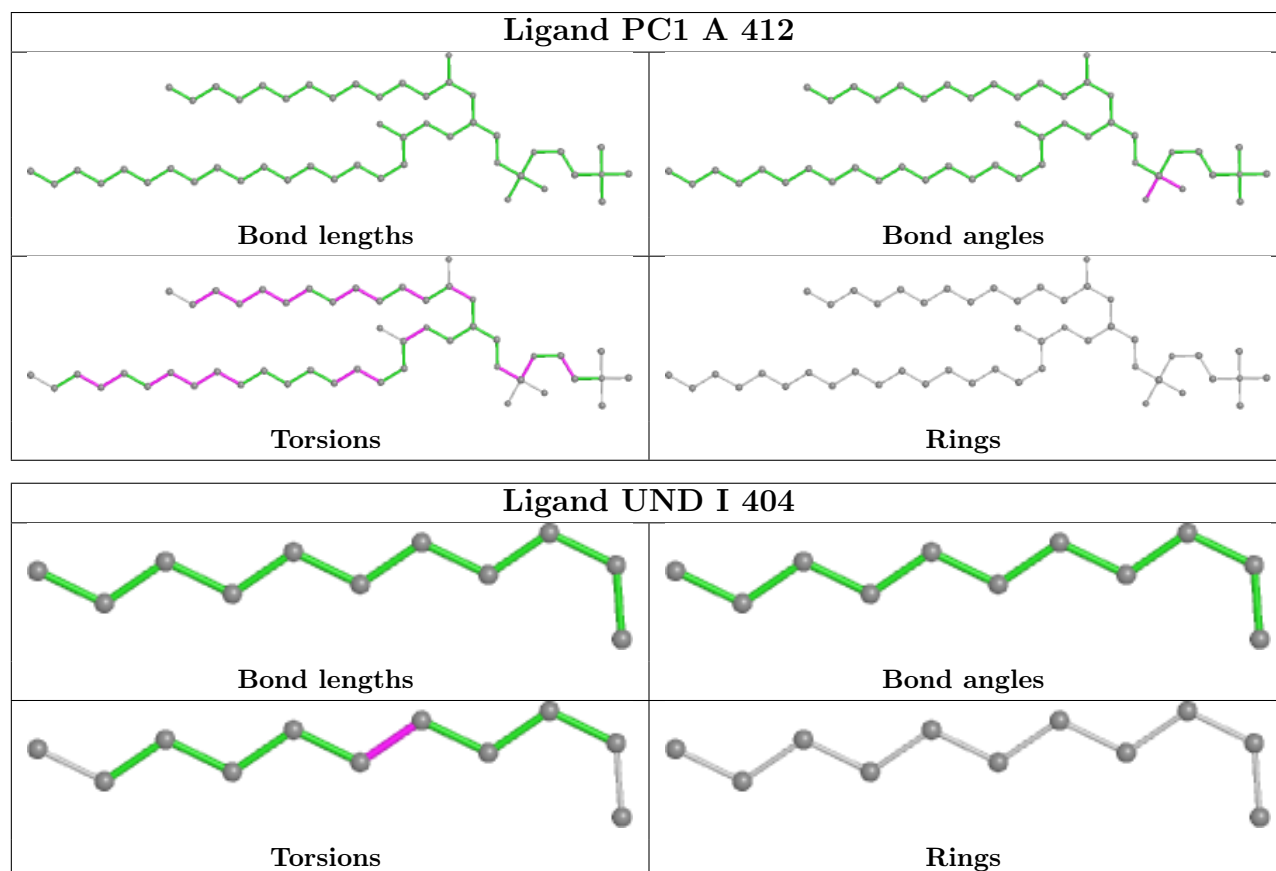
There are no ring outliers.

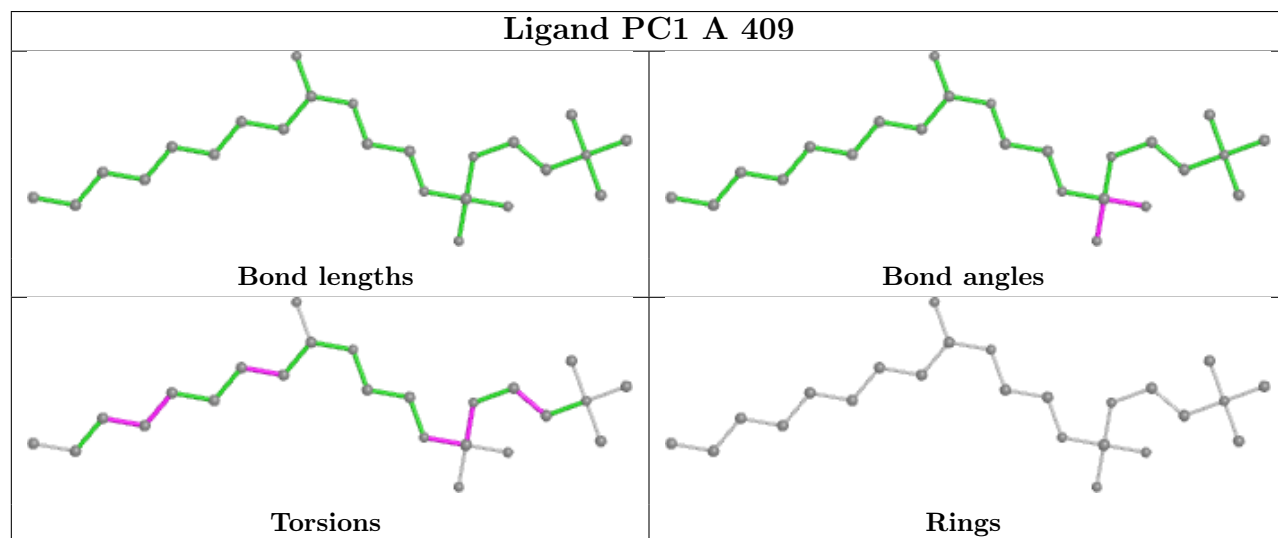
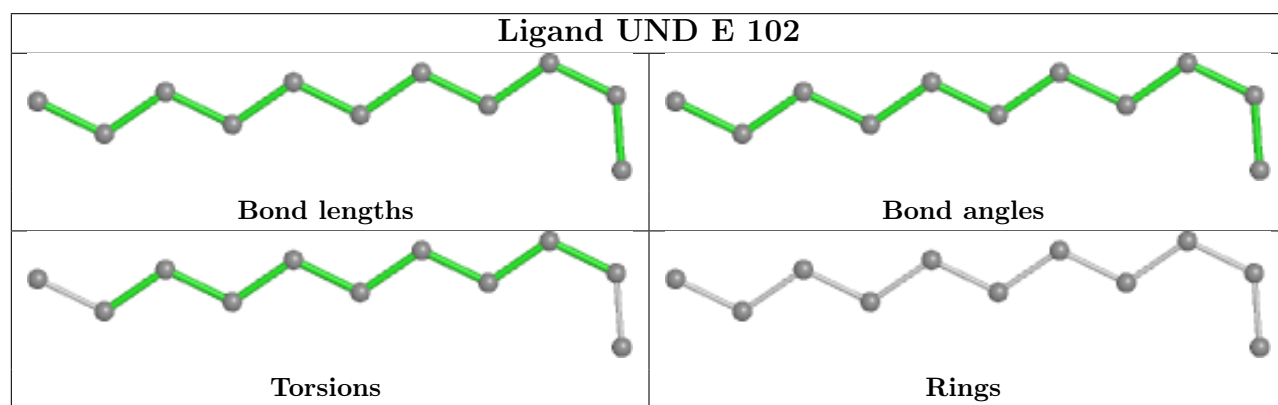
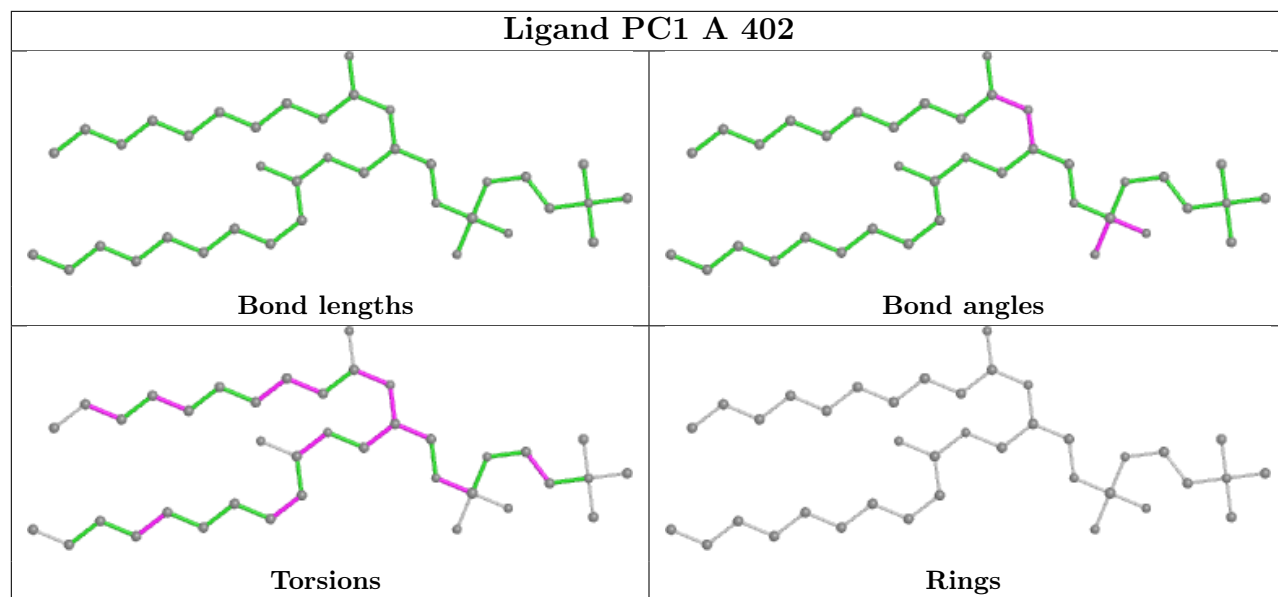
16 monomers are involved in 16 short contacts:

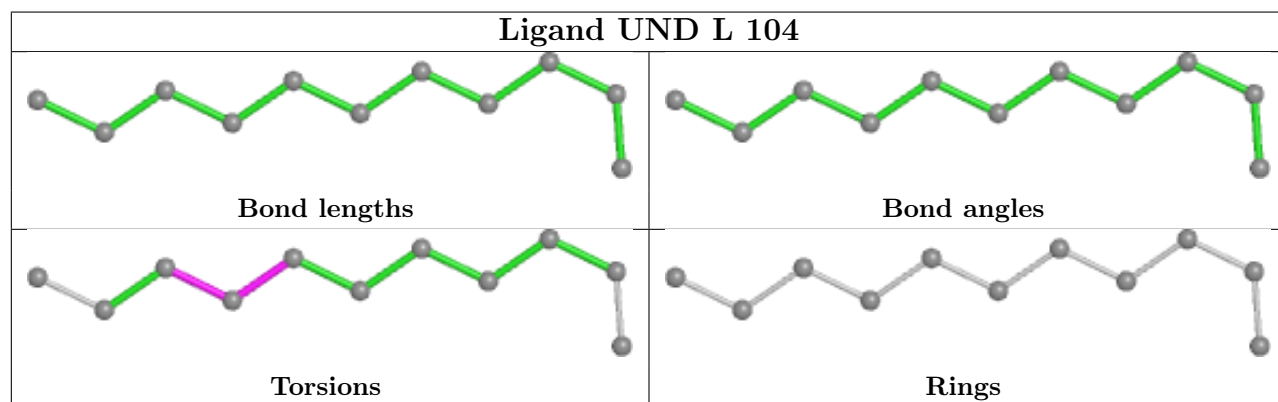
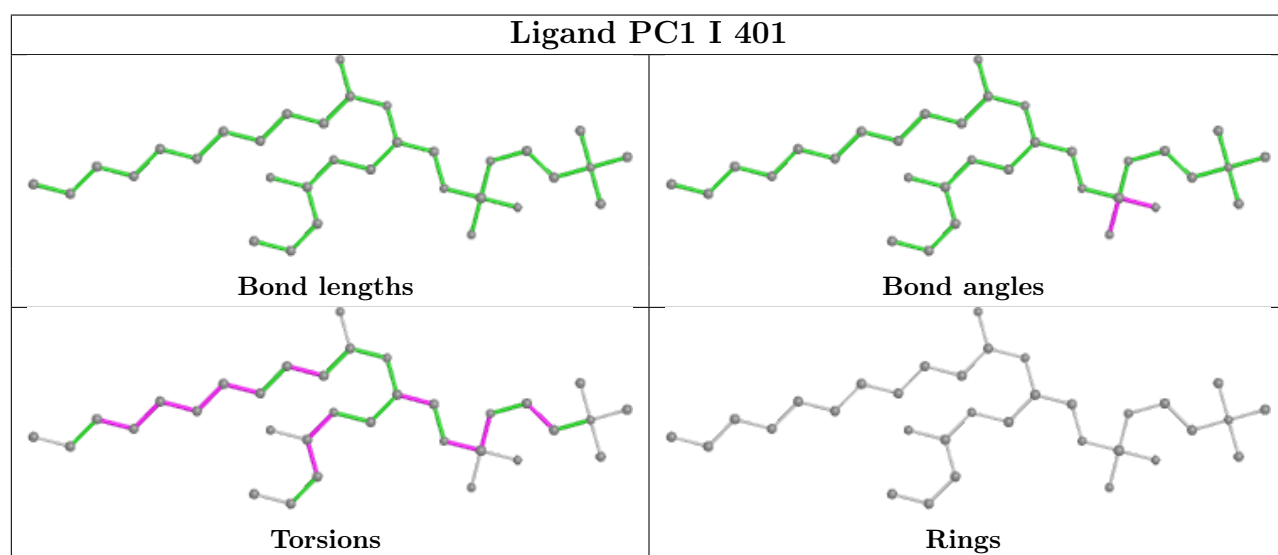
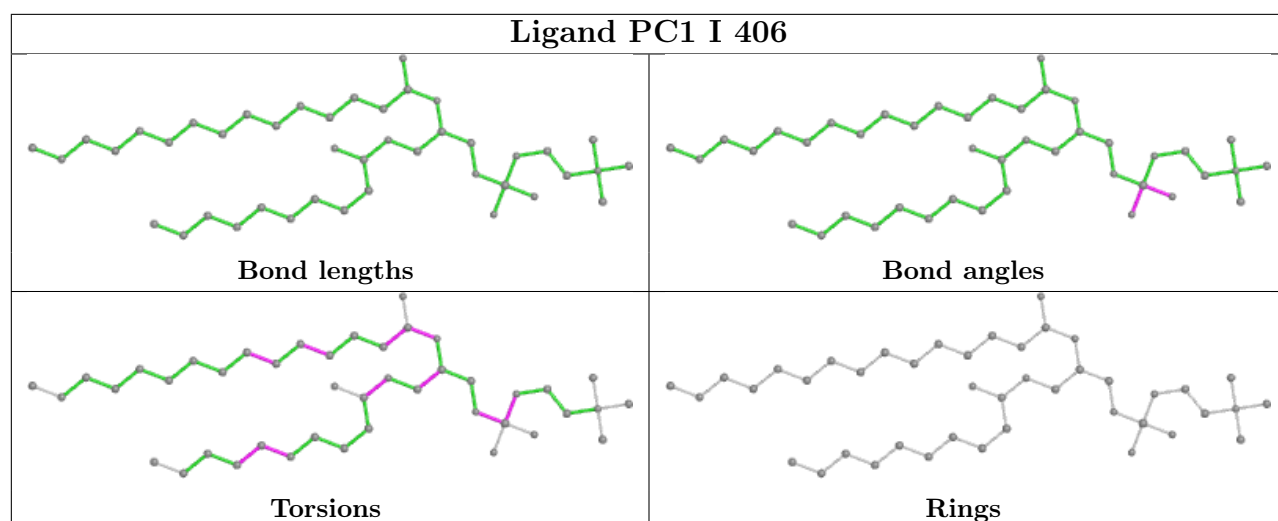
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	406	PC1	1	0
7	I	401	PC1	1	0
6	A	401	UND	1	0
7	I	408	PC1	1	0
7	D	104	PC1	2	0
7	I	410	PC1	3	0
7	I	409	PC1	1	0
6	C	102	UND	1	0
6	E	101	UND	1	0
6	D	106	UND	1	0
7	A	403	PC1	1	0
7	E	103	PC1	1	0
6	A	406	UND	1	0
7	A	405	PC1	1	0
7	I	403	PC1	1	0
6	B	201	UND	1	0

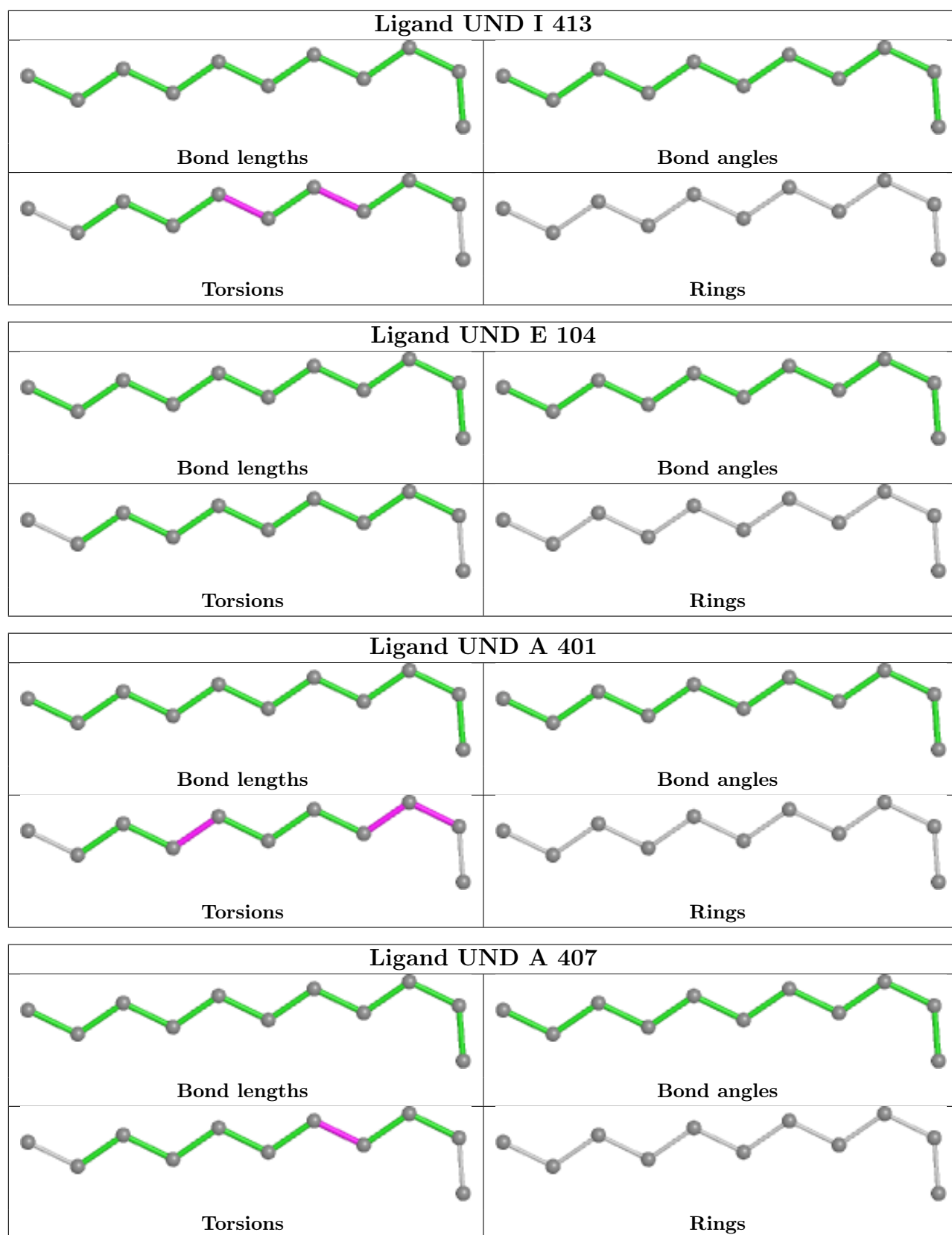
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

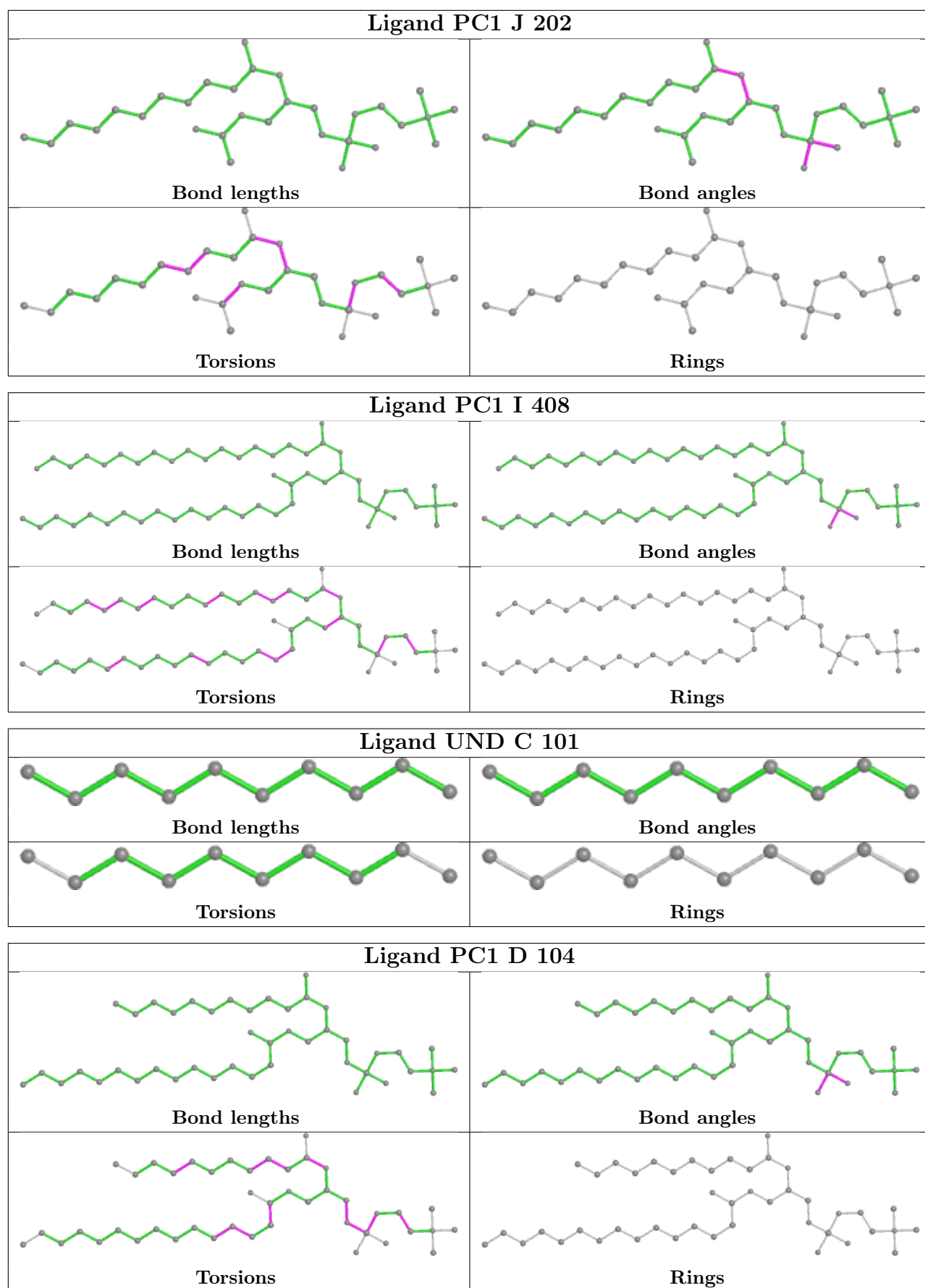
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

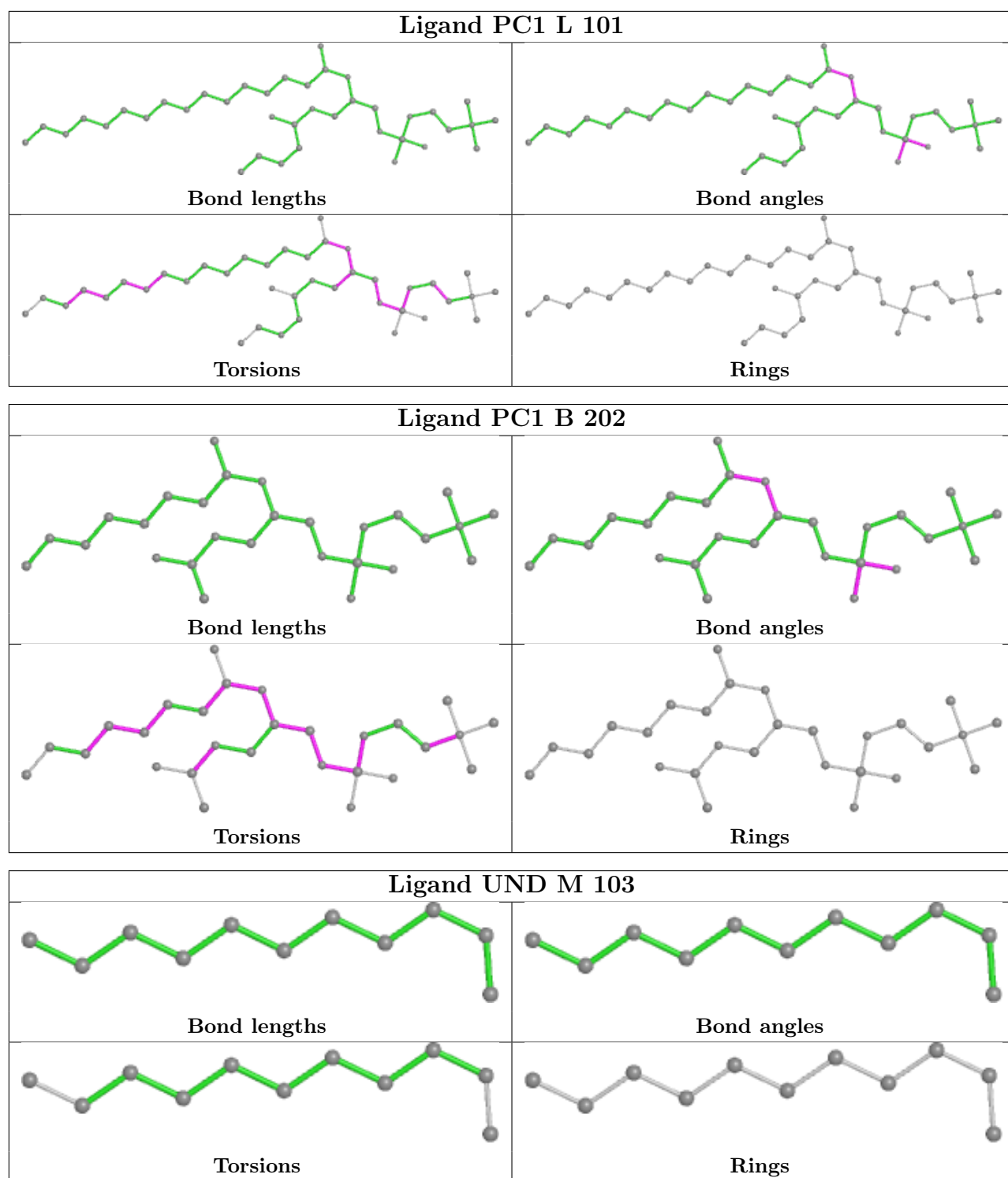


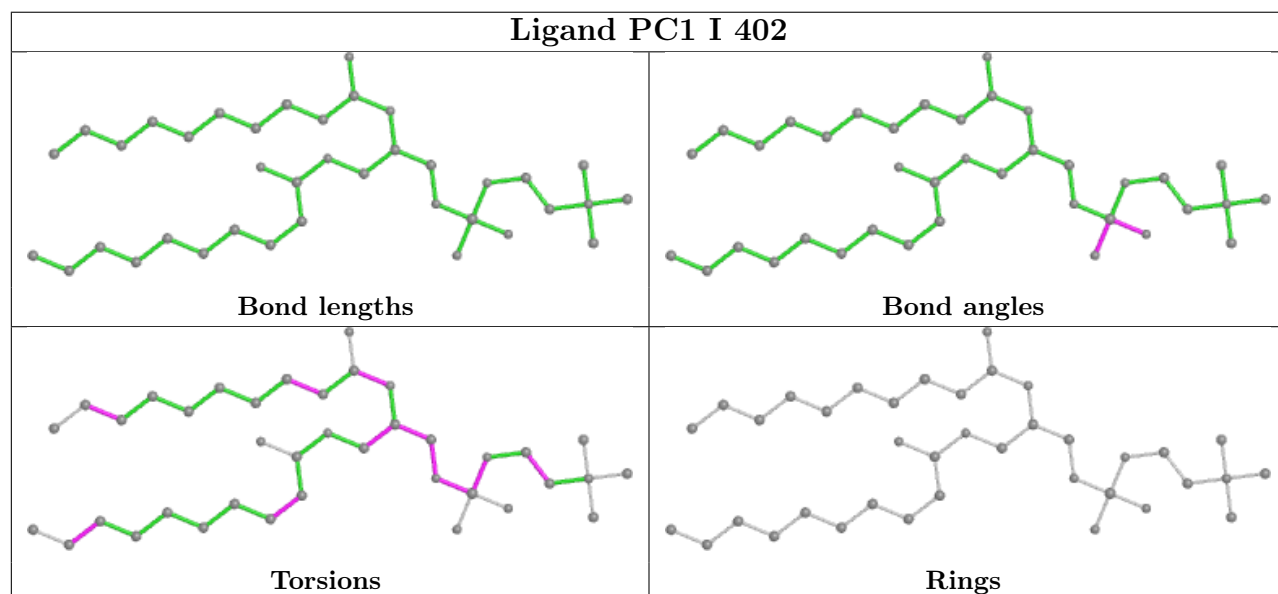
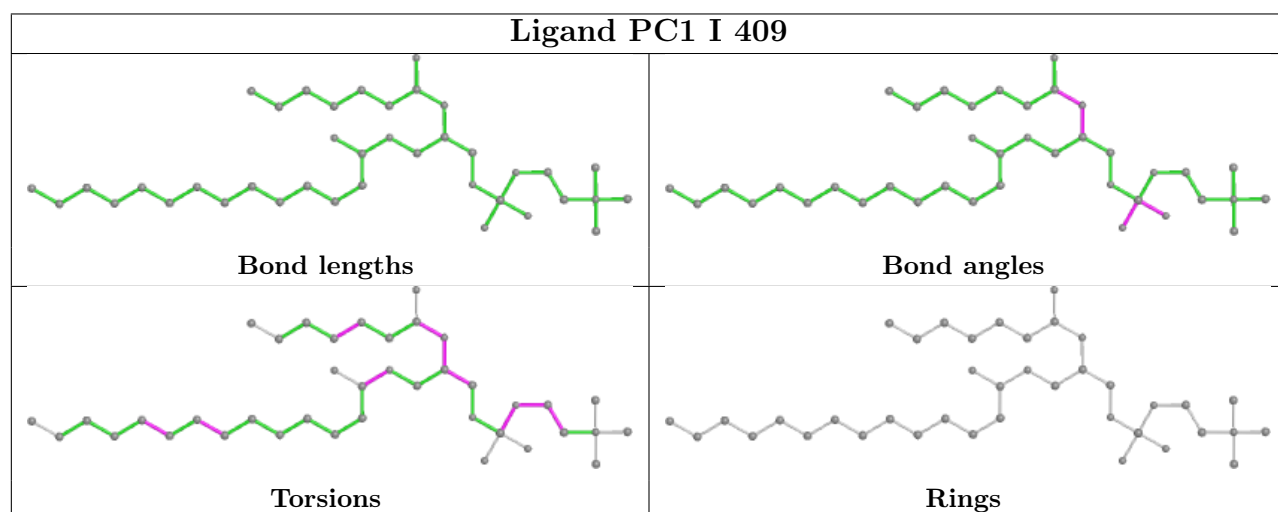
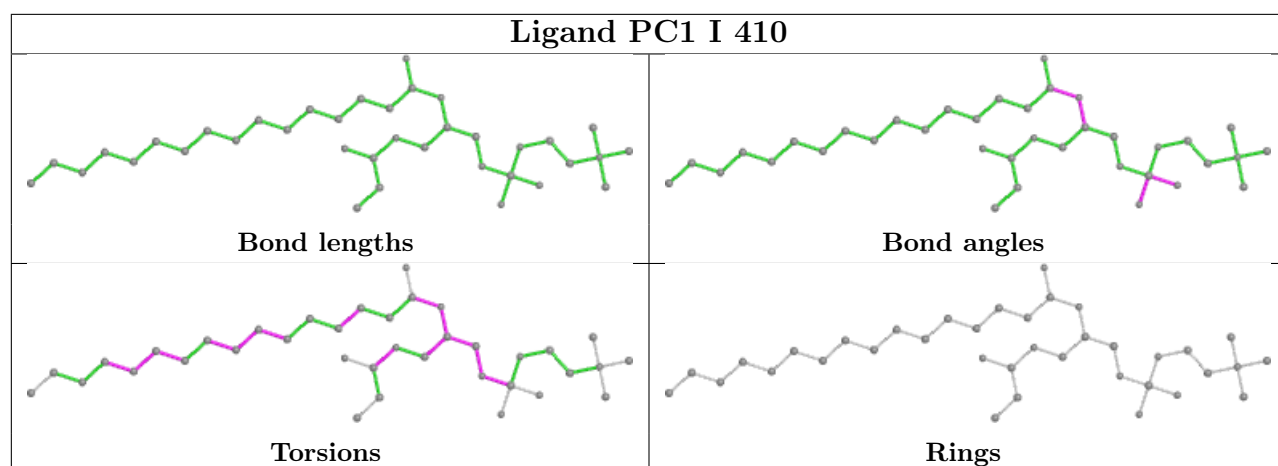


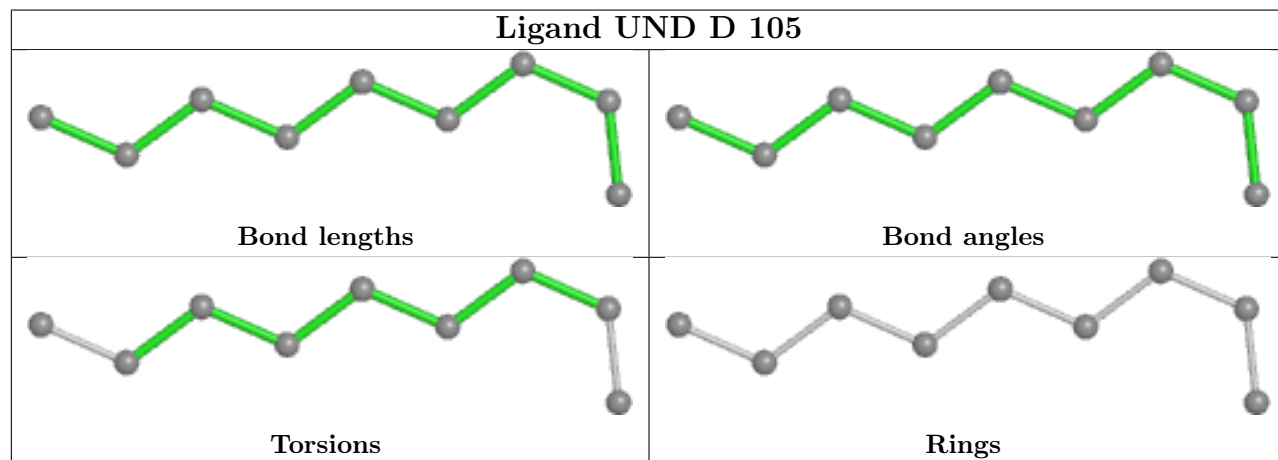
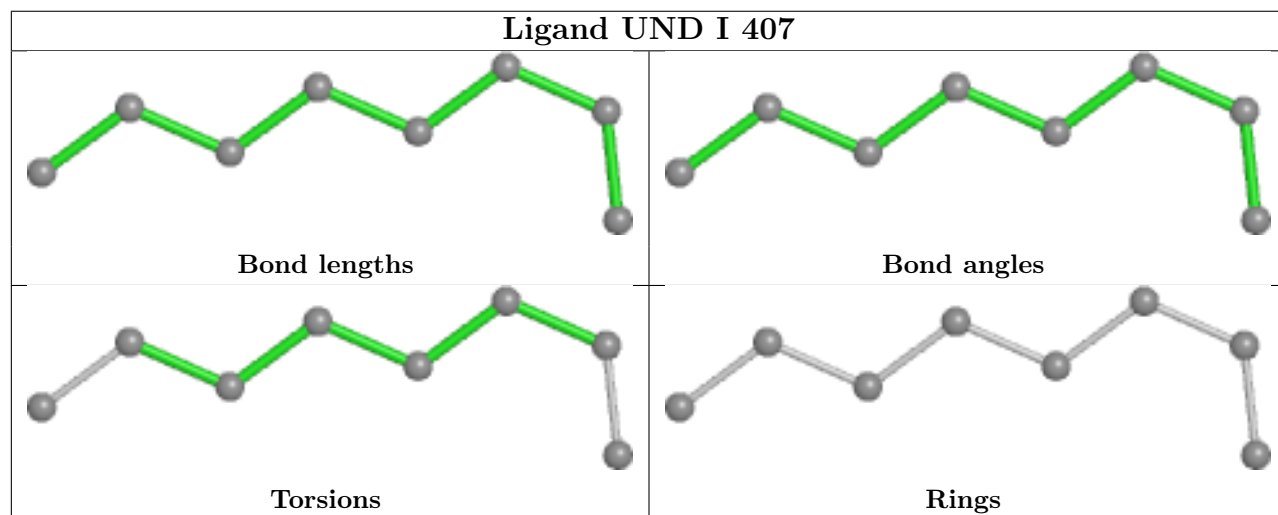
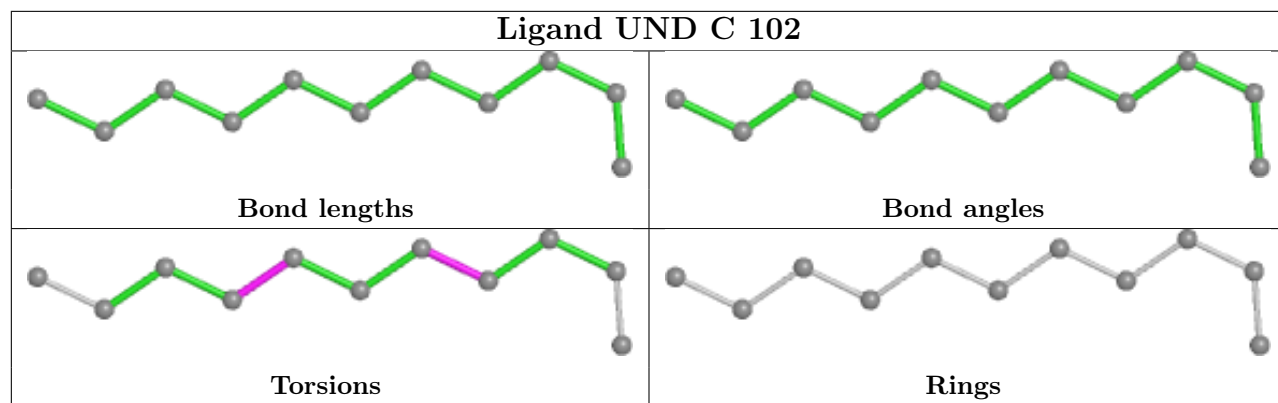


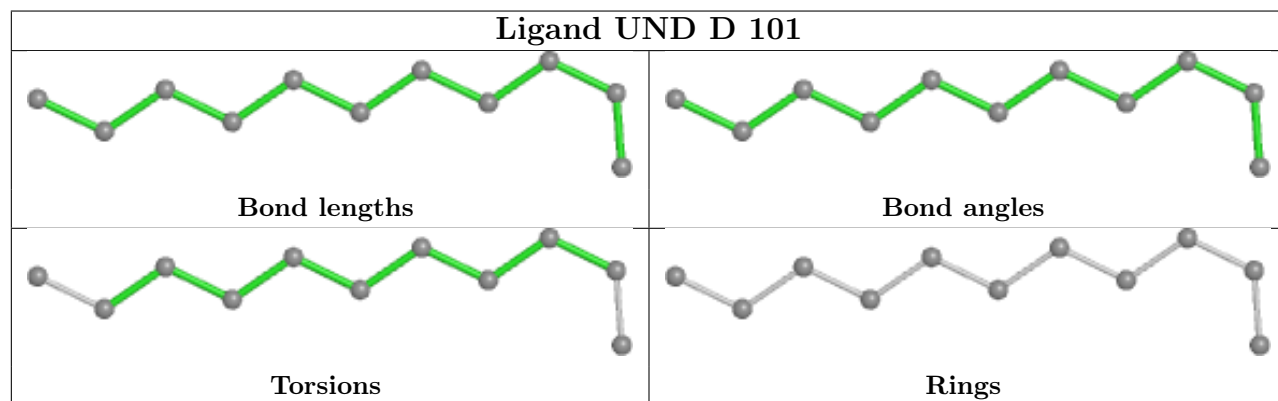
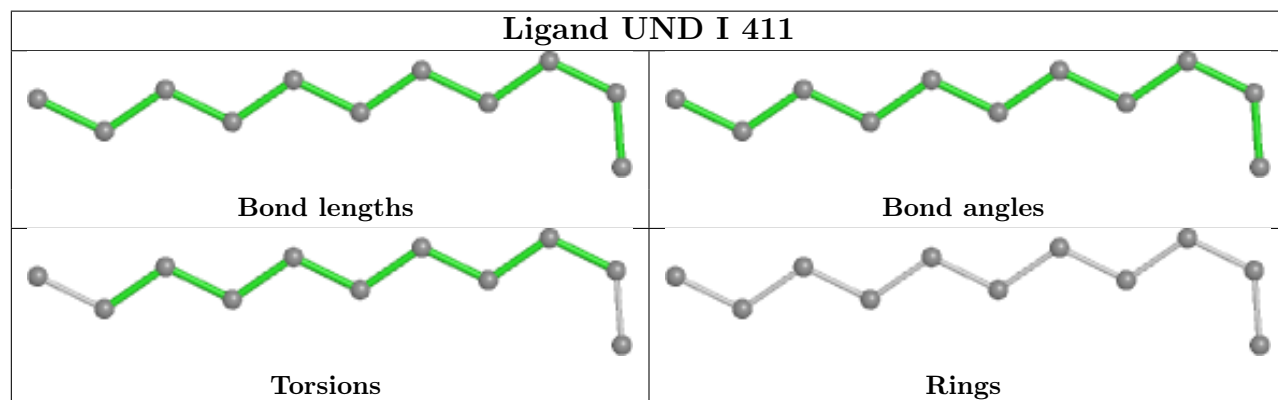
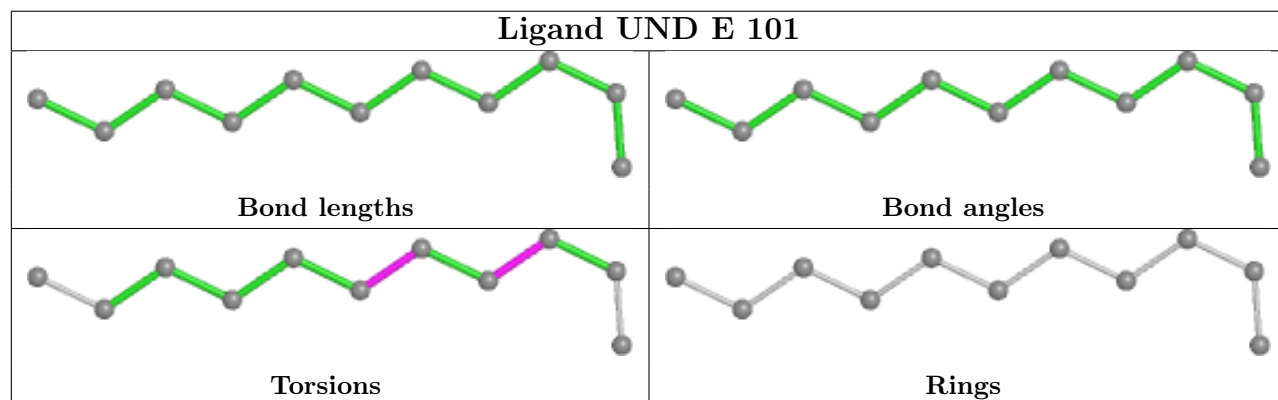
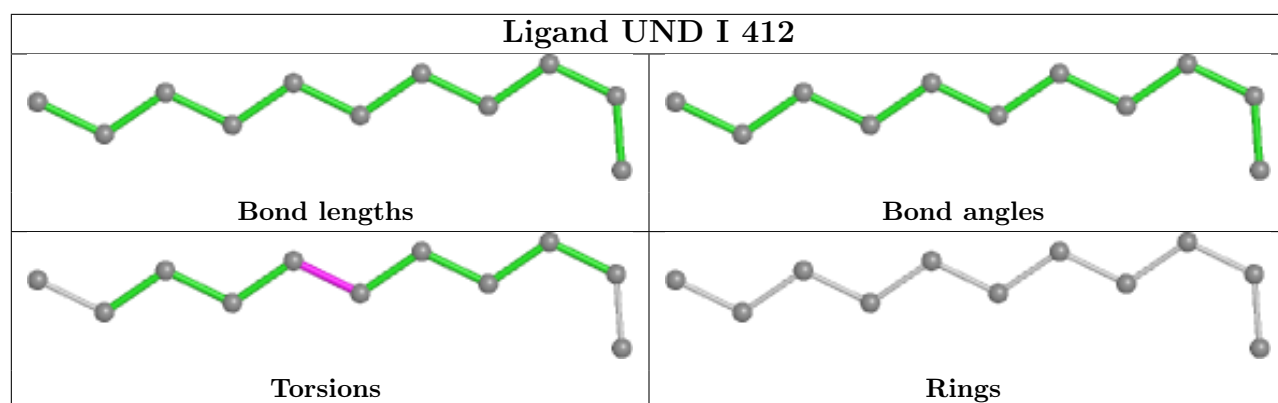


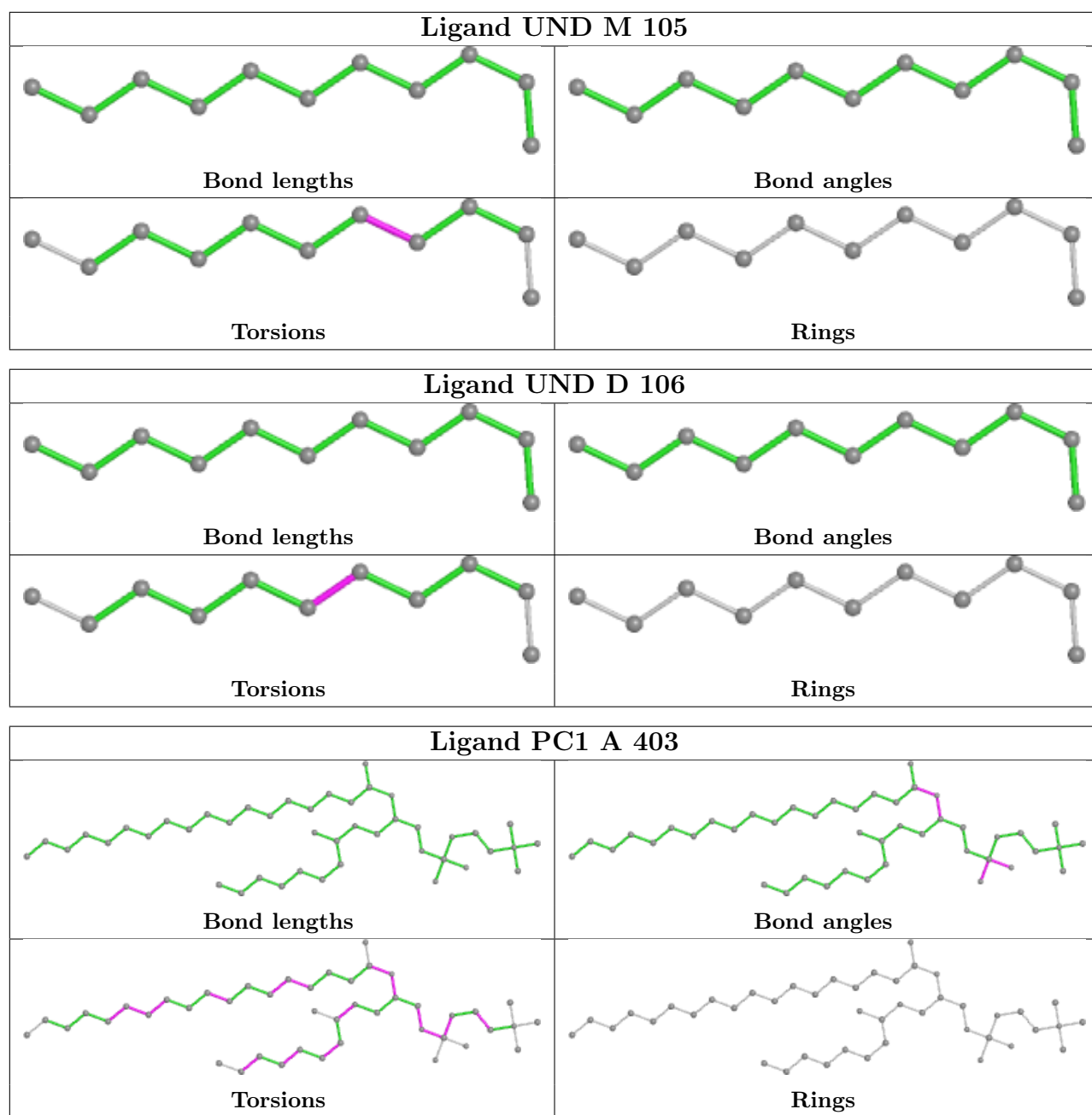


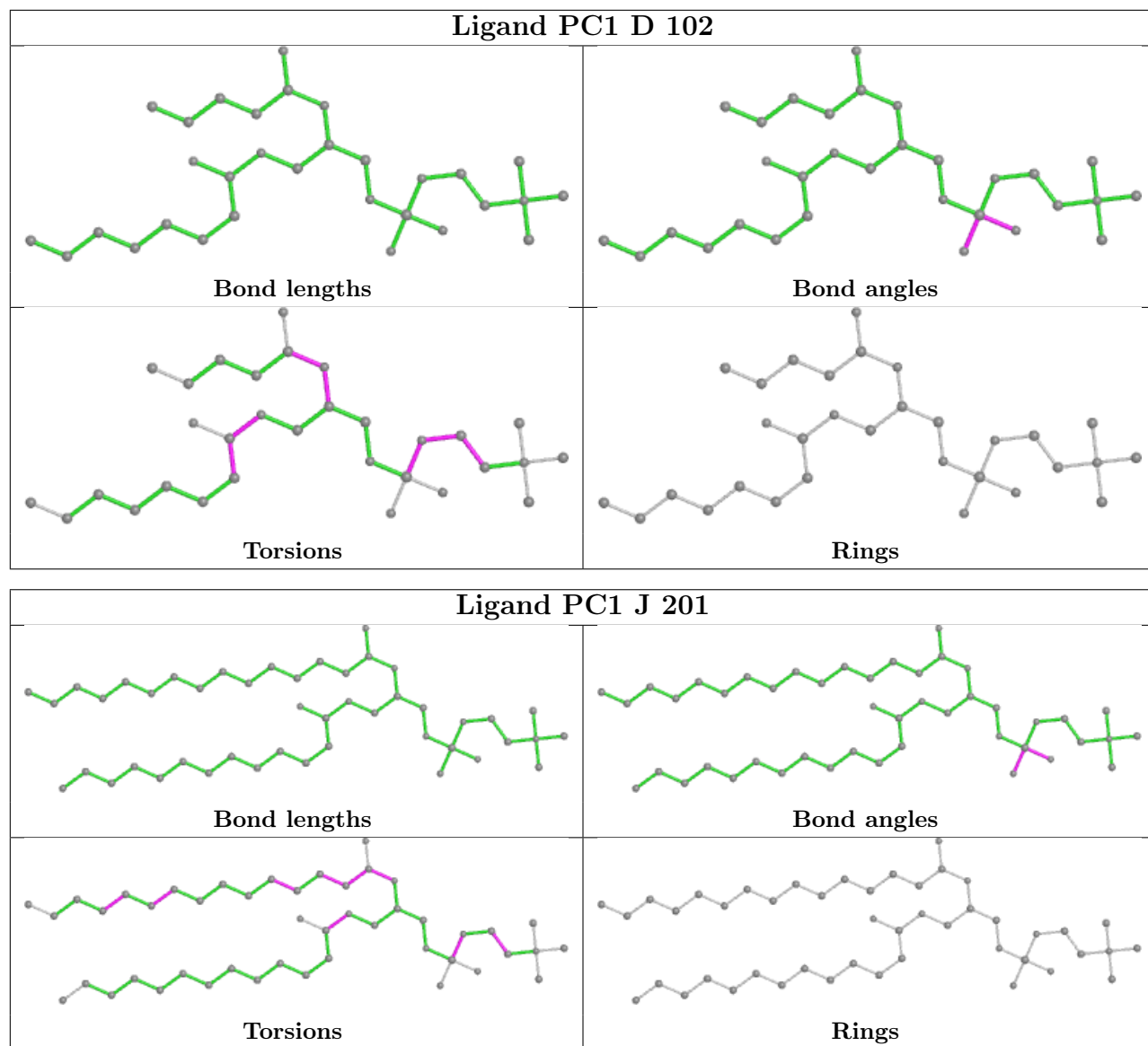


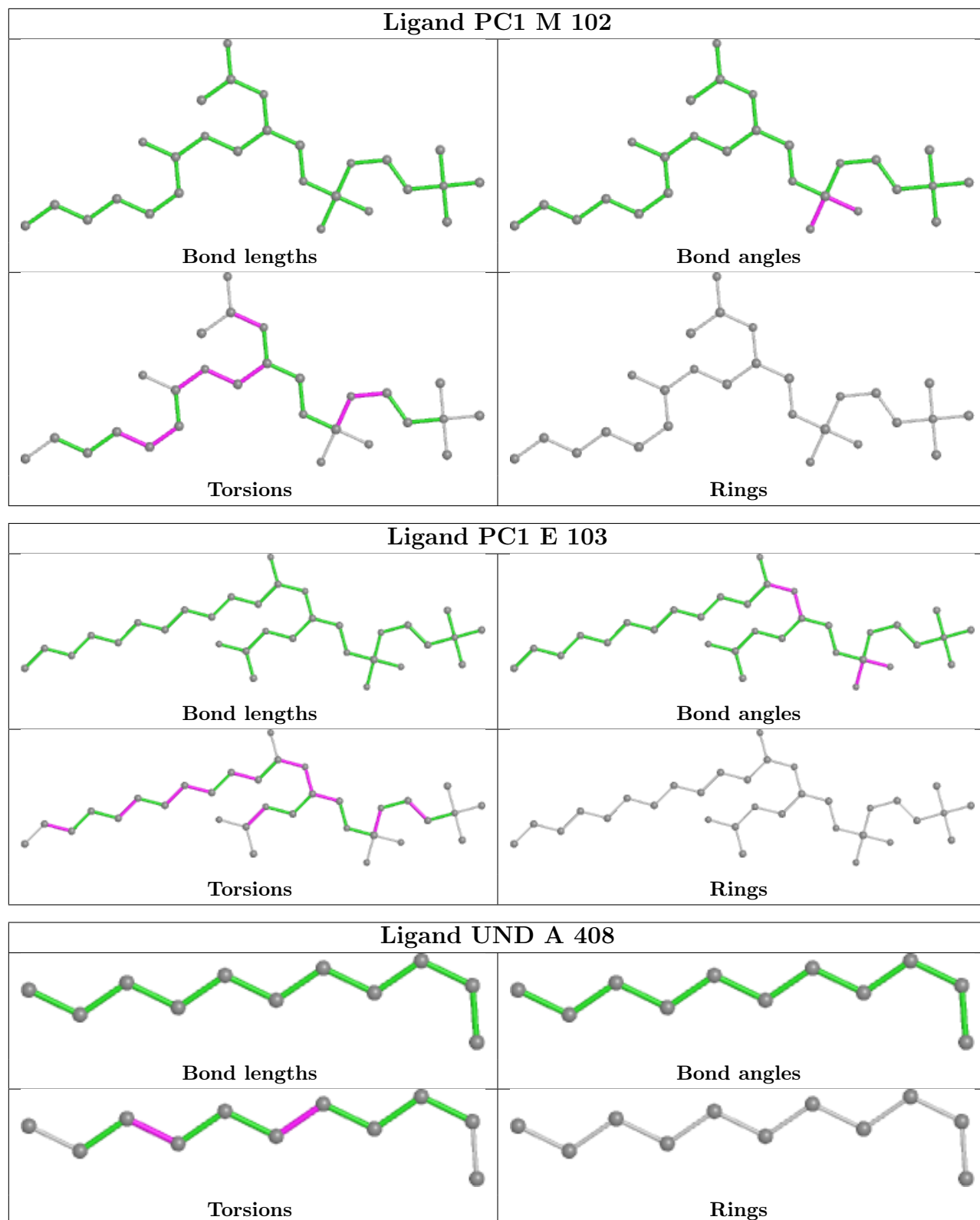


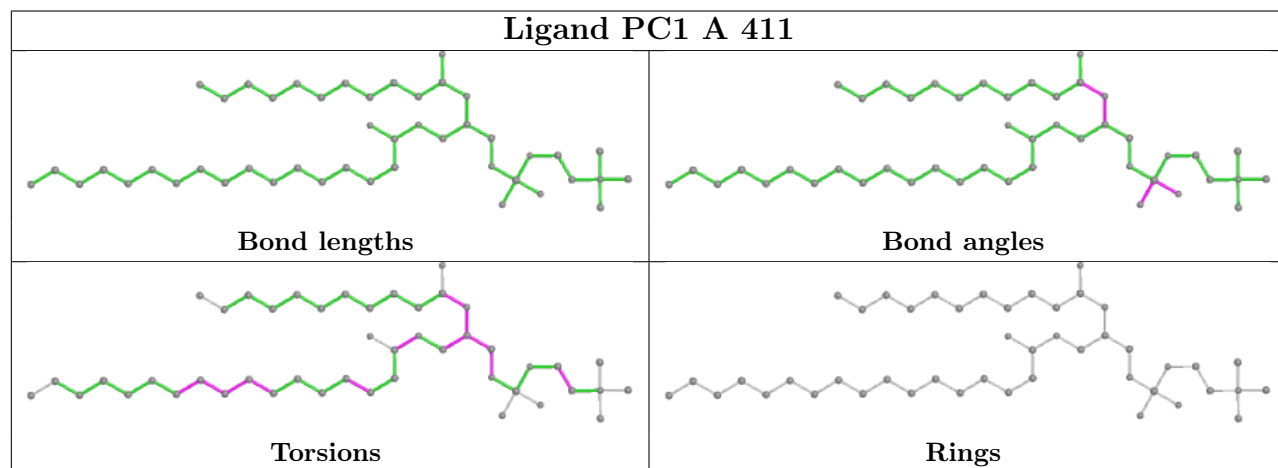
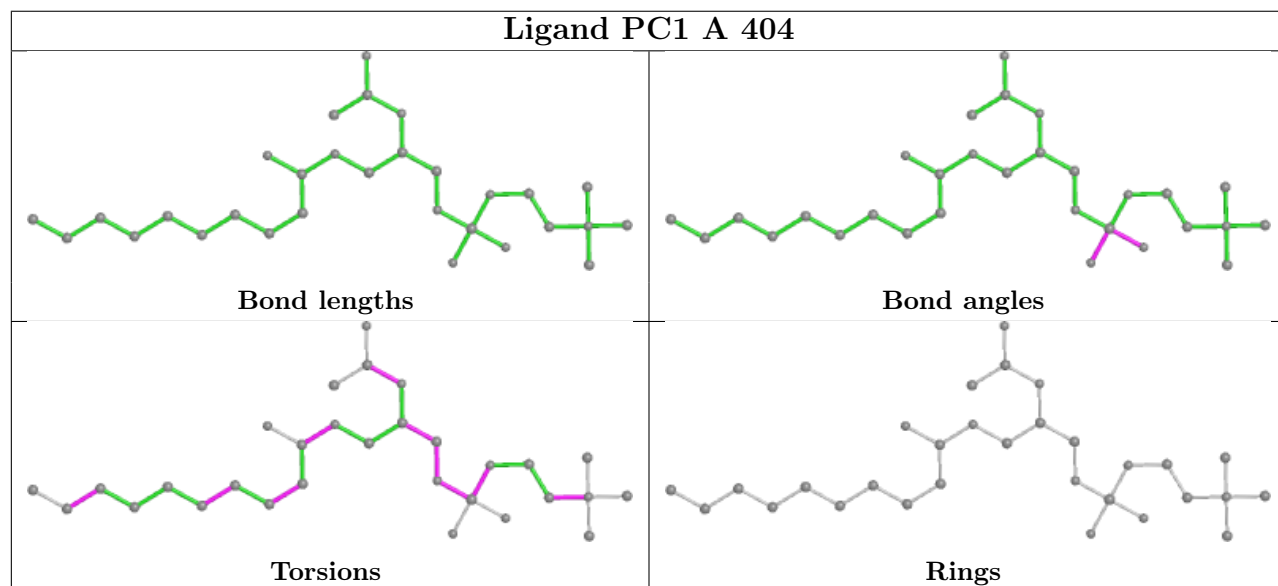
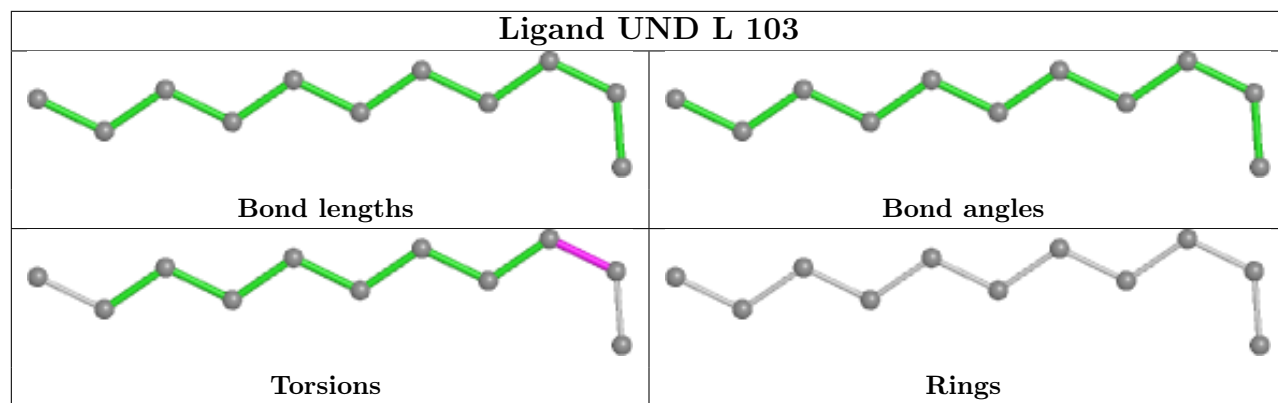


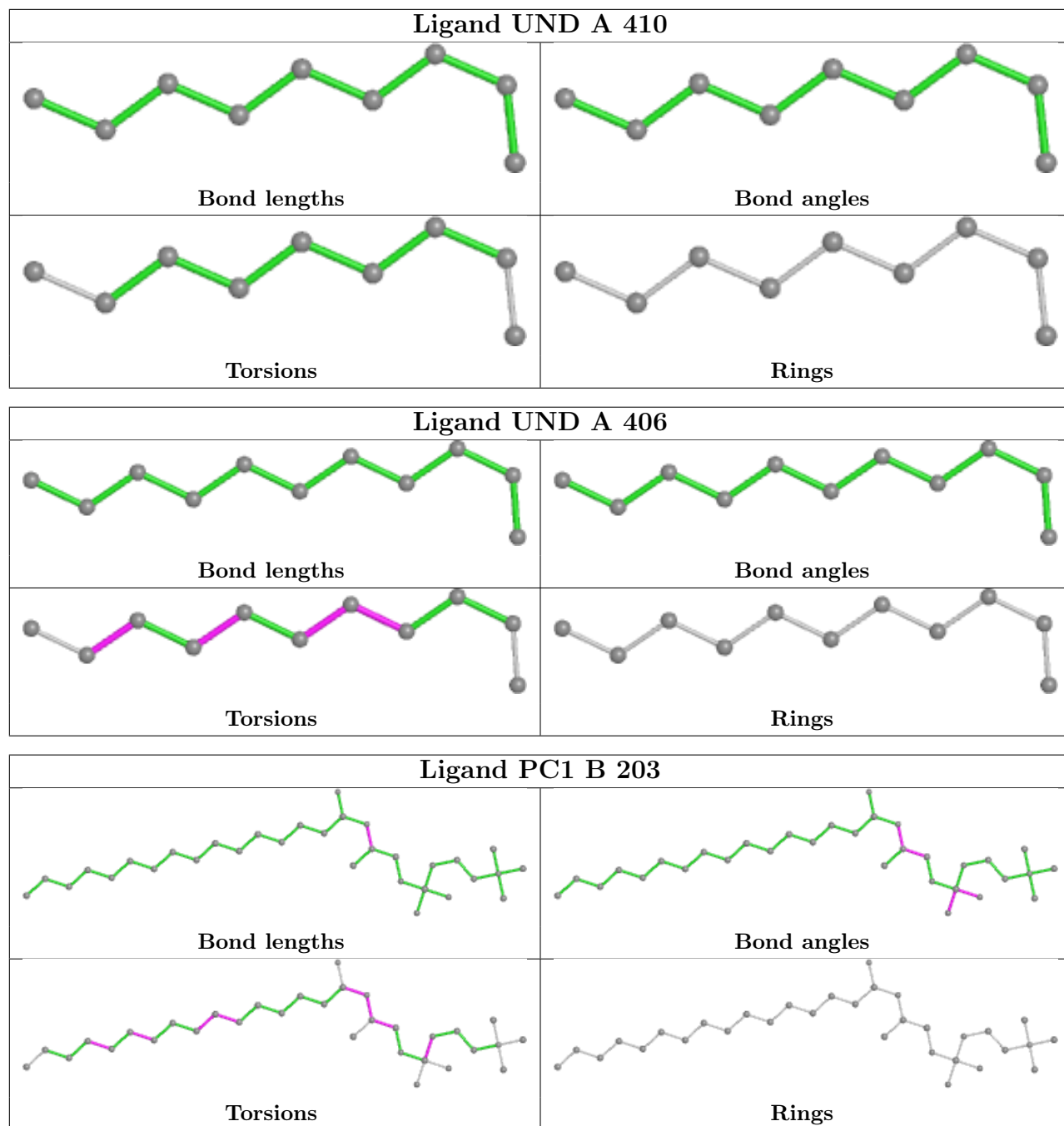


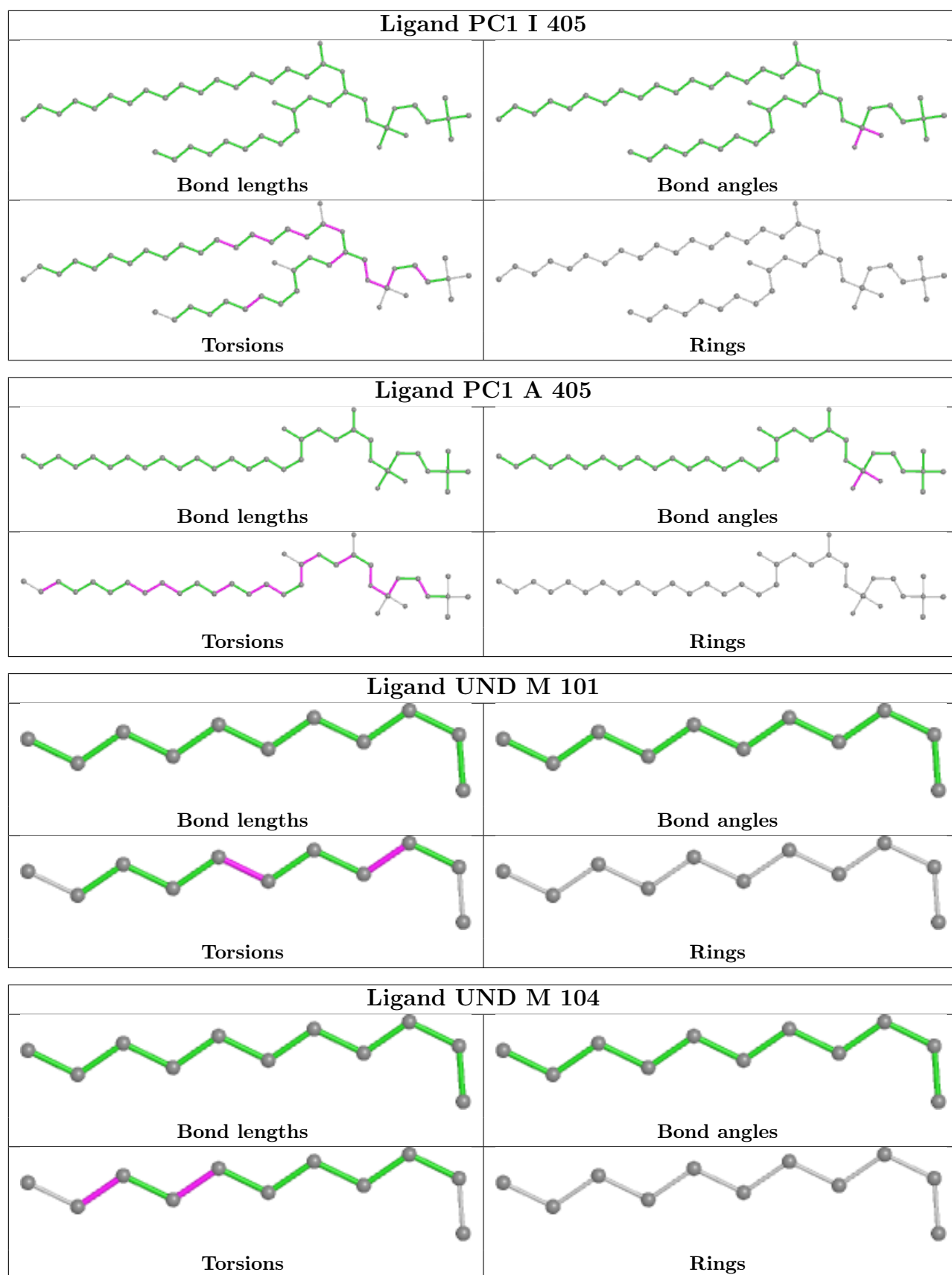


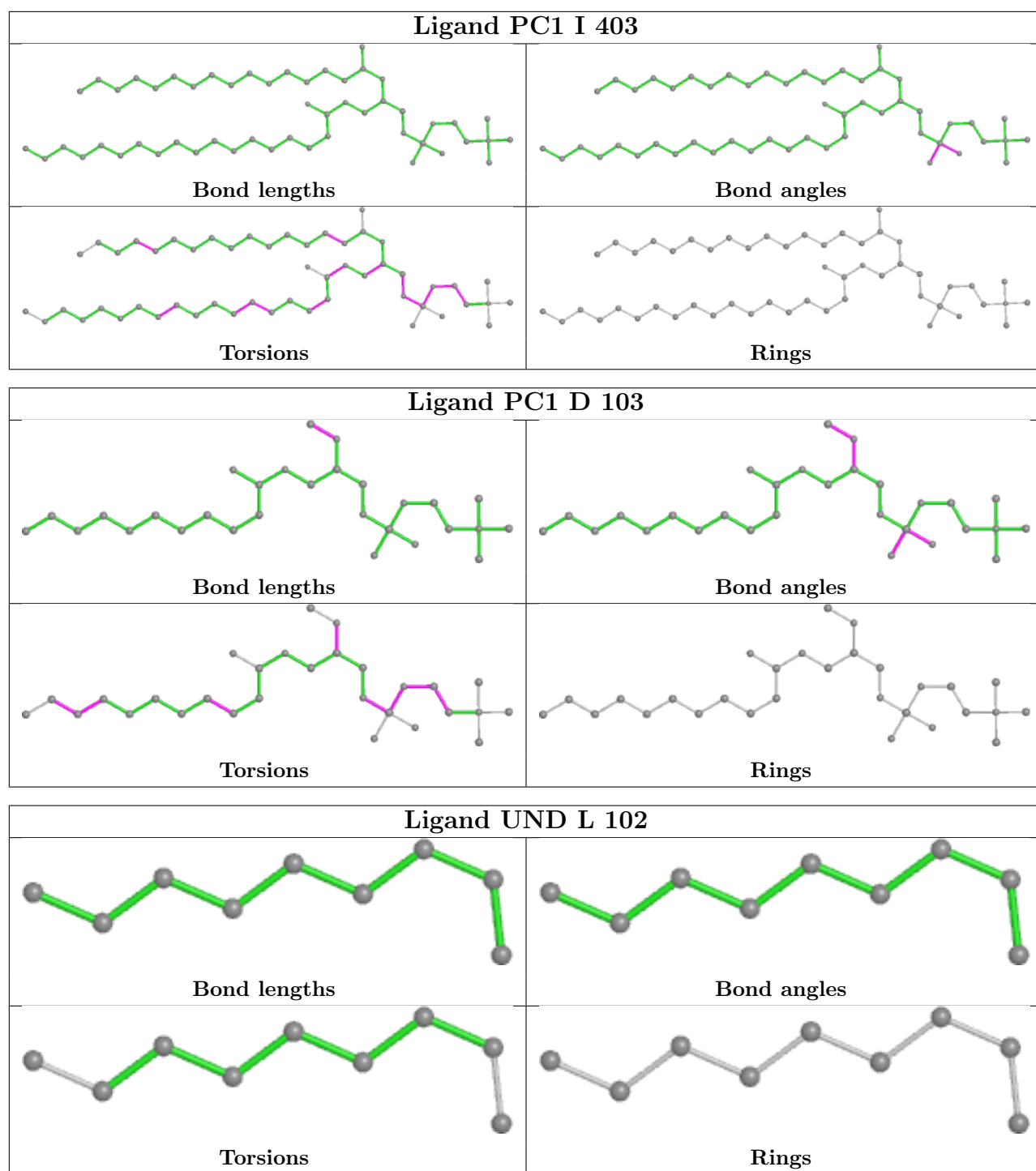


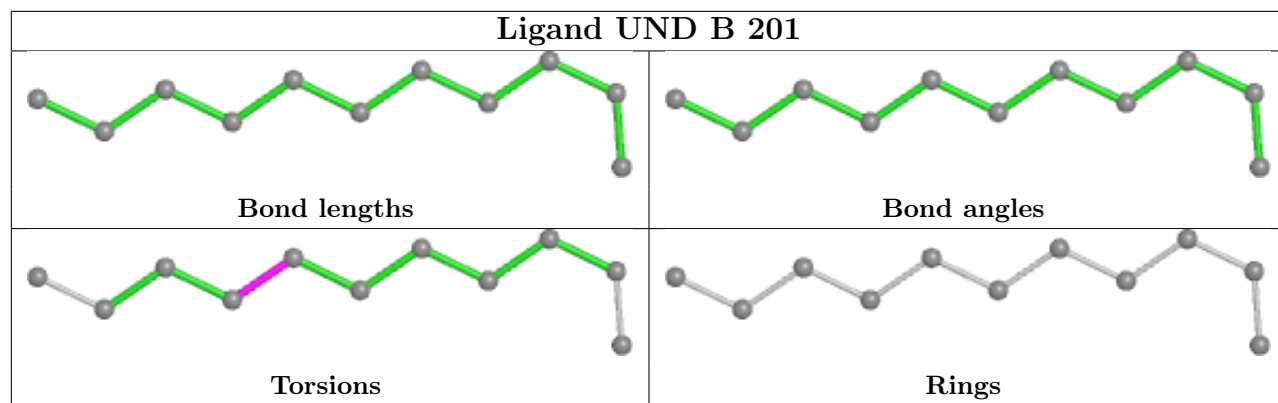












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

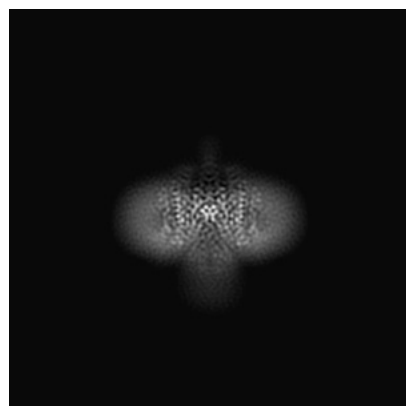
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61256. These allow visual inspection of the internal detail of the map and identification of artifacts.

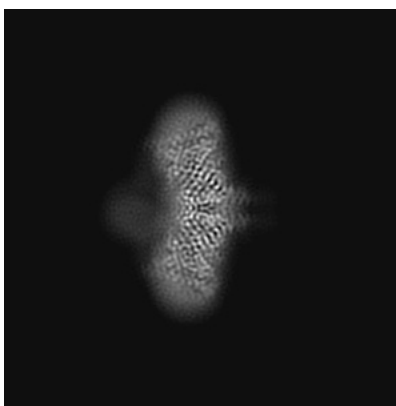
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

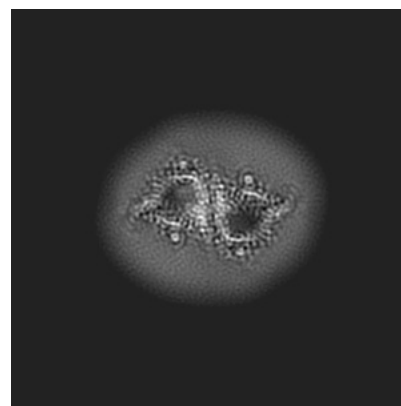
6.1.1 Primary map



X

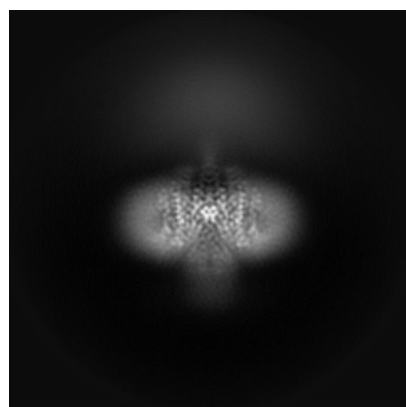


Y

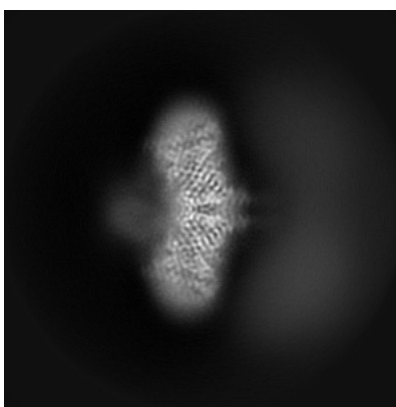


Z

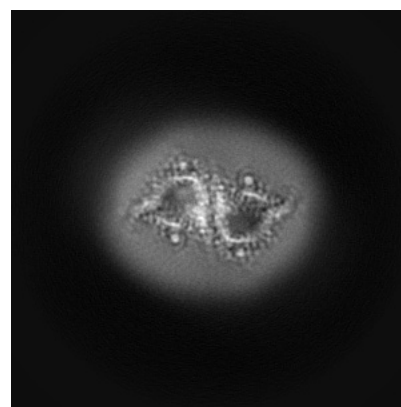
6.1.2 Raw map



X



Y

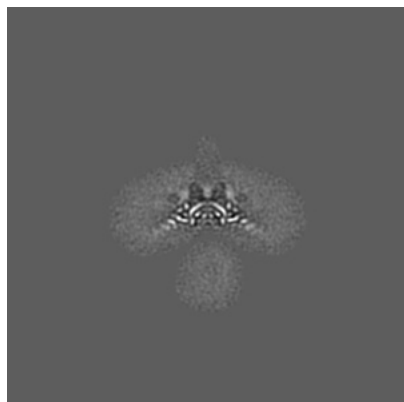


Z

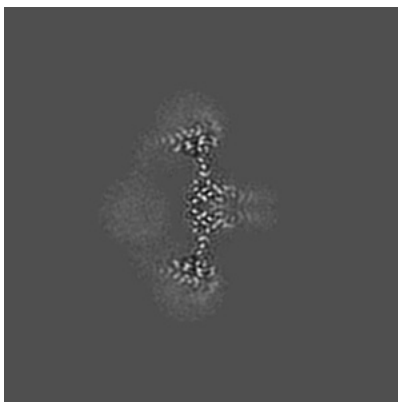
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

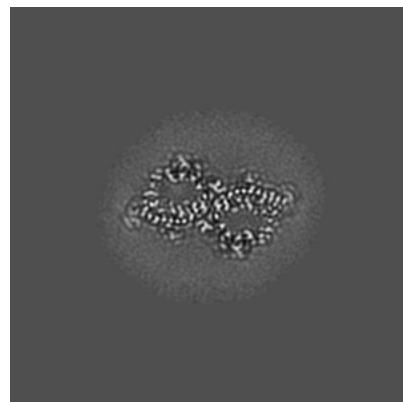
6.2.1 Primary map



X Index: 150

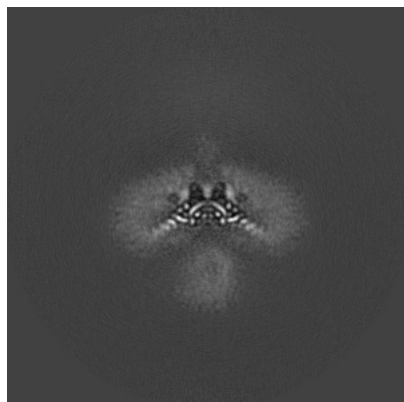


Y Index: 150

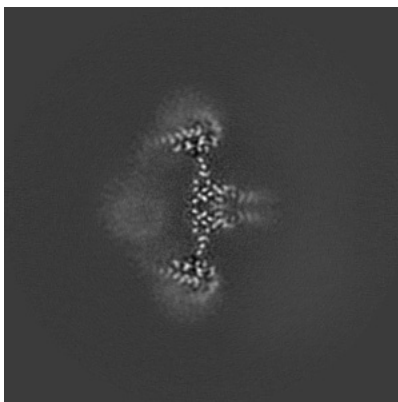


Z Index: 150

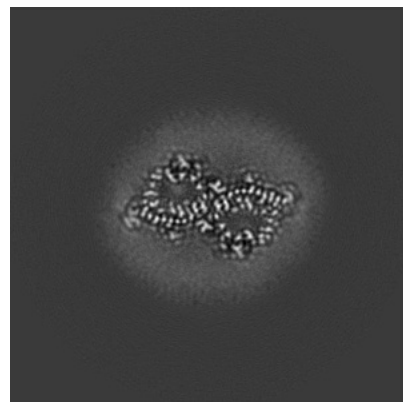
6.2.2 Raw map



X Index: 150



Y Index: 150

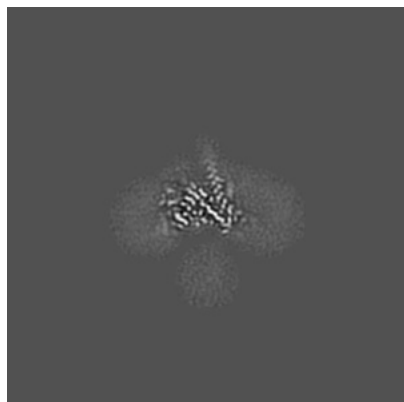


Z Index: 150

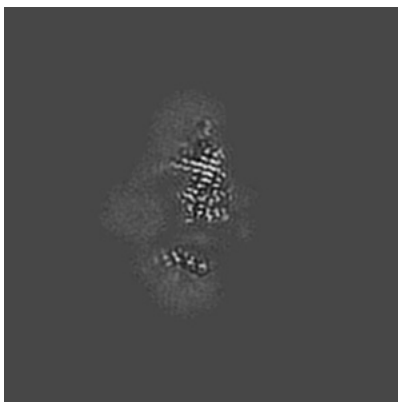
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

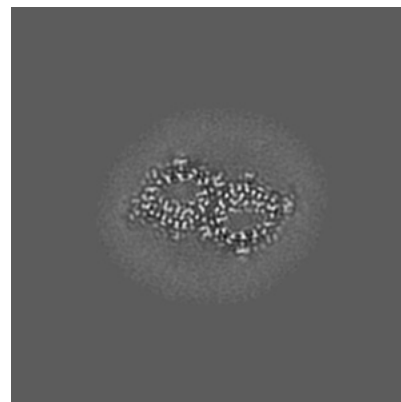
6.3.1 Primary map



X Index: 157

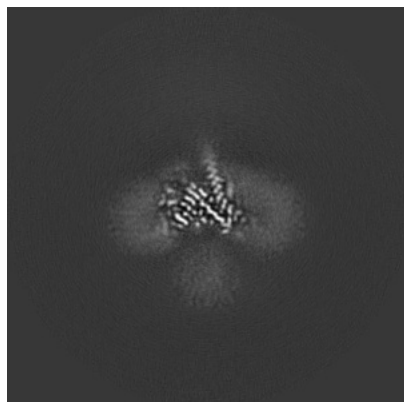


Y Index: 161

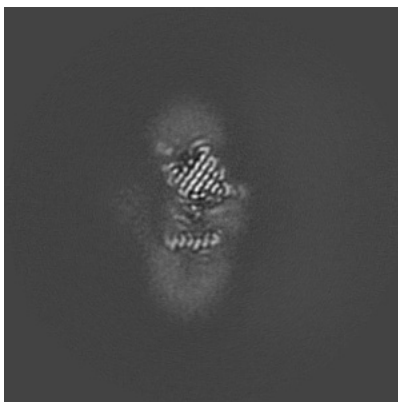


Z Index: 146

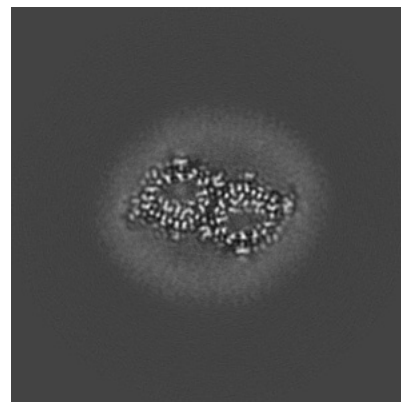
6.3.2 Raw map



X Index: 157



Y Index: 127

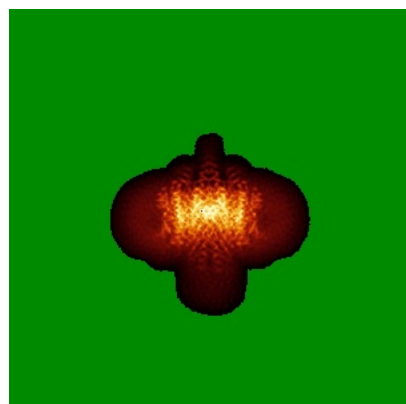


Z Index: 146

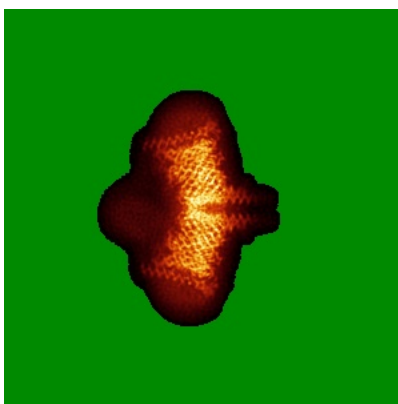
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

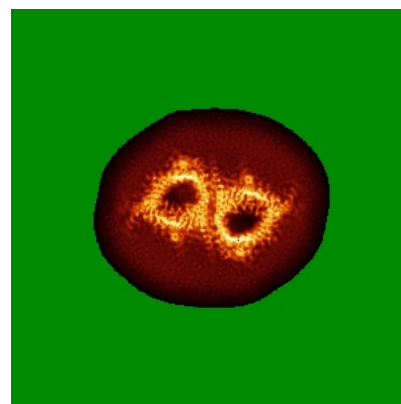
6.4.1 Primary map



X

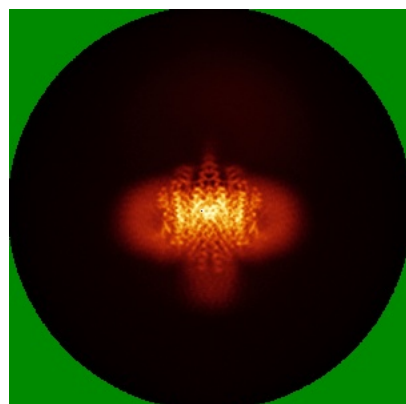


Y

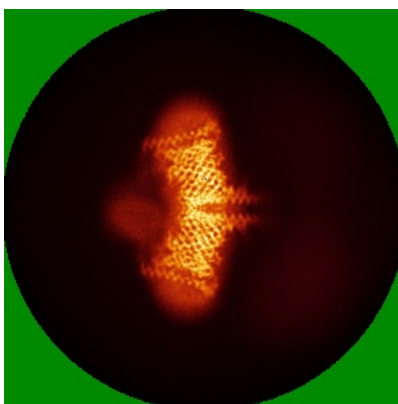


Z

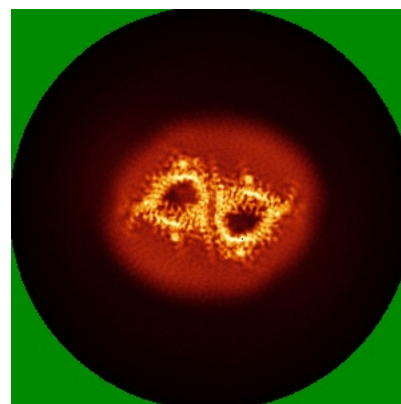
6.4.2 Raw map



X



Y

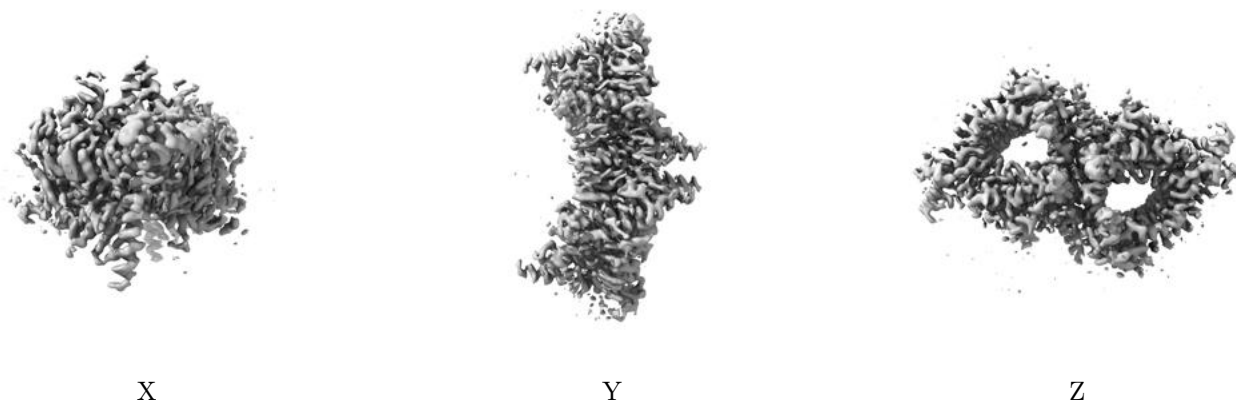


Z

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.

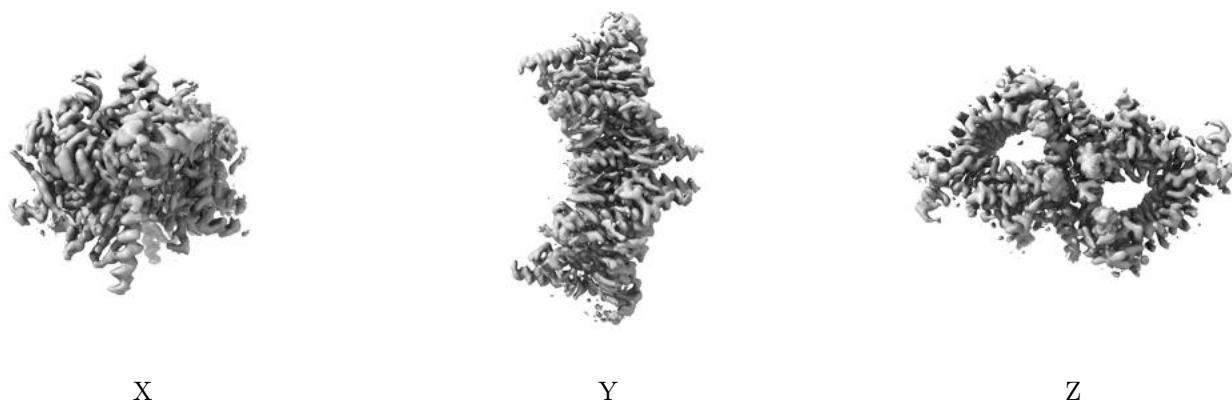
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0082. 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



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.

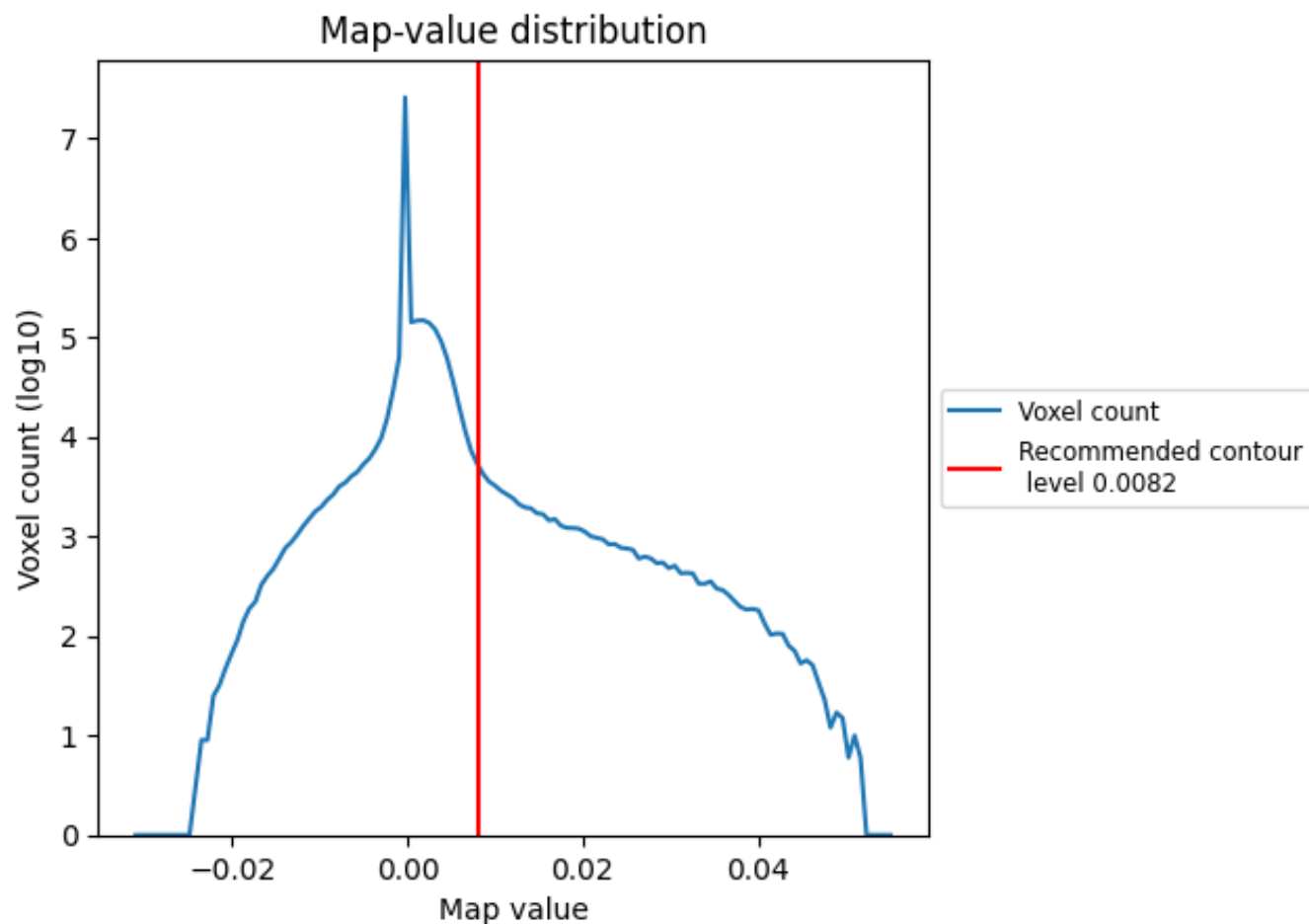
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

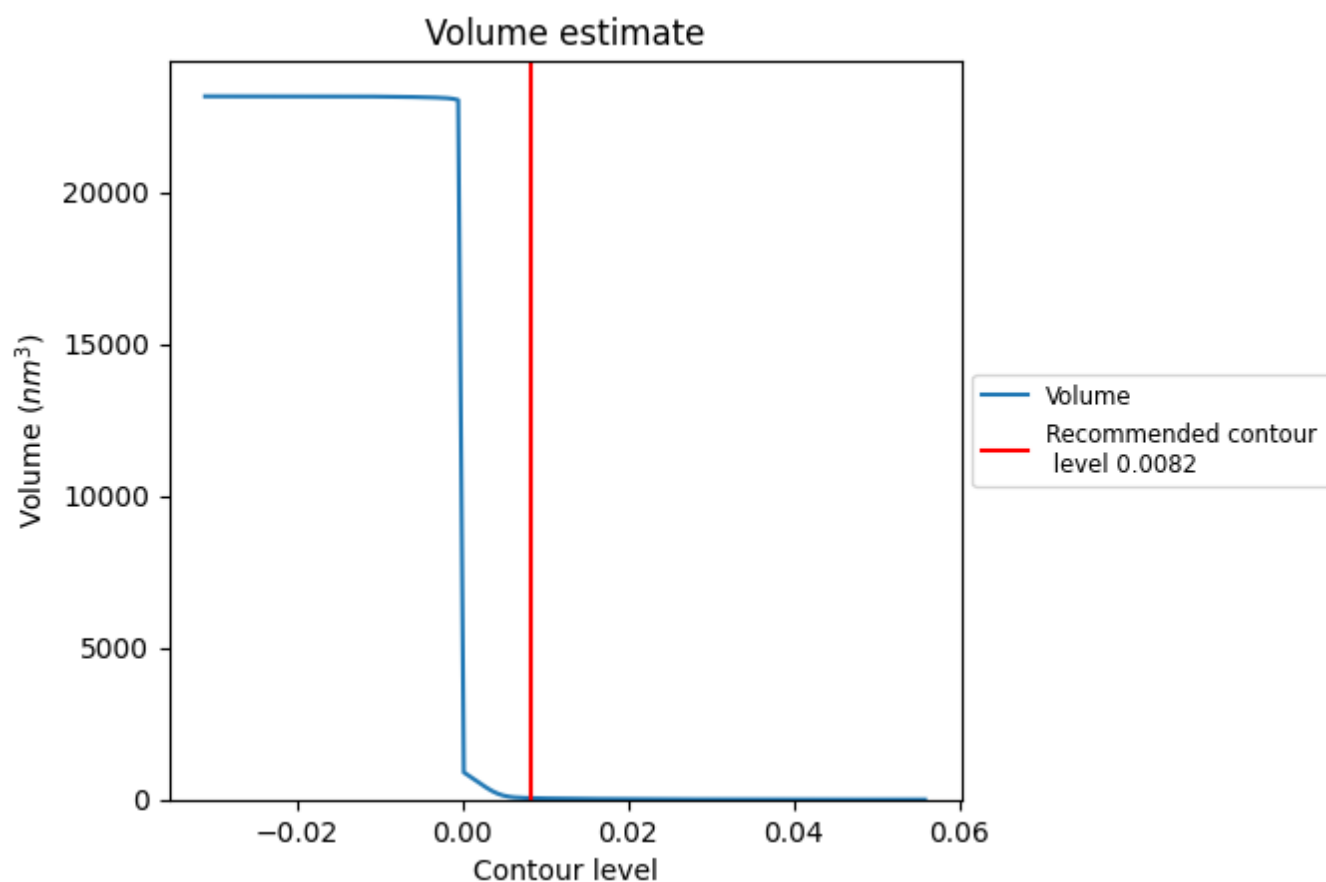
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

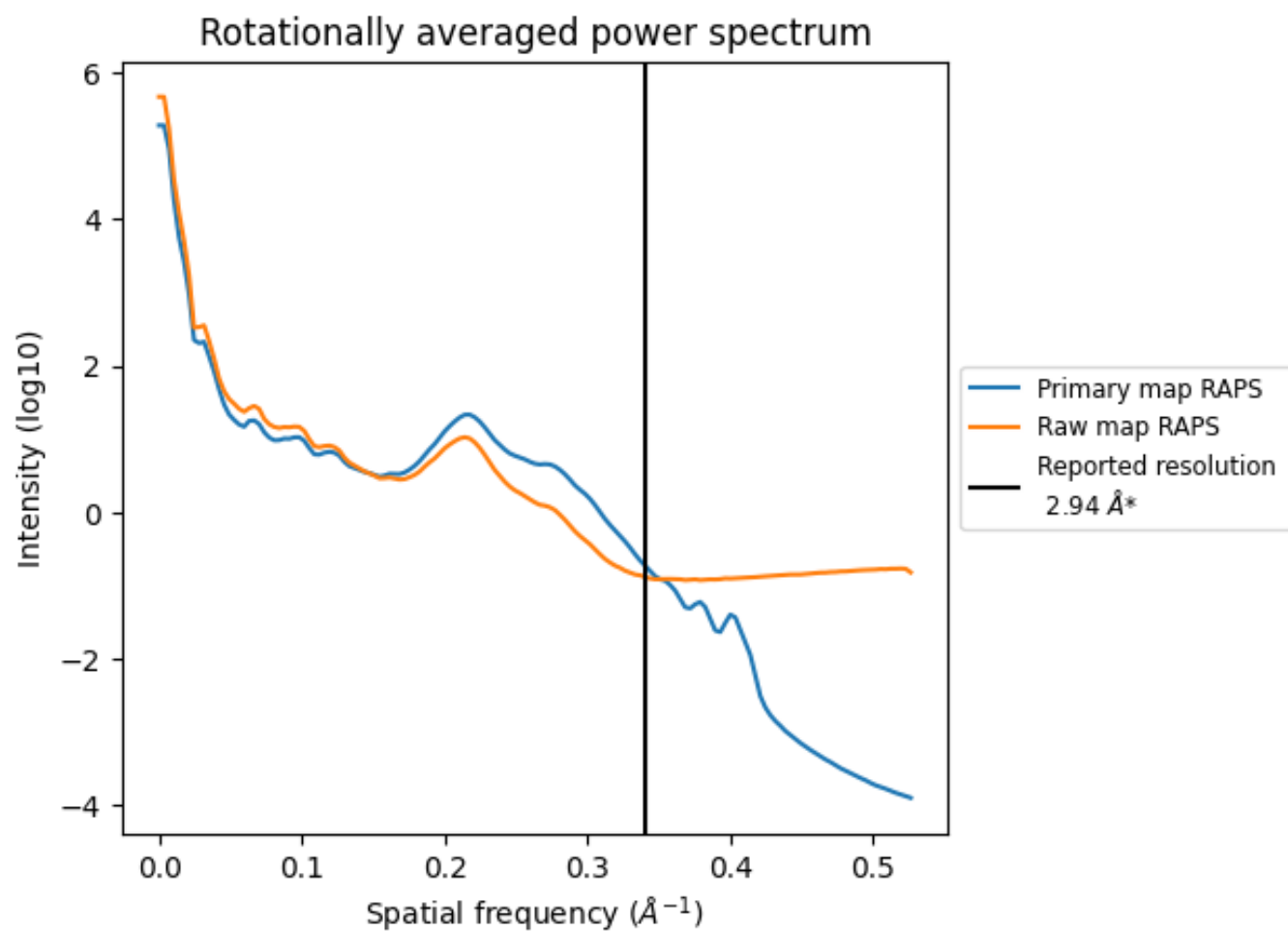
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 48 nm³; this corresponds to an approximate mass of 44 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 ⓘ

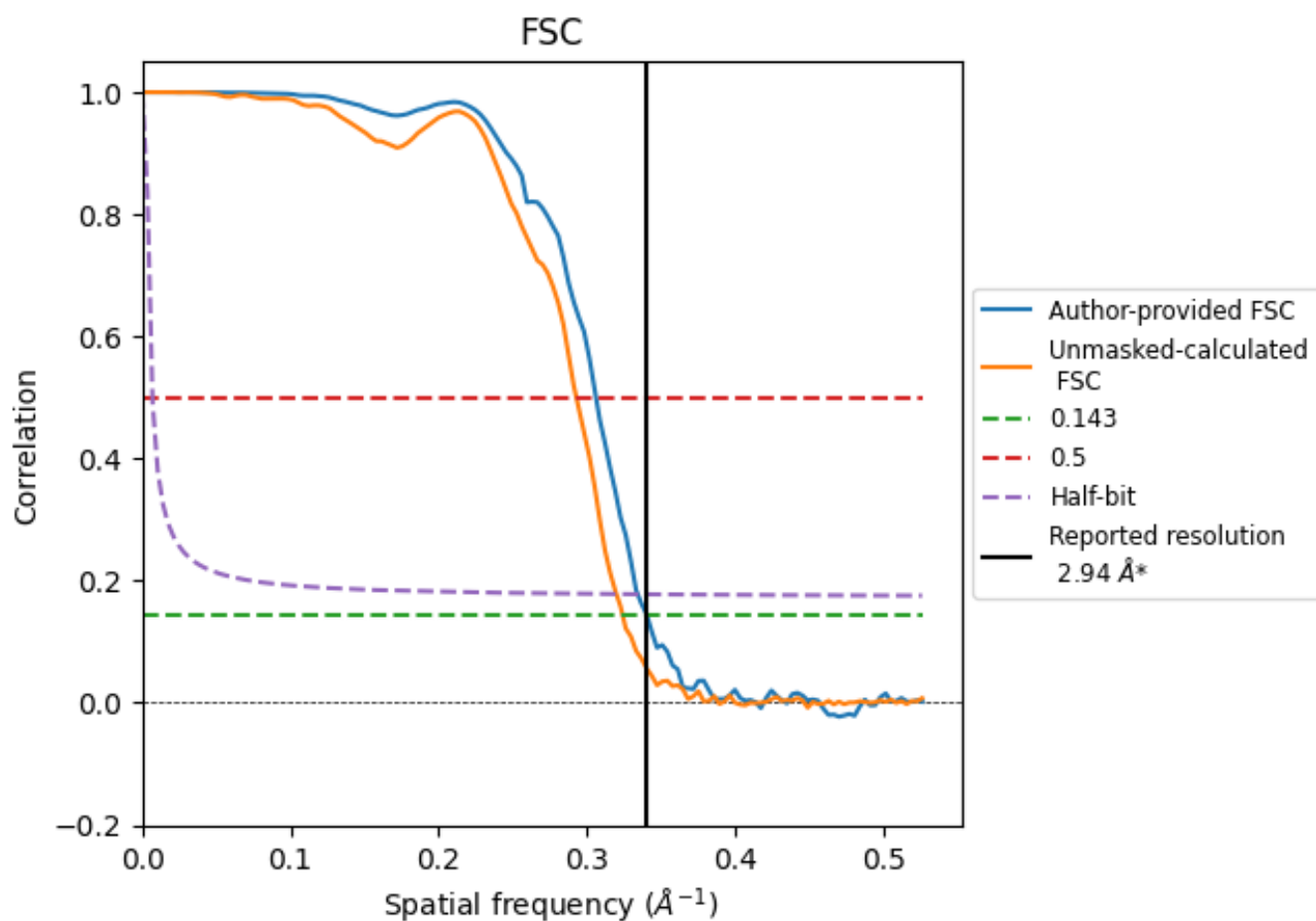


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 \AA^{-1}

8.2 Resolution estimates [i](#)

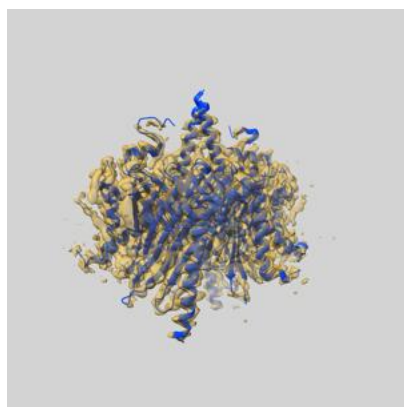
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.94	3.27	2.99
Unmasked-calculated*	3.08	3.41	3.12

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

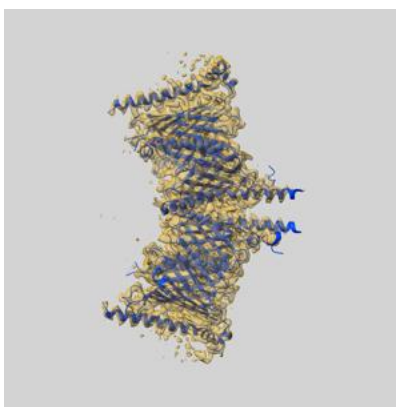
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61256 and PDB model 9J99. Per-residue inclusion information can be found in section [3](#) on page [9](#).

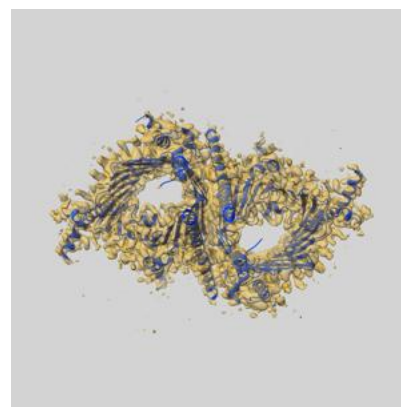
9.1 Map-model overlay [i](#)



X



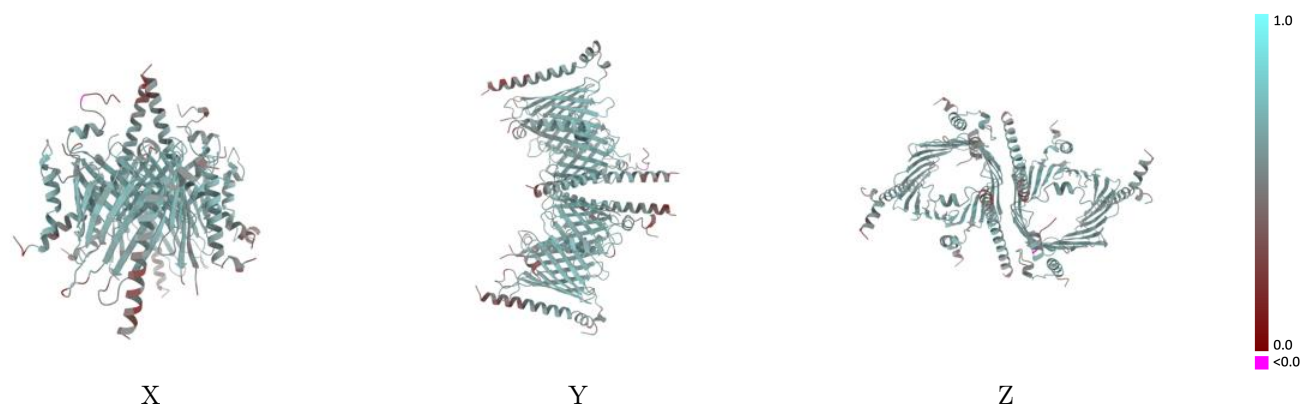
Y



Z

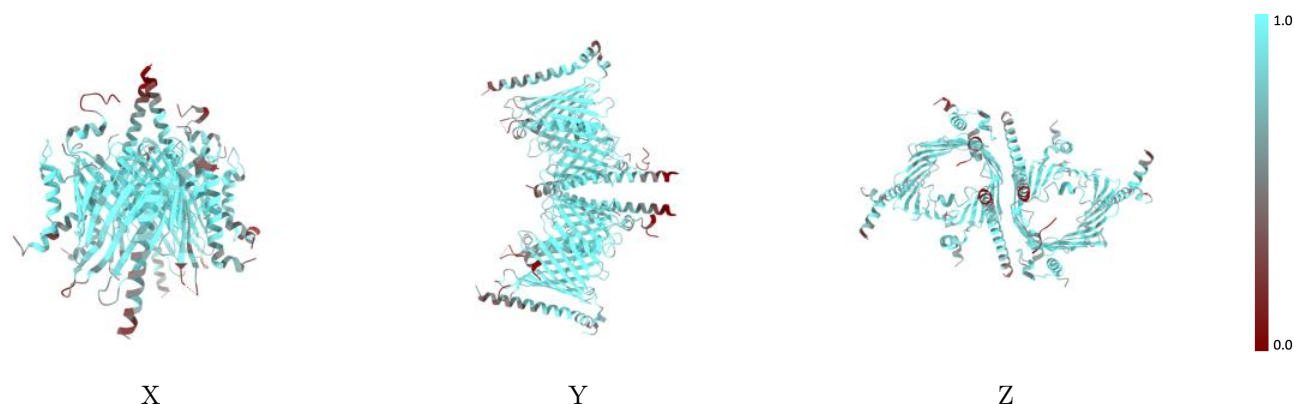
The images above show the 3D surface view of the map at the recommended contour level 0.0082 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



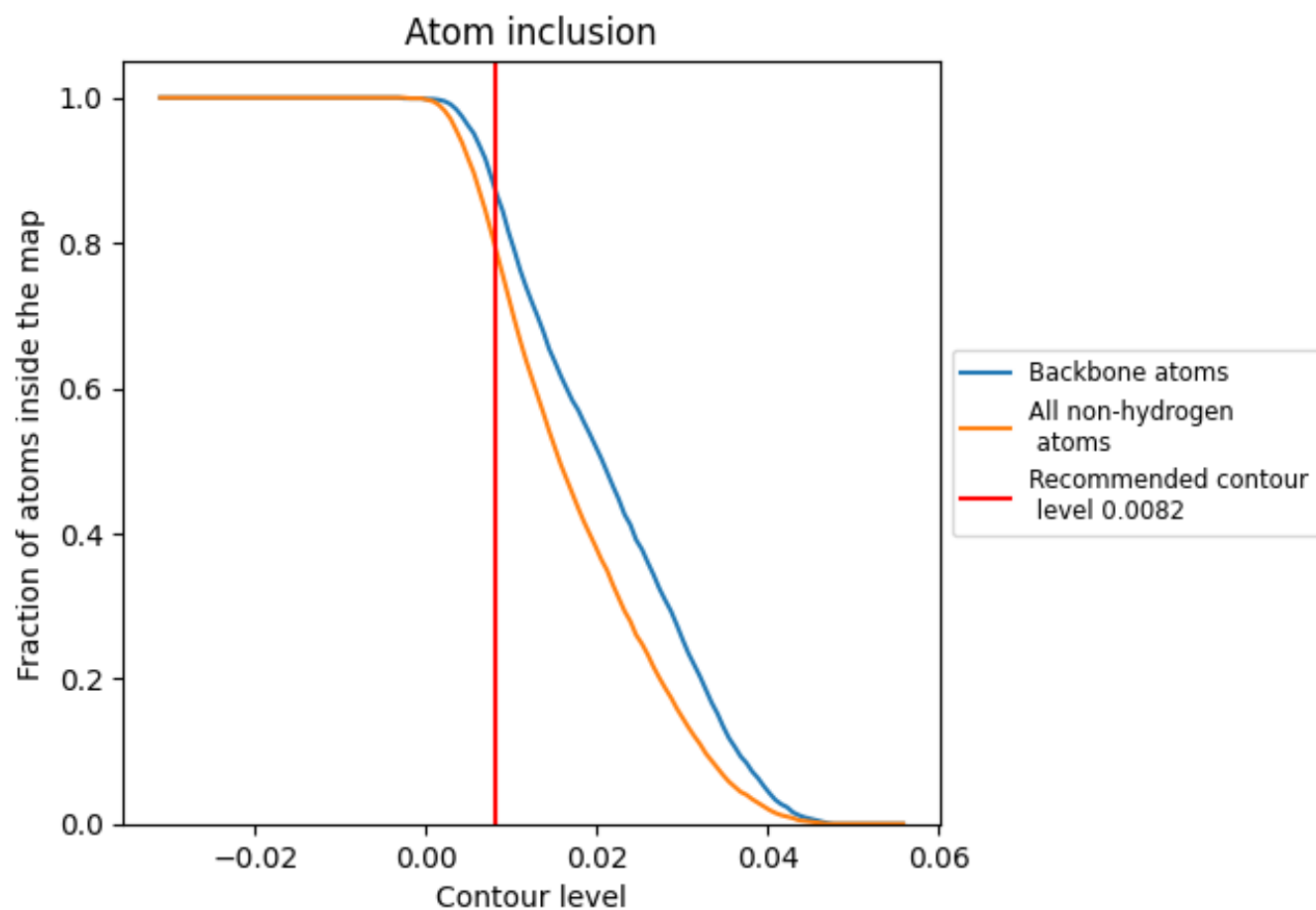
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0082).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.0082) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7910	<div></div> 0.5670
A	<div></div> 0.8370	<div></div> 0.5870
B	<div></div> 0.6680	<div></div> 0.5230
C	<div></div> 0.6600	<div></div> 0.4890
D	<div></div> 0.7440	<div></div> 0.5650
E	<div></div> 0.8230	<div></div> 0.5490
I	<div></div> 0.8360	<div></div> 0.5890
J	<div></div> 0.6350	<div></div> 0.5190
K	<div></div> 0.6570	<div></div> 0.4720
L	<div></div> 0.7340	<div></div> 0.5520
M	<div></div> 0.7680	<div></div> 0.5700

1.0

0.0

<0.0