



Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 06:17 AM JST

PDB ID : 6M0R
EMDB ID : EMD-30034
Title : 2.7A Yeast Vo state3
Authors : Roh, S.H.; Shekhar, M.; Pintilie, G.; Chipot, C.; Wilkens, S.; Singharoy, A.;
Chiu, W.
Deposited on : 2020-02-22
Resolution : 2.70 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:

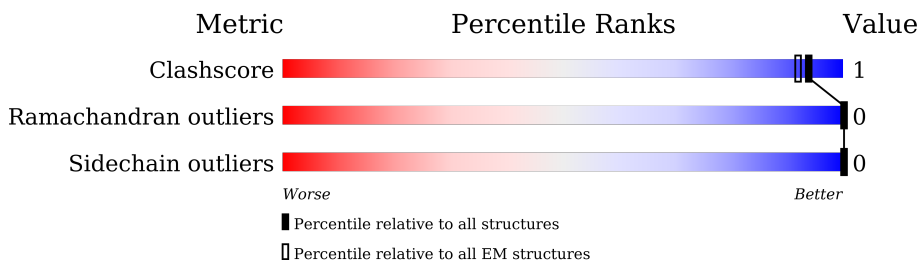
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



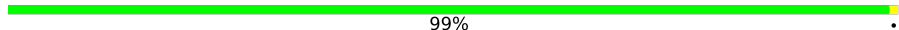

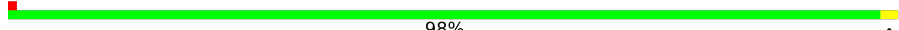
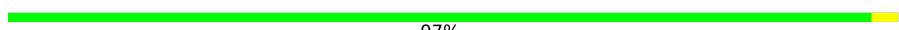
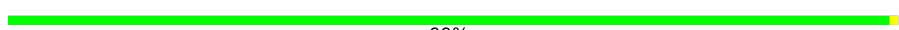



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	D	158	98%
2	C	198	95% 5%
3	N	52	98%
4	M	71	99%
5	E	159	99%
5	F	159	100%
5	G	159	100%
5	H	159	99%

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Mol	Chain	Length	Quality of chain
5	I	159	 99%
5	J	159	 100%
5	K	159	 98%
5	L	159	 97%
6	O	69	 99%
7	B	345	 93% 7%
8	A	825	 86% 5% 9%
9	P	5	 40% 100%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 48160 atoms, of which 24493 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 c'.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	D	158	2340	756	1196	180	196	12	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit c''.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	C	198	3012	980	1540	228	257	7	0	0

- Molecule 3 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	N	52	830	267	430	59	72	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	M	71	1159	381	589	93	90	6	0	0

- Molecule 5 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	159	2344	749	1207	182	199	7	0	0
5	F	159	2344	749	1207	182	199	7	0	0
5	G	159	2344	749	1207	182	199	7	0	0
5	H	159	2344	749	1207	182	199	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
5	I	159	Total	C	H	N	O	S	0	0
			2344	749	1207	182	199	7		
5	J	159	Total	C	H	N	O	S	0	0
			2344	749	1207	182	199	7		
5	K	159	Total	C	H	N	O	S	0	0
			2344	749	1207	182	199	7		
5	L	159	Total	C	H	N	O	S	0	0
			2344	749	1207	182	199	7		

- Molecule 6 is a protein called Uncharacterized protein YPR170W-B.

Mol	Chain	Residues	Atoms					AltConf	Trace	
6	O	69	Total	C	H	N	O	S	0	0
			1044	353	515	81	92	3		

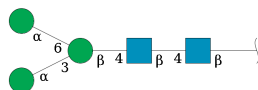
- Molecule 7 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace	
7	B	345	Total	C	H	N	O	S	0	0
			5490	1779	2689	454	554	14		

- Molecule 8 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

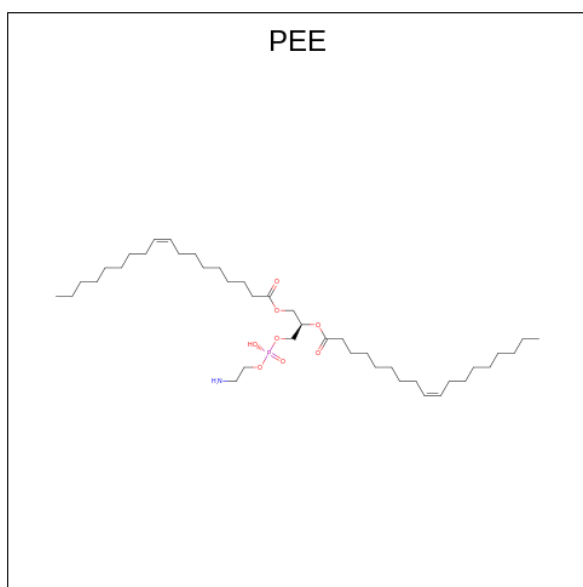
Mol	Chain	Residues	Atoms					AltConf	Trace	
8	A	750	Total	C	H	N	O	S	0	0
			12161	3977	6072	991	1086	35		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace	
9	P	5	Total	C	N	O	0	0
			62	34	2	26		

- Molecule 10 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



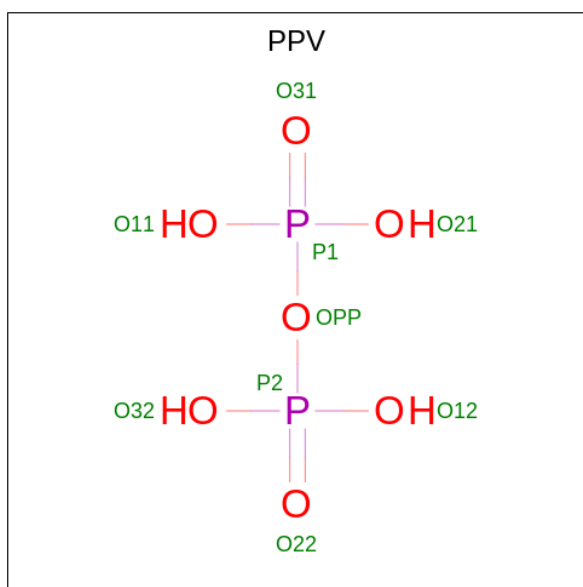
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
10	C	1	124	39	75	1	8	1	0
10	C	1	118	37	71	1	8	1	0
10	C	1	100	31	59	1	8	1	0
10	C	1	91	29	52	1	8	1	0
10	C	1	103	33	60	1	8	1	0
10	C	1	85	27	48	1	8	1	0
10	C	1	91	29	52	1	8	1	0
10	C	1	91	29	52	1	8	1	0
10	C	1	85	27	48	1	8	1	0
10	C	1	91	29	52	1	8	1	0
10	M	1	124	39	75	1	8	1	0
10	M	1	118	37	71	1	8	1	0
10	E	1	97	31	56	1	8	1	0
10	E	1	91	29	52	1	8	1	0

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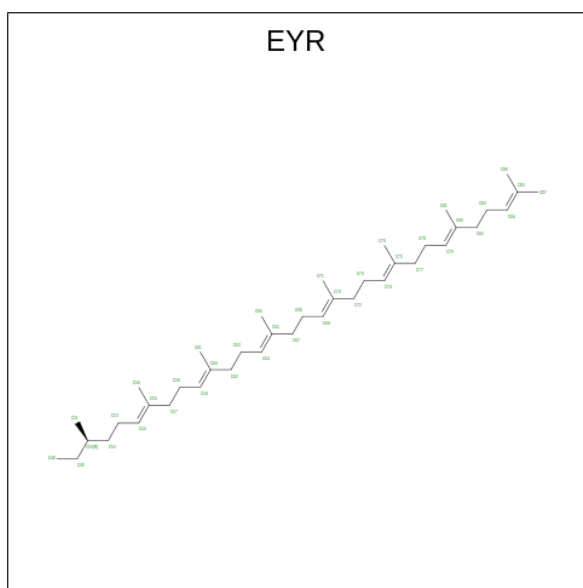
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
10	O	1	Total 79	C 25	H 44	N 1	O 8	P 1	0
10	F	1	Total 91	C 29	H 52	N 1	O 8	P 1	0
10	G	1	Total 109	C 35	H 64	N 1	O 8	P 1	0
10	H	1	Total 85	C 27	H 48	N 1	O 8	P 1	0
10	I	1	Total 103	C 33	H 60	N 1	O 8	P 1	0
10	I	1	Total 109	C 35	H 64	N 1	O 8	P 1	0
10	J	1	Total 97	C 31	H 56	N 1	O 8	P 1	0
10	J	1	Total 94	C 29	H 55	N 1	O 8	P 1	0
10	K	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
10	K	1	Total 109	C 35	H 64	N 1	O 8	P 1	0
10	B	1	Total 112	C 35	H 67	N 1	O 8	P 1	0
10	A	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
10	A	1	Total 97	C 31	H 56	N 1	O 8	P 1	0
10	A	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
10	A	1	Total 106	C 33	H 63	N 1	O 8	P 1	0
10	A	1	Total 79	C 25	H 44	N 1	O 8	P 1	0

- Molecule 11 is PYROPHOSPHATE (three-letter code: PPV) (formula: H₄O₇P₂).



Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	O	P	0
			8	6	2	

- Molecule 12 is (6 {E},10 {E},14 {E},18 {E},22 {E},26 {E},30 {R})-2,6,10,14,18,22,26,30-octamethyldotriaconta-2,6,10,14,18,22,26-heptaene (three-letter code: EYR) (formula: $C_{40}H_{68}$).



Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	C	0
			40	40	

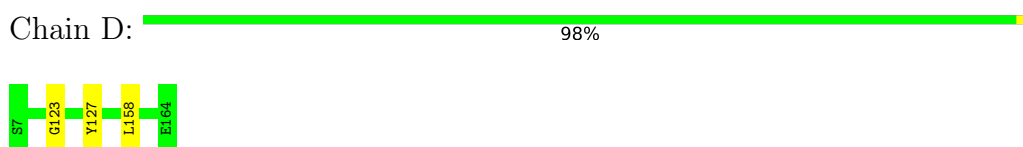
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	AltConf
13	D	8	Total O 8 8	0
13	C	15	Total O 15 15	0
13	N	2	Total O 2 2	0
13	M	5	Total O 5 5	0
13	E	7	Total O 7 7	0
13	O	2	Total O 2 2	0
13	F	9	Total O 9 9	0
13	G	9	Total O 9 9	0
13	H	8	Total O 8 8	0
13	I	10	Total O 10 10	0
13	J	6	Total O 6 6	0
13	K	7	Total O 7 7	0
13	L	18	Total O 18 18	0
13	B	14	Total O 14 14	0
13	A	64	Total O 64 64	0

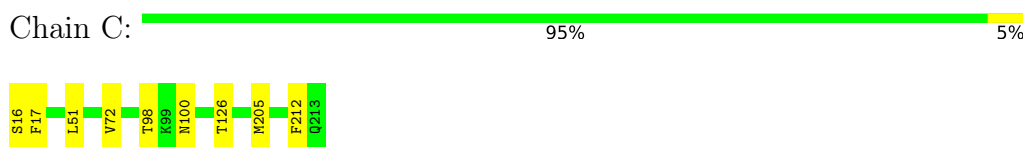
3 Residue-property plots

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.

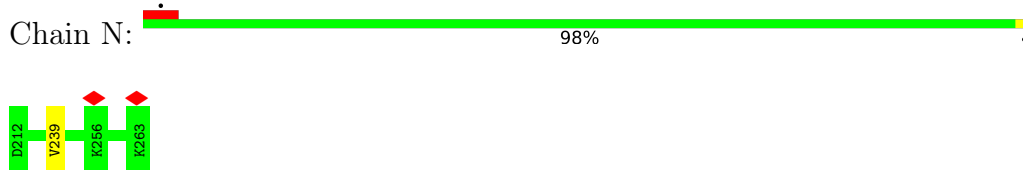
- Molecule 1: V-type proton ATPase subunit c'



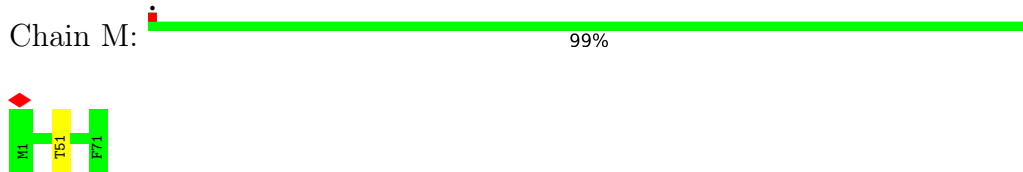
- Molecule 2: V-type proton ATPase subunit c''



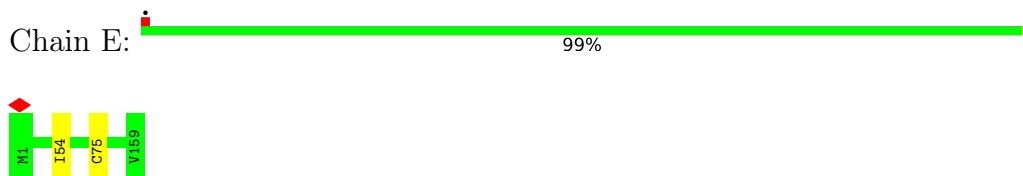
- Molecule 3: V0 assembly protein 1



- Molecule 4: V-type proton ATPase subunit e



- Molecule 5: V-type proton ATPase subunit c



- Molecule 5: V-type proton ATPase subunit c

Chain F:  100%



- Molecule 5: V-type proton ATPase subunit c

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: V-type proton ATPase subunit c

Chain H:  99%



- Molecule 5: V-type proton ATPase subunit c

Chain I:  99%



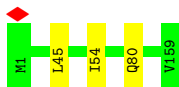
- Molecule 5: V-type proton ATPase subunit c

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: V-type proton ATPase subunit c

Chain K:  98%



- Molecule 5: V-type proton ATPase subunit c

Chain L:  97%



- Molecule 6: Uncharacterized protein YPR170W-B

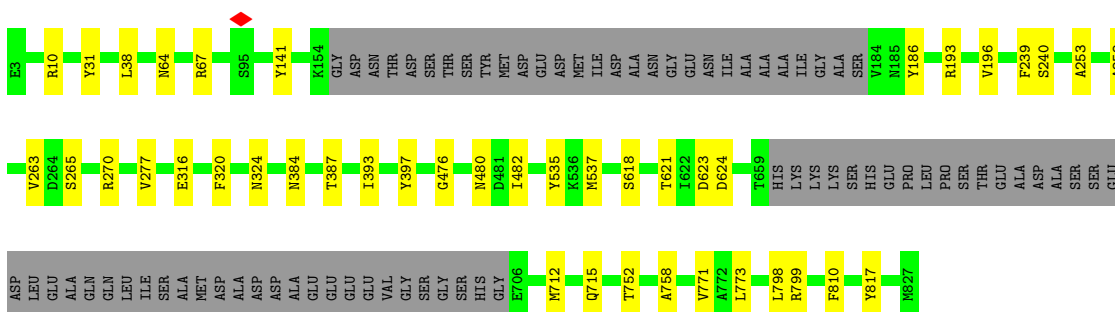
Chain O:  99%



- Molecule 7: V-type proton ATPase subunit d



- Molecule 8: V-type proton ATPase subunit a, vacuolar isoform



- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117948	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	216.00002, 216.00002, 216.00002	wwPDB
Map dimensions	200, 200, 200	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: PPV, BMA, MAN, PEE, EYR, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	D	0.49	0/1167	0.54	0/1582
2	C	0.50	0/1502	0.54	0/2041
3	N	0.43	0/406	0.51	0/553
4	M	0.47	0/587	0.51	0/801
5	E	0.48	0/1155	0.55	0/1571
5	F	0.48	0/1155	0.54	0/1571
5	G	0.46	0/1155	0.56	0/1571
5	H	0.44	0/1155	0.56	0/1571
5	I	0.46	0/1155	0.55	0/1571
5	J	0.49	0/1155	0.56	0/1571
5	K	0.47	0/1155	0.55	0/1571
5	L	0.50	0/1155	0.60	0/1571
6	O	0.39	0/545	0.46	0/747
7	B	0.47	0/2860	0.56	0/3880
8	A	0.43	0/6242	0.54	0/8448
All	All	0.46	0/22549	0.55	0/30620

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1144	1196	1196	2	0
2	C	1472	1540	1540	7	0
3	N	400	430	430	1	0
4	M	570	589	589	1	0
5	E	1137	1207	1207	2	0
5	F	1137	1207	1207	0	0
5	G	1137	1207	1207	0	0
5	H	1137	1207	1207	1	0
5	I	1137	1207	1207	2	0
5	J	1137	1207	1207	0	0
5	K	1137	1207	1207	3	0
5	L	1137	1207	1207	4	0
6	O	529	515	515	1	0
7	B	2801	2689	2689	14	0
8	A	6089	6072	6071	29	0
9	P	62	0	53	0	0
10	A	221	327	327	2	0
10	B	45	67	67	2	0
10	C	410	569	569	0	0
10	E	80	108	108	0	0
10	F	39	52	52	0	0
10	G	45	64	64	0	0
10	H	37	48	48	0	0
10	I	88	124	124	0	0
10	J	80	111	111	0	0
10	K	96	146	146	0	0
10	M	96	146	146	0	0
10	O	35	44	44	0	0
11	A	8	0	0	0	0
12	A	40	0	0	0	0
13	A	64	0	0	4	0
13	B	14	0	0	0	0
13	C	15	0	0	3	0
13	D	8	0	0	0	0
13	E	7	0	0	0	0
13	F	9	0	0	0	0
13	G	9	0	0	0	0
13	H	8	0	0	0	0
13	I	10	0	0	0	0
13	J	6	0	0	0	0
13	K	7	0	0	1	0
13	L	18	0	0	1	0
13	M	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	2	0	0	0	0
13	O	2	0	0	0	0
All	All	23667	24493	24545	59	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 1.

All (59) 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)
8:A:31:TYR:OH	8:A:316:GLU:OE1	2.04	0.76
8:A:810:PHE:O	13:A:1001:HOH:O	2.08	0.72
5:L:117:ARG:NH2	7:B:86:GLN:OE1	2.23	0.71
8:A:799:ARG:NH1	13:A:1003:HOH:O	2.25	0.70
8:A:537:MET:SD	13:A:1054:HOH:O	2.50	0.69
7:B:182:ASN:OD1	7:B:219:ARG:NH2	2.27	0.68
8:A:186:TYR:OH	8:A:263:VAL:O	2.12	0.67
2:C:205:MET:O	13:C:401:HOH:O	2.11	0.67
2:C:51:LEU:O	13:C:402:HOH:O	2.13	0.67
6:O:62:TYR:OH	8:A:771:VAL:O	2.13	0.67
8:A:752:THR:OG1	13:A:1002:HOH:O	2.12	0.66
7:B:90:SER:OG	7:B:199:GLU:OE2	2.12	0.65
8:A:384:ASN:ND2	10:A:903:PEE:O4	2.30	0.65
7:B:215:GLU:OE1	7:B:218:ARG:NH2	2.31	0.64
5:L:110:ILE:O	13:L:201:HOH:O	2.16	0.62
7:B:81:ASN:OD1	7:B:84:ARG:NH2	2.36	0.59
4:M:51:THR:OG1	8:A:535:TYR:OH	2.15	0.58
7:B:5:TYR:OH	10:B:401:PEE:O5	2.21	0.58
8:A:64:ASN:OD1	8:A:67:ARG:NH2	2.37	0.57
8:A:38:LEU:O	8:A:817:TYR:OH	2.23	0.55
8:A:10:ARG:NH2	10:A:902:PEE:O2P	2.40	0.55
1:D:158:LEU:HD23	5:E:75:CYS:SG	2.49	0.53
7:B:186:LYS:NZ	7:B:242:LEU:O	2.41	0.52
8:A:193:ARG:O	8:A:196:VAL:HG12	2.11	0.50
2:C:16:SER:OG	2:C:17:PHE:N	2.45	0.49
8:A:239:PHE:O	8:A:240:SER:OG	2.29	0.49
5:K:80:GLN:O	13:K:301:HOH:O	2.20	0.48
7:B:283:ASN:O	7:B:287:HIS:ND1	2.41	0.48
7:B:76:LEU:HD13	7:B:316:LYS:HD2	1.95	0.47
8:A:618:SER:O	8:A:621:THR:OG1	2.28	0.47
7:B:211:LEU:HD13	7:B:310:TRP:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:54:ILE:O	5:E:54:ILE:HG22	2.14	0.47
8:A:141:TYR:CD2	8:A:277:VAL:HG21	2.50	0.46
8:A:141:TYR:HD2	8:A:277:VAL:HG21	1.80	0.46
8:A:253:ALA:O	8:A:258:ALA:HB3	2.16	0.45
5:K:45:LEU:O	8:A:193:ARG:NH1	2.50	0.45
7:B:214:PHE:CE1	7:B:291:LEU:HD23	2.52	0.44
8:A:265:SER:O	8:A:270:ARG:NH1	2.51	0.44
8:A:476:GLY:O	8:A:480:ASN:N	2.51	0.43
8:A:758:ALA:HB2	8:A:773:LEU:HD12	2.01	0.43
7:B:108:ALA:O	7:B:112:THR:HG23	2.18	0.43
8:A:712:MET:O	8:A:715:GLN:N	2.50	0.43
2:C:72:VAL:HG13	5:L:139:LEU:HB3	2.01	0.43
8:A:482:ILE:HG23	8:A:482:ILE:O	2.18	0.43
8:A:623:ASP:OD1	8:A:624:ASP:N	2.49	0.43
2:C:98:THR:HG21	8:A:397:TYR:HA	2.01	0.42
5:I:155:THR:HG22	5:I:155:THR:O	2.20	0.42
5:L:129:MET:SD	5:L:133:LEU:HD22	2.60	0.42
8:A:384:ASN:H	8:A:387:THR:HG1	1.67	0.41
1:D:123:GLY:O	1:D:127:TYR:N	2.53	0.41
5:H:4:LEU:HD23	5:I:7:VAL:HG12	2.02	0.41
7:B:153:LEU:HD13	7:B:162:PHE:CE2	2.55	0.41
2:C:100:ASN:ND2	13:C:403:HOH:O	2.54	0.41
3:N:239:VAL:HG11	10:B:401:PEE:H66	2.03	0.41
8:A:393:ILE:HG23	8:A:798:LEU:HD11	2.03	0.40
7:B:214:PHE:HE1	7:B:291:LEU:HD23	1.86	0.40
8:A:320:PHE:O	8:A:324:ASN:N	2.53	0.40
5:K:54:ILE:O	5:K:54:ILE:HG22	2.22	0.40
2:C:126:THR:OG1	2:C:212:PHE:O	2.33	0.40

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	D	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
2	C	196/198 (99%)	195 (100%)	1 (0%)	0	100	100
3	N	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
4	M	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
5	E	157/159 (99%)	156 (99%)	1 (1%)	0	100	100
5	F	157/159 (99%)	157 (100%)	0	0	100	100
5	G	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
5	H	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
5	I	157/159 (99%)	157 (100%)	0	0	100	100
5	J	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
5	K	157/159 (99%)	156 (99%)	1 (1%)	0	100	100
5	L	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
6	O	67/69 (97%)	67 (100%)	0	0	100	100
7	B	343/345 (99%)	337 (98%)	6 (2%)	0	100	100
8	A	744/825 (90%)	726 (98%)	18 (2%)	0	100	100
All	All	2881/2990 (96%)	2841 (99%)	40 (1%)	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	D	119/120 (99%)	119 (100%)	0	100	100
2	C	154/154 (100%)	154 (100%)	0	100	100
3	N	46/47 (98%)	46 (100%)	0	100	100
4	M	63/64 (98%)	63 (100%)	0	100	100
5	E	117/118 (99%)	117 (100%)	0	100	100
5	F	117/118 (99%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	117/118 (99%)	117 (100%)	0	100	100
5	H	117/118 (99%)	117 (100%)	0	100	100
5	I	117/118 (99%)	117 (100%)	0	100	100
5	J	117/118 (99%)	117 (100%)	0	100	100
5	K	117/118 (99%)	117 (100%)	0	100	100
5	L	117/118 (99%)	117 (100%)	0	100	100
6	O	57/57 (100%)	57 (100%)	0	100	100
7	B	309/309 (100%)	309 (100%)	0	100	100
8	A	658/718 (92%)	658 (100%)	0	100	100
All	All	2342/2413 (97%)	2342 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

5 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
9	NAG	P	1	9,11	15,15,15	1.81	4 (26%)	21,21,21	1.46	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	P	2	9	14,14,15	2.09	5 (35%)	17,19,21	1.35	3 (17%)
9	BMA	P	3	9	11,11,12	1.57	3 (27%)	15,15,17	1.15	2 (13%)
9	MAN	P	4	9	11,11,12	1.73	3 (27%)	15,15,17	1.21	1 (6%)
9	MAN	P	5	9	11,11,12	1.56	3 (27%)	15,15,17	1.02	1 (6%)

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
9	NAG	P	1	9,11	-	1/6/26/26	0/1/1/1
9	NAG	P	2	9	-	0/6/23/26	0/1/1/1
9	BMA	P	3	9	-	0/2/19/22	0/1/1/1
9	MAN	P	4	9	-	2/2/19/22	0/1/1/1
9	MAN	P	5	9	-	2/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	2	NAG	C7-N2	3.93	1.47	1.34
9	P	2	NAG	O5-C1	3.87	1.49	1.43
9	P	4	MAN	O5-C1	3.85	1.49	1.43
9	P	1	NAG	C7-N2	3.47	1.46	1.34
9	P	3	BMA	O5-C5	3.22	1.50	1.43
9	P	2	NAG	C2-N2	3.20	1.51	1.46
9	P	1	NAG	C3-C2	-3.13	1.47	1.53
9	P	4	MAN	C2-C3	-2.95	1.48	1.52
9	P	5	MAN	O5-C5	2.86	1.49	1.43
9	P	1	NAG	C2-N2	2.84	1.50	1.45
9	P	2	NAG	C8-C7	2.46	1.55	1.50
9	P	1	NAG	O5-C1	2.44	1.49	1.42
9	P	5	MAN	C2-C3	-2.37	1.49	1.52
9	P	5	MAN	O5-C1	2.24	1.47	1.43
9	P	2	NAG	C3-C2	-2.15	1.47	1.52
9	P	3	BMA	C4-C3	-2.07	1.47	1.52
9	P	4	MAN	O5-C5	2.06	1.47	1.43
9	P	3	BMA	O3-C3	2.01	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	5	MAN	C1-C2-C3	2.80	113.11	109.67
9	P	1	NAG	O5-C5-C4	2.77	114.73	109.69
9	P	4	MAN	C1-C2-C3	2.71	113.00	109.67
9	P	1	NAG	C1-C2-C3	-2.58	107.03	110.54
9	P	2	NAG	C2-N2-C7	-2.37	119.53	122.90
9	P	2	NAG	C8-C7-N2	2.36	120.10	116.10
9	P	1	NAG	C3-C4-C5	2.36	114.45	110.24
9	P	3	BMA	C1-C2-C3	2.09	112.23	109.67
9	P	1	NAG	C1-O5-C5	-2.07	109.75	113.66
9	P	3	BMA	C6-C5-C4	-2.05	108.21	113.00
9	P	2	NAG	C1-C2-N2	-2.03	107.02	110.49

There are no chirality outliers.

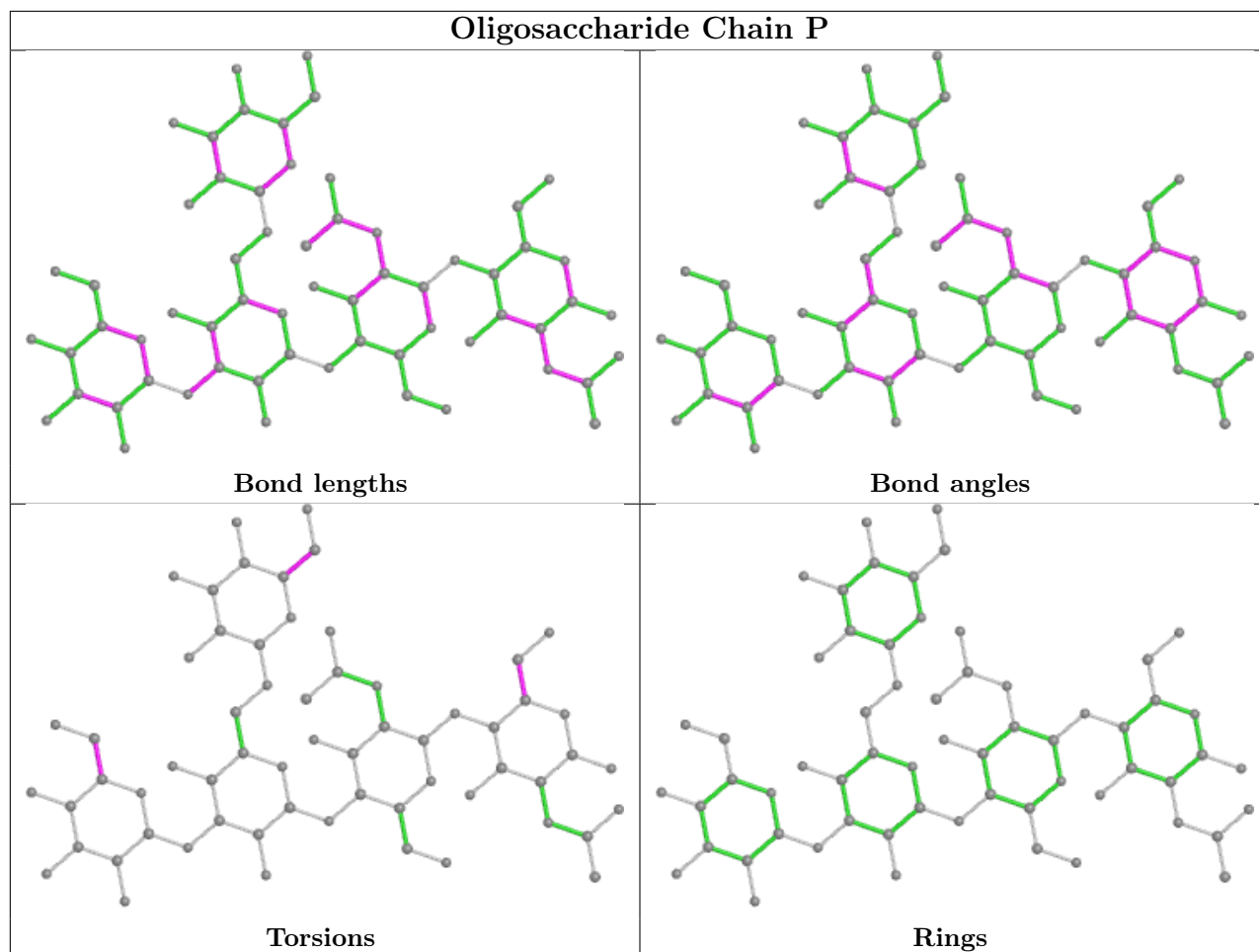
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	P	4	MAN	O5-C5-C6-O6
9	P	5	MAN	O5-C5-C6-O6
9	P	5	MAN	C4-C5-C6-O6
9	P	4	MAN	C4-C5-C6-O6
9	P	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

32 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$
10	PEE	B	401	-	44,44,50	0.78	2 (4%)	46,49,55	0.53	0
10	PEE	K	202	-	44,44,50	0.80	2 (4%)	47,49,55	0.53	0
10	PEE	K	201	-	50,50,50	0.74	2 (4%)	53,55,55	0.57	0
10	PEE	C	306	-	36,36,50	0.85	2 (5%)	38,41,55	0.55	0
10	PEE	A	903	-	50,50,50	0.73	2 (4%)	53,55,55	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PEE	J	202	-	38,38,50	0.64	1 (2%)	41,43,55	0.49	0
10	PEE	G	201	-	44,44,50	0.77	2 (4%)	47,49,55	0.58	0
10	PEE	C	302	-	46,46,50	0.77	2 (4%)	49,51,55	0.53	0
10	PEE	C	301	-	48,48,50	0.76	2 (4%)	51,53,55	0.53	0
10	PEE	H	201	-	36,36,50	0.86	2 (5%)	38,41,55	0.58	0
10	PEE	E	201	-	40,40,50	0.80	2 (5%)	42,45,55	0.53	0
10	PEE	M	101	-	48,48,50	0.75	2 (4%)	51,53,55	0.49	0
10	PEE	C	305	-	42,42,50	0.79	2 (4%)	44,47,55	0.53	0
10	PEE	M	102	-	46,46,50	0.75	2 (4%)	49,51,55	0.56	0
10	PEE	E	202	-	38,38,50	0.83	2 (5%)	39,43,55	0.53	0
10	PEE	A	905	-	34,34,50	0.88	2 (5%)	37,39,55	0.67	0
10	PEE	I	202	-	44,44,50	0.76	2 (4%)	47,49,55	0.60	0
10	PEE	A	902	-	40,40,50	0.82	2 (5%)	42,45,55	0.54	0
12	EYR	A	907	11	39,39,39	1.32	4 (10%)	46,46,46	1.79	14 (30%)
10	PEE	C	309	-	36,36,50	0.64	1 (2%)	39,41,55	0.50	0
10	PEE	J	201	-	40,40,50	0.82	2 (5%)	42,45,55	0.54	0
10	PEE	A	901	-	50,50,50	0.72	2 (4%)	53,55,55	0.53	0
10	PEE	A	904	-	42,42,50	0.77	2 (4%)	45,47,55	0.61	0
10	PEE	C	304	-	38,38,50	0.84	2 (5%)	41,43,55	0.61	0
10	PEE	C	307	-	38,38,50	0.84	2 (5%)	39,43,55	0.45	0
10	PEE	O	101	-	34,34,50	0.88	2 (5%)	37,39,55	0.61	0
10	PEE	I	201	-	42,42,50	0.79	2 (4%)	45,47,55	0.53	0
10	PEE	C	308	-	38,38,50	0.84	2 (5%)	39,43,55	0.51	0
11	PPV	A	906	12,9	3,7,8	1.95	1 (33%)	6,10,13	1.02	1 (16%)
10	PEE	F	201	-	38,38,50	0.85	2 (5%)	39,43,55	0.54	0
10	PEE	C	310	-	38,38,50	0.84	2 (5%)	39,43,55	0.52	0
10	PEE	C	303	-	40,40,50	0.64	1 (2%)	43,45,55	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PEE	B	401	-	-	11/48/48/54	-
10	PEE	K	202	-	-	12/48/48/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PEE	K	201	-	-	18/54/54/54	-
10	PEE	C	306	-	-	9/40/40/54	-
10	PEE	A	903	-	-	11/54/54/54	-
10	PEE	J	202	-	-	15/42/42/54	-
10	PEE	G	201	-	-	15/48/48/54	-
10	PEE	C	302	-	-	13/50/50/54	-
10	PEE	C	301	-	-	7/52/52/54	-
10	PEE	H	201	-	-	13/40/40/54	-
10	PEE	E	201	-	-	11/44/44/54	-
10	PEE	M	101	-	-	13/52/52/54	-
10	PEE	C	305	-	-	10/46/46/54	-
10	PEE	M	102	-	-	11/50/50/54	-
10	PEE	E	202	-	-	12/42/42/54	-
10	PEE	A	905	-	-	10/38/38/54	-
10	PEE	I	202	-	-	12/48/48/54	-
10	PEE	A	902	-	-	11/44/44/54	-
12	EYR	A	907	11	-	13/44/44/44	-
10	PEE	C	309	-	-	9/40/40/54	-
10	PEE	J	201	-	-	18/44/44/54	-
10	PEE	A	901	-	-	16/54/54/54	-
10	PEE	A	904	-	-	10/46/46/54	-
10	PEE	C	304	-	-	9/42/42/54	-
10	PEE	C	307	-	-	13/42/42/54	-
10	PEE	O	101	-	-	6/38/38/54	-
10	PEE	I	201	-	-	9/46/46/54	-
10	PEE	C	308	-	-	11/42/42/54	-
11	PPV	A	906	12,9	-	1/2/5/6	-
10	PEE	F	201	-	-	13/42/42/54	-
10	PEE	C	310	-	-	12/42/42/54	-
10	PEE	C	303	-	-	9/44/44/54	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	202	PEE	C39-C38	3.51	1.52	1.31
10	J	202	PEE	C18-C19	3.43	1.51	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	202	PEE	C18-C19	3.43	1.51	1.31
10	C	303	PEE	C18-C19	3.42	1.51	1.31
10	C	310	PEE	C18-C19	3.41	1.51	1.31
10	A	902	PEE	C39-C38	3.41	1.51	1.31
10	F	201	PEE	C39-C38	3.41	1.51	1.31
10	C	304	PEE	C18-C19	3.40	1.51	1.31
10	C	307	PEE	C18-C19	3.40	1.51	1.31
10	E	202	PEE	C39-C38	3.40	1.51	1.31
10	A	902	PEE	C18-C19	3.38	1.51	1.31
10	C	308	PEE	C18-C19	3.38	1.51	1.31
10	I	201	PEE	C18-C19	3.37	1.51	1.31
10	C	304	PEE	C39-C38	3.37	1.51	1.28
10	C	307	PEE	C39-C38	3.36	1.51	1.31
10	C	306	PEE	C19-C18	3.36	1.51	1.28
10	G	201	PEE	C18-C19	3.36	1.51	1.31
10	A	903	PEE	C39-C38	3.36	1.51	1.31
10	A	905	PEE	C39-C38	3.36	1.51	1.28
10	C	302	PEE	C39-C38	3.35	1.51	1.31
10	A	904	PEE	C39-C38	3.35	1.51	1.28
10	O	101	PEE	C39-C38	3.35	1.51	1.28
10	I	201	PEE	C39-C38	3.35	1.51	1.31
10	A	905	PEE	C19-C18	3.35	1.51	1.28
10	C	305	PEE	C18-C19	3.35	1.51	1.31
10	M	101	PEE	C18-C19	3.35	1.51	1.31
10	C	308	PEE	C39-C38	3.35	1.51	1.31
10	C	302	PEE	C18-C19	3.34	1.51	1.31
10	H	201	PEE	C19-C18	3.34	1.51	1.28
10	J	201	PEE	C18-C19	3.34	1.51	1.31
10	F	201	PEE	C18-C19	3.34	1.51	1.31
10	C	305	PEE	C39-C38	3.33	1.51	1.31
10	O	101	PEE	C19-C18	3.33	1.51	1.28
10	C	310	PEE	C39-C38	3.33	1.51	1.31
10	E	201	PEE	C18-C19	3.32	1.51	1.31
10	H	201	PEE	C39-C38	3.32	1.51	1.31
10	G	201	PEE	C39-C38	3.32	1.51	1.31
10	C	301	PEE	C39-C38	3.32	1.51	1.31
10	J	201	PEE	C39-C38	3.31	1.51	1.31
10	E	202	PEE	C18-C19	3.31	1.51	1.31
10	A	903	PEE	C18-C19	3.31	1.51	1.31
10	K	201	PEE	C39-C38	3.31	1.50	1.31
10	A	901	PEE	C18-C19	3.29	1.50	1.31
10	M	102	PEE	C18-C19	3.29	1.50	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	202	PEE	C18-C19	3.28	1.50	1.31
10	B	401	PEE	C18-C19	3.28	1.50	1.31
10	C	309	PEE	C18-C19	3.27	1.50	1.31
10	C	301	PEE	C18-C19	3.26	1.50	1.31
10	C	306	PEE	C39-C38	3.25	1.50	1.31
10	K	201	PEE	C18-C19	3.25	1.50	1.31
10	M	102	PEE	C39-C38	3.24	1.50	1.31
10	A	901	PEE	C39-C38	3.24	1.50	1.31
10	I	202	PEE	C39-C38	3.23	1.50	1.31
10	M	101	PEE	C39-C38	3.22	1.50	1.31
10	B	401	PEE	C39-C38	3.21	1.50	1.31
10	A	904	PEE	C18-C19	3.20	1.50	1.31
10	E	201	PEE	C39-C38	3.20	1.50	1.31
11	A	906	PPV	P2-O32	3.20	1.67	1.54
12	A	907	EYR	C57-C55	3.09	1.57	1.51
12	A	907	EYR	C77-C75	2.13	1.55	1.51
12	A	907	EYR	C53-C54	2.13	1.57	1.50
12	A	907	EYR	C82-C80	2.06	1.55	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	907	EYR	C63-C64-C65	-3.40	119.46	127.66
12	A	907	EYR	C73-C74-C75	-3.36	119.56	127.66
12	A	907	EYR	C78-C79-C80	-3.31	119.69	127.66
12	A	907	EYR	C56-C55-C57	3.25	120.75	115.27
12	A	907	EYR	C68-C69-C70	-3.14	120.11	127.66
12	A	907	EYR	C53-C54-C55	-2.99	120.46	127.66
12	A	907	EYR	C76-C75-C77	2.95	120.24	115.27
12	A	907	EYR	C61-C60-C62	2.89	120.14	115.27
12	A	907	EYR	C81-C80-C82	2.86	120.09	115.27
12	A	907	EYR	C58-C59-C60	-2.76	121.02	127.66
12	A	907	EYR	C83-C84-C85	-2.70	118.53	127.75
12	A	907	EYR	C66-C65-C67	2.64	119.72	115.27
12	A	907	EYR	C87-C85-C86	2.57	120.28	114.60
12	A	907	EYR	C71-C70-C72	2.41	119.32	115.27
11	A	906	PPV	O12-P2-OPP	2.01	111.36	104.64

There are no chirality outliers.

All (363) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	302	PEE	O2-C2-C3-O3
10	C	303	PEE	C17-C18-C19-C20
10	C	305	PEE	C1-O3P-P-O1P
10	C	306	PEE	C2-C1-O3P-P
10	C	309	PEE	C1-O3P-P-O4P
10	C	310	PEE	C2-C1-O3P-P
10	C	310	PEE	C1-O3P-P-O1P
10	M	101	PEE	C4-O4P-P-O1P
10	M	102	PEE	C4-O4P-P-O1P
10	M	102	PEE	C5-C4-O4P-P
10	E	201	PEE	C18-C19-C20-C21
10	E	201	PEE	C2-C1-O3P-P
10	E	202	PEE	C11-C10-O2-C2
10	G	201	PEE	C1-O3P-P-O1P
10	G	201	PEE	C1-O3P-P-O4P
10	G	201	PEE	O5-C30-O3-C3
10	H	201	PEE	C2-C1-O3P-P
10	H	201	PEE	C1-O3P-P-O4P
10	I	202	PEE	C5-C4-O4P-P
10	J	201	PEE	C1-O3P-P-O1P
10	J	201	PEE	C4-O4P-P-O3P
10	J	202	PEE	C5-C4-O4P-P
10	K	201	PEE	C1-O3P-P-O2P
10	A	901	PEE	C2-C1-O3P-P
10	A	901	PEE	C1-O3P-P-O1P
10	A	901	PEE	C4-O4P-P-O1P
10	A	901	PEE	C37-C38-C39-C40
10	A	902	PEE	C4-O4P-P-O1P
10	A	905	PEE	C5-C4-O4P-P
12	A	907	EYR	C50-C52-C53-C54
12	A	907	EYR	C69-C70-C72-C73
12	A	907	EYR	C71-C70-C72-C73
12	A	907	EYR	C79-C80-C82-C83
12	A	907	EYR	C81-C80-C82-C83
12	A	907	EYR	C80-C82-C83-C84
10	G	201	PEE	C31-C30-O3-C3
10	I	202	PEE	O5-C30-O3-C3
10	E	202	PEE	O4-C10-O2-C2
10	I	202	PEE	C31-C30-O3-C3
10	C	305	PEE	C17-C18-C19-C20
10	M	101	PEE	C17-C18-C19-C20
10	I	201	PEE	C17-C18-C19-C20
10	J	201	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
10	A	902	PEE	C37-C38-C39-C40
10	A	903	PEE	C17-C18-C19-C20
10	A	902	PEE	C11-C10-O2-C2
12	A	907	EYR	C70-C72-C73-C74
12	A	907	EYR	C75-C77-C78-C79
10	C	307	PEE	C17-C18-C19-C20
10	A	902	PEE	O4-C10-O2-C2
10	C	308	PEE	C10-C11-C12-C13
10	C	308	PEE	C17-C18-C19-C20
10	O	101	PEE	C4-O4P-P-O3P
10	A	901	PEE	C1-O3P-P-O4P
10	J	201	PEE	C11-C10-O2-C2
10	K	202	PEE	C11-C10-O2-C2
10	A	901	PEE	C33-C34-C35-C36
10	C	306	PEE	C16-C17-C18-C19
10	A	905	PEE	C16-C17-C18-C19
10	J	201	PEE	C30-C31-C32-C33
10	J	201	PEE	C33-C34-C35-C36
10	M	101	PEE	C34-C35-C36-C37
10	C	305	PEE	C10-C11-C12-C13
10	K	201	PEE	C21-C22-C23-C24
10	E	201	PEE	C30-C31-C32-C33
10	J	201	PEE	O4-C10-O2-C2
10	K	202	PEE	O4-C10-O2-C2
10	H	201	PEE	C31-C30-O3-C3
10	H	201	PEE	C38-C39-C40-C41
10	J	201	PEE	C38-C39-C40-C41
10	B	401	PEE	C18-C19-C20-C21
10	G	201	PEE	C40-C41-C42-C43
10	C	309	PEE	C32-C33-C34-C35
10	A	903	PEE	C40-C41-C42-C43
10	G	201	PEE	C2-C3-O3-C30
10	B	401	PEE	C14-C15-C16-C17
10	C	309	PEE	C11-C10-O2-C2
10	K	201	PEE	C41-C42-C43-C44
10	C	307	PEE	O2-C2-C3-O3
10	M	101	PEE	C21-C22-C23-C24
10	H	201	PEE	O5-C30-O3-C3
10	A	903	PEE	C34-C35-C36-C37
10	J	201	PEE	C1-O3P-P-O4P
10	C	308	PEE	O3P-C1-C2-C3
10	K	202	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	K	201	PEE	C10-C11-C12-C13
10	A	904	PEE	C1-C2-C3-O3
10	C	306	PEE	O3P-C1-C2-O2
10	A	902	PEE	O3P-C1-C2-O2
10	C	303	PEE	C13-C14-C15-C16
10	C	303	PEE	C15-C16-C17-C18
10	A	904	PEE	O2-C2-C3-O3
10	K	201	PEE	C32-C33-C34-C35
10	A	905	PEE	O3-C30-C31-C32
10	A	903	PEE	C36-C37-C38-C39
10	F	201	PEE	O3P-C1-C2-C3
10	J	201	PEE	O3P-C1-C2-C3
10	J	202	PEE	O3P-C1-C2-C3
10	E	202	PEE	O2-C10-C11-C12
10	G	201	PEE	C10-C11-C12-C13
10	C	307	PEE	C1-C2-C3-O3
10	C	305	PEE	C37-C38-C39-C40
10	C	310	PEE	C1-O3P-P-O4P
10	A	905	PEE	C4-O4P-P-O3P
10	C	303	PEE	C10-C11-C12-C13
10	C	308	PEE	O3P-C1-C2-O2
10	J	202	PEE	O3P-C1-C2-O2
10	F	201	PEE	C31-C30-O3-C3
10	J	201	PEE	O2-C2-C3-O3
10	H	201	PEE	O2-C10-C11-C12
10	F	201	PEE	C2-C1-O3P-P
10	B	401	PEE	C34-C35-C36-C37
10	J	202	PEE	C10-C11-C12-C13
10	C	305	PEE	C18-C19-C20-C21
10	C	306	PEE	C38-C39-C40-C41
10	C	307	PEE	C18-C19-C20-C21
10	C	307	PEE	C38-C39-C40-C41
10	C	308	PEE	C18-C19-C20-C21
10	C	308	PEE	C38-C39-C40-C41
10	C	310	PEE	C18-C19-C20-C21
10	C	310	PEE	C38-C39-C40-C41
10	E	202	PEE	C18-C19-C20-C21
10	E	202	PEE	C38-C39-C40-C41
10	F	201	PEE	C18-C19-C20-C21
10	F	201	PEE	C38-C39-C40-C41
10	A	902	PEE	C38-C39-C40-C41
10	C	306	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	A	907	EYR	C49-C50-C52-C53
10	B	401	PEE	C38-C39-C40-C41
12	A	907	EYR	C48-C49-C50-C52
10	C	302	PEE	C1-C2-C3-O3
10	F	201	PEE	O3P-C1-C2-O2
10	A	905	PEE	O2-C10-C11-C12
10	C	304	PEE	C36-C37-C38-C39
10	O	101	PEE	C36-C37-C38-C39
10	H	201	PEE	C16-C17-C18-C19
10	C	309	PEE	O4-C10-O2-C2
10	F	201	PEE	O5-C30-O3-C3
10	C	302	PEE	O5-C30-O3-C3
10	C	302	PEE	C31-C30-O3-C3
10	C	304	PEE	C4-O4P-P-O3P
10	C	307	PEE	C1-O3P-P-O4P
10	O	101	PEE	C1-O3P-P-O4P
10	B	401	PEE	C1-O3P-P-O4P
10	A	902	PEE	C4-O4P-P-O3P
10	B	401	PEE	C40-C41-C42-C43
10	C	309	PEE	C1-O3P-P-O2P
10	O	101	PEE	C4-O4P-P-O2P
10	H	201	PEE	C1-O3P-P-O2P
10	J	201	PEE	C4-O4P-P-O2P
10	C	310	PEE	O3P-C1-C2-C3
10	A	904	PEE	C36-C37-C38-C39
10	A	905	PEE	C36-C37-C38-C39
10	C	303	PEE	C5-C4-O4P-P
10	C	304	PEE	C5-C4-O4P-P
10	C	305	PEE	C5-C4-O4P-P
10	C	307	PEE	C5-C4-O4P-P
10	C	310	PEE	C5-C4-O4P-P
10	J	201	PEE	C5-C4-O4P-P
10	B	401	PEE	C5-C4-O4P-P
10	A	901	PEE	C5-C4-O4P-P
10	F	201	PEE	C34-C35-C36-C37
10	C	310	PEE	O3P-C1-C2-O2
10	K	202	PEE	O3P-C1-C2-O2
10	C	303	PEE	C16-C17-C18-C19
10	A	904	PEE	O5-C30-O3-C3
10	G	201	PEE	C32-C33-C34-C35
10	M	101	PEE	C10-C11-C12-C13
10	M	102	PEE	O2-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
10	M	102	PEE	C37-C38-C39-C40
10	C	301	PEE	C36-C37-C38-C39
10	K	201	PEE	C38-C39-C40-C41
12	A	907	EYR	C48-C49-C50-C51
10	K	201	PEE	C31-C30-O3-C3
12	A	907	EYR	C51-C50-C52-C53
12	A	907	EYR	C55-C57-C58-C59
10	J	202	PEE	C22-C23-C24-C25
10	A	903	PEE	C35-C36-C37-C38
10	B	401	PEE	C37-C38-C39-C40
10	E	202	PEE	C33-C34-C35-C36
10	E	201	PEE	C38-C39-C40-C41
10	I	202	PEE	C1-C2-O2-C10
10	A	902	PEE	O3P-C1-C2-C3
10	E	201	PEE	O5-C30-O3-C3
10	C	309	PEE	C16-C17-C18-C19
10	E	201	PEE	C31-C30-O3-C3
10	K	201	PEE	C17-C18-C19-C20
10	O	101	PEE	C16-C17-C18-C19
10	C	302	PEE	C11-C10-O2-C2
10	J	202	PEE	C11-C10-O2-C2
10	F	201	PEE	C36-C37-C38-C39
10	H	201	PEE	C36-C37-C38-C39
10	I	201	PEE	C16-C17-C18-C19
10	C	301	PEE	C4-O4P-P-O3P
10	C	302	PEE	C1-O3P-P-O4P
10	C	302	PEE	C4-O4P-P-O3P
10	C	305	PEE	C1-O3P-P-O4P
10	C	306	PEE	C1-O3P-P-O4P
10	C	306	PEE	C4-O4P-P-O3P
10	C	307	PEE	C4-O4P-P-O3P
10	C	308	PEE	C4-O4P-P-O3P
10	C	310	PEE	C4-O4P-P-O3P
10	M	102	PEE	C4-O4P-P-O3P
10	E	201	PEE	C1-O3P-P-O4P
10	E	201	PEE	C4-O4P-P-O3P
10	E	202	PEE	C4-O4P-P-O3P
10	F	201	PEE	C1-O3P-P-O4P
10	H	201	PEE	C4-O4P-P-O3P
10	I	202	PEE	C4-O4P-P-O3P
10	J	202	PEE	C1-O3P-P-O4P
10	J	202	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
10	K	202	PEE	C4-O4P-P-O3P
10	A	901	PEE	C4-O4P-P-O3P
10	A	903	PEE	C4-O4P-P-O3P
10	A	904	PEE	C1-O3P-P-O4P
10	A	905	PEE	C1-O3P-P-O4P
10	C	302	PEE	C16-C17-C18-C19
10	C	302	PEE	C36-C37-C38-C39
10	I	201	PEE	C38-C39-C40-C41
10	C	309	PEE	C12-C13-C14-C15
10	C	305	PEE	C36-C37-C38-C39
10	E	201	PEE	C36-C37-C38-C39
10	I	202	PEE	C38-C39-C40-C41
10	K	202	PEE	C16-C17-C18-C19
10	A	901	PEE	C38-C39-C40-C41
10	A	903	PEE	C38-C39-C40-C41
10	A	904	PEE	C31-C30-O3-C3
10	K	201	PEE	O5-C30-O3-C3
10	M	101	PEE	C18-C19-C20-C21
10	K	201	PEE	C36-C37-C38-C39
10	H	201	PEE	O3P-C1-C2-O2
10	C	310	PEE	C16-C17-C18-C19
10	J	201	PEE	C18-C19-C20-C21
10	C	304	PEE	C16-C17-C18-C19
10	I	202	PEE	C16-C17-C18-C19
10	K	201	PEE	C16-C17-C18-C19
10	A	901	PEE	C16-C17-C18-C19
10	A	903	PEE	C16-C17-C18-C19
10	A	905	PEE	O5-C30-C31-C32
10	C	301	PEE	C19-C20-C21-C22
10	A	904	PEE	C33-C34-C35-C36
10	C	304	PEE	C18-C19-C20-C21
10	J	201	PEE	C16-C17-C18-C19
10	A	902	PEE	C16-C17-C18-C19
10	C	304	PEE	C1-O3P-P-O4P
11	A	906	PPV	P1-OPP-P2-O12
10	A	904	PEE	O2-C10-C11-C12
10	K	201	PEE	C30-C31-C32-C33
10	I	202	PEE	O3P-C1-C2-O2
10	M	101	PEE	C24-C25-C26-C27
10	H	201	PEE	O3P-C1-C2-C3
10	I	202	PEE	C18-C19-C20-C21
10	J	202	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
10	C	308	PEE	O2-C2-C3-O3
10	C	303	PEE	C14-C15-C16-C17
10	G	201	PEE	C17-C18-C19-C20
10	C	302	PEE	C18-C19-C20-C21
10	K	201	PEE	C18-C19-C20-C21
10	A	903	PEE	C18-C19-C20-C21
10	M	102	PEE	C34-C35-C36-C37
10	K	202	PEE	C32-C33-C34-C35
10	C	302	PEE	C38-C39-C40-C41
10	C	307	PEE	C14-C15-C16-C17
10	K	201	PEE	C34-C35-C36-C37
10	A	901	PEE	C23-C24-C25-C26
10	C	306	PEE	C11-C12-C13-C14
10	C	310	PEE	C36-C37-C38-C39
10	J	201	PEE	O3P-C1-C2-O2
10	I	201	PEE	C2-C3-O3-C30
10	A	901	PEE	C13-C14-C15-C16
10	C	302	PEE	C12-C13-C14-C15
10	E	201	PEE	C16-C17-C18-C19
10	I	202	PEE	O2-C10-C11-C12
10	C	301	PEE	C16-C17-C18-C19
10	C	303	PEE	C18-C19-C20-C21
10	C	305	PEE	C16-C17-C18-C19
10	C	307	PEE	C16-C17-C18-C19
10	M	101	PEE	C36-C37-C38-C39
10	M	102	PEE	C16-C17-C18-C19
10	M	102	PEE	C36-C37-C38-C39
10	M	102	PEE	C38-C39-C40-C41
10	G	201	PEE	C18-C19-C20-C21
10	G	201	PEE	C36-C37-C38-C39
10	J	202	PEE	C18-C19-C20-C21
10	K	202	PEE	C18-C19-C20-C21
10	A	901	PEE	C18-C19-C20-C21
10	E	202	PEE	C1-C2-O2-C10
10	C	301	PEE	C38-C39-C40-C41
10	C	306	PEE	C36-C37-C38-C39
10	C	308	PEE	C16-C17-C18-C19
10	C	308	PEE	C36-C37-C38-C39
10	M	101	PEE	C38-C39-C40-C41
10	F	201	PEE	C16-C17-C18-C19
10	G	201	PEE	C38-C39-C40-C41
10	J	202	PEE	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
10	K	202	PEE	C36-C37-C38-C39
10	K	202	PEE	C38-C39-C40-C41
10	A	901	PEE	C36-C37-C38-C39
10	G	201	PEE	C42-C43-C44-C45
10	E	202	PEE	O4-C10-C11-C12
10	J	202	PEE	C12-C13-C14-C15
10	A	901	PEE	O2-C10-C11-C12
10	M	101	PEE	C16-C17-C18-C19
10	I	201	PEE	C36-C37-C38-C39
10	B	401	PEE	C16-C17-C18-C19
10	H	201	PEE	O4-C10-C11-C12
10	C	308	PEE	C11-C10-O2-C2
10	J	202	PEE	O4-C10-O2-C2
10	C	305	PEE	C38-C39-C40-C41
10	C	307	PEE	C36-C37-C38-C39
10	C	309	PEE	C18-C19-C20-C21
10	E	202	PEE	C16-C17-C18-C19
10	E	202	PEE	C36-C37-C38-C39
10	I	201	PEE	C18-C19-C20-C21
10	A	902	PEE	C18-C19-C20-C21
10	K	201	PEE	C11-C10-O2-C2
10	M	102	PEE	C18-C19-C20-C21
10	G	201	PEE	C16-C17-C18-C19
10	I	202	PEE	O4-C10-C11-C12
10	C	301	PEE	C4-O4P-P-O1P
10	C	302	PEE	C4-O4P-P-O1P
10	C	304	PEE	C1-O3P-P-O1P
10	C	307	PEE	C4-O4P-P-O1P
10	C	310	PEE	C4-O4P-P-O1P
10	M	101	PEE	C1-O3P-P-O1P
10	E	201	PEE	C1-O3P-P-O1P
10	I	202	PEE	C4-O4P-P-O1P
10	J	202	PEE	C4-O4P-P-O1P
10	K	201	PEE	C1-O3P-P-O1P
10	K	202	PEE	C1-O3P-P-O1P
10	B	401	PEE	C4-O4P-P-O2P
10	A	904	PEE	C1-O3P-P-O1P
10	A	904	PEE	C4-O4P-P-O1P
10	A	905	PEE	C4-O4P-P-O2P
10	C	301	PEE	O3P-C1-C2-C3
10	M	102	PEE	C40-C41-C42-C43
10	C	307	PEE	O4P-C4-C5-N

Continued on next page...

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Mol	Chain	Res	Type	Atoms
10	E	202	PEE	O4P-C4-C5-N
10	B	401	PEE	O4P-C4-C5-N
10	A	901	PEE	O4-C10-C11-C12
10	J	201	PEE	O2-C10-C11-C12
10	A	905	PEE	C33-C34-C35-C36
10	K	201	PEE	C5-C4-O4P-P
10	M	101	PEE	O2-C10-C11-C12
10	F	201	PEE	O2-C10-C11-C12
10	I	201	PEE	O2-C10-C11-C12
10	K	201	PEE	C44-C45-C46-C47
10	C	304	PEE	O3-C30-C31-C32
10	C	309	PEE	O2-C10-C11-C12
10	G	201	PEE	O2-C10-C11-C12
10	K	202	PEE	O3-C30-C31-C32
10	C	303	PEE	O3-C30-C31-C32
10	A	902	PEE	O3-C30-C31-C32
10	A	903	PEE	C31-C32-C33-C34
10	C	304	PEE	O5-C30-C31-C32
10	M	101	PEE	O4-C10-C11-C12
10	F	201	PEE	O4-C10-C11-C12
10	I	201	PEE	O4-C10-C11-C12
10	J	201	PEE	O4-C10-C11-C12
10	J	202	PEE	O3-C30-C31-C32
10	O	101	PEE	C12-C13-C14-C15
10	I	201	PEE	C12-C13-C14-C15
10	A	903	PEE	C33-C34-C35-C36

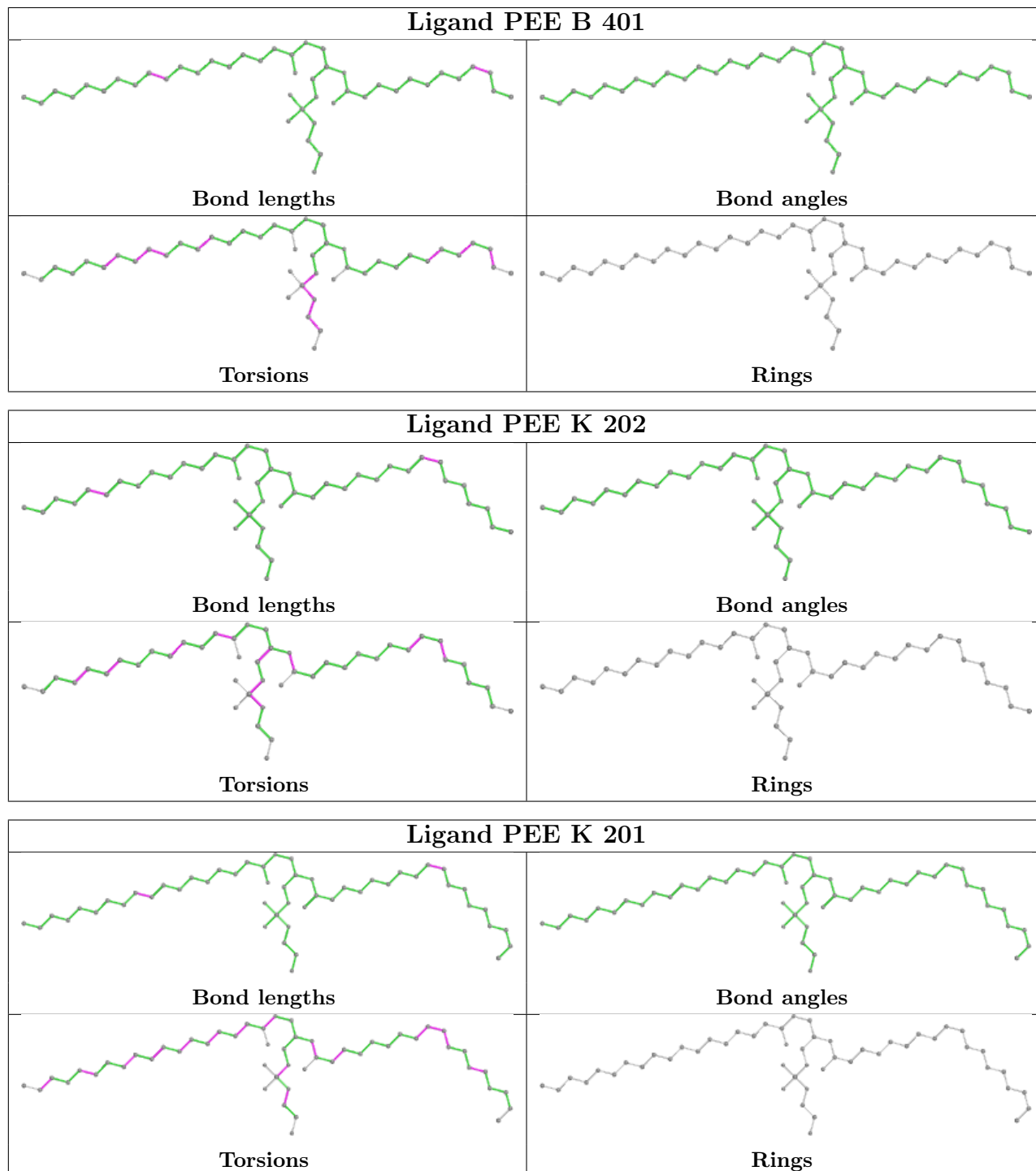
There are no ring outliers.

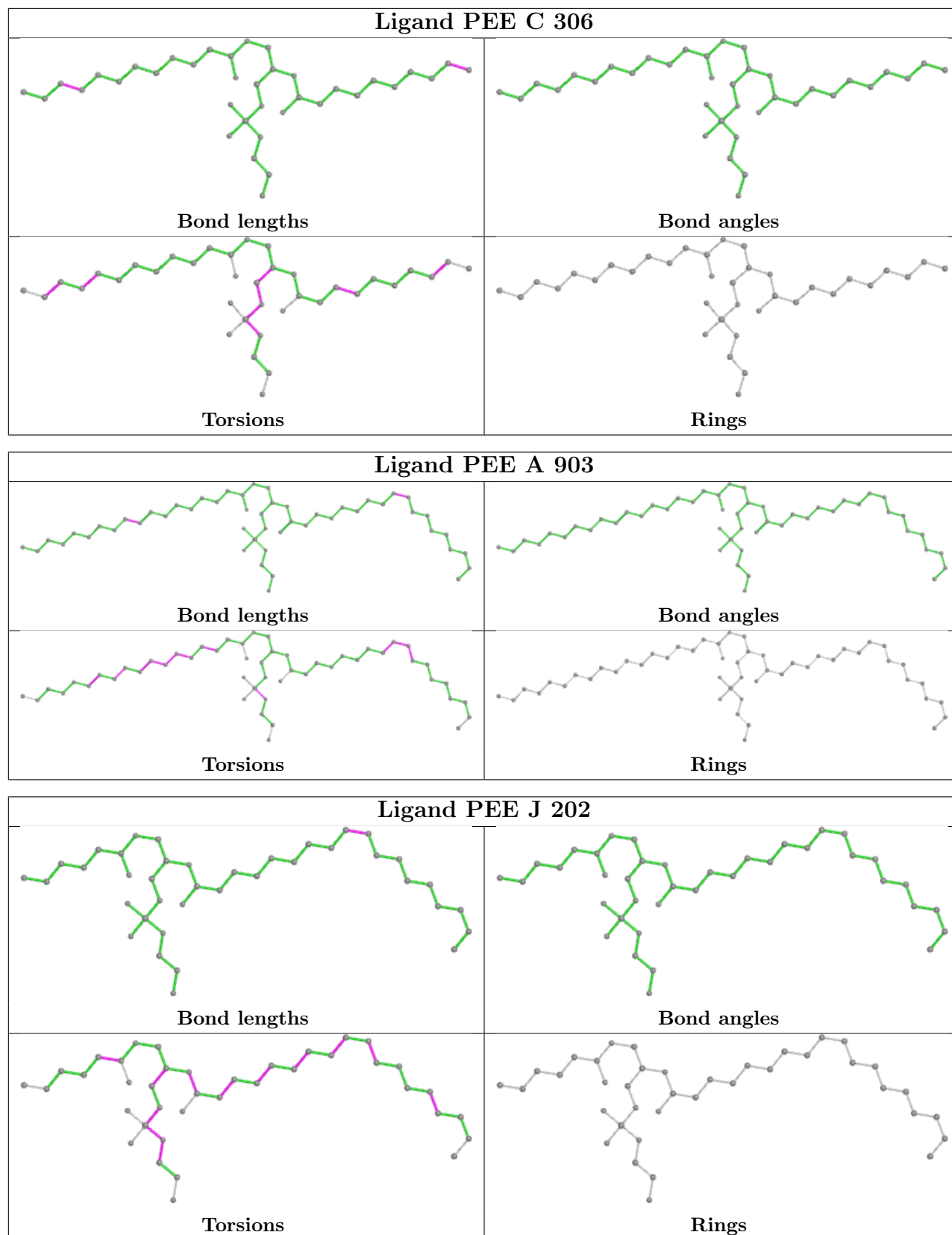
3 monomers are involved in 4 short contacts:

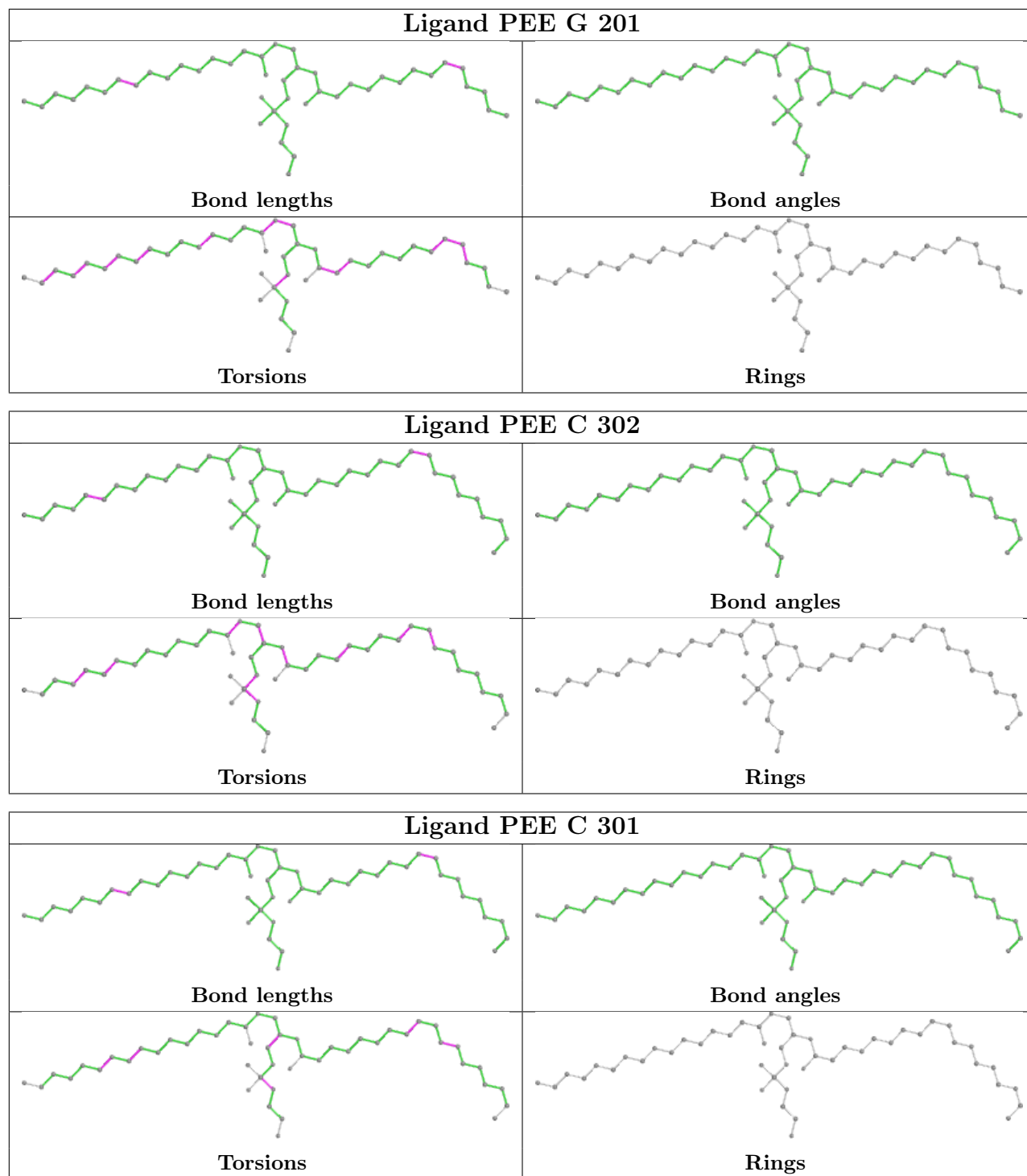
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	401	PEE	2	0
10	A	903	PEE	1	0
10	A	902	PEE	1	0

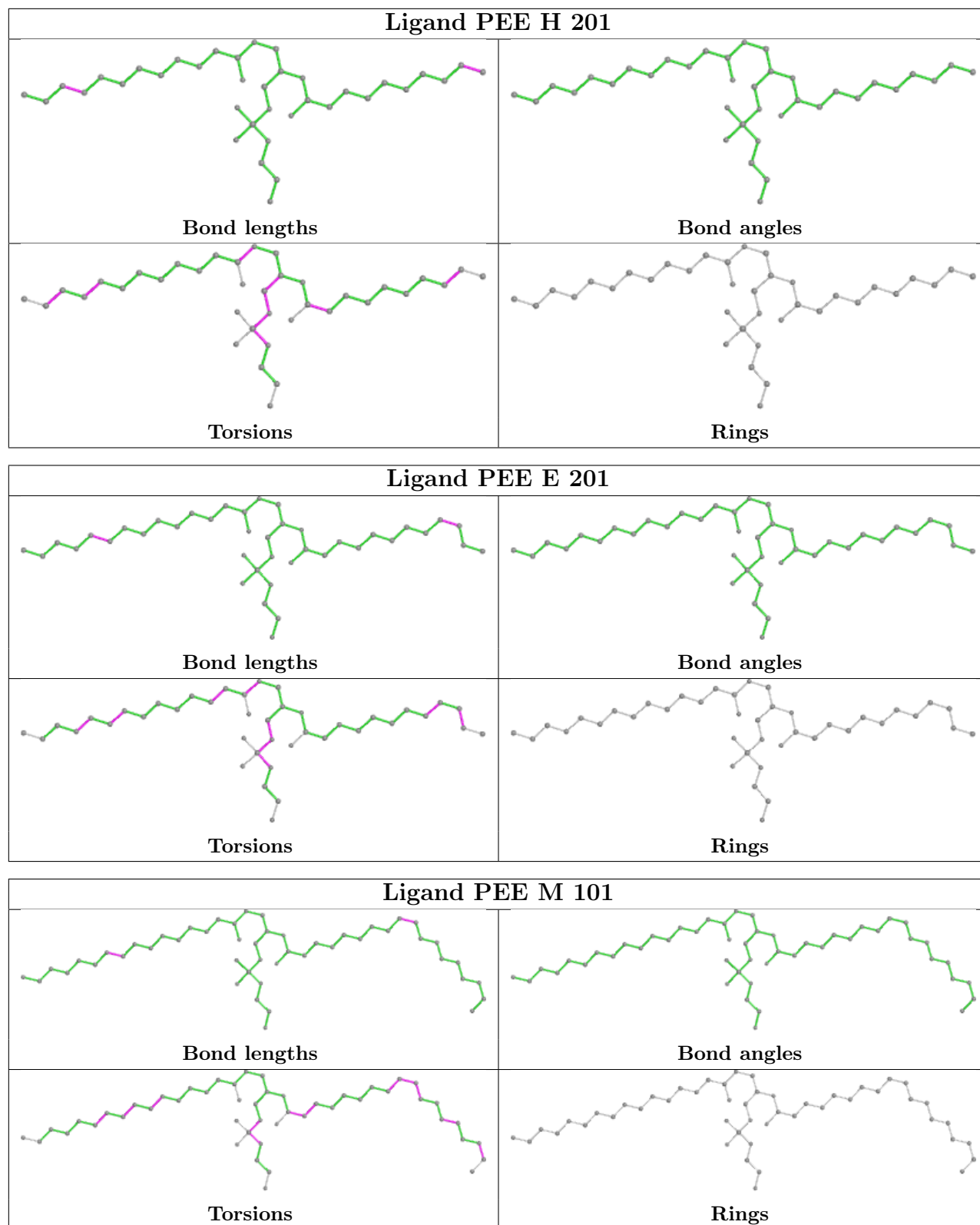
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

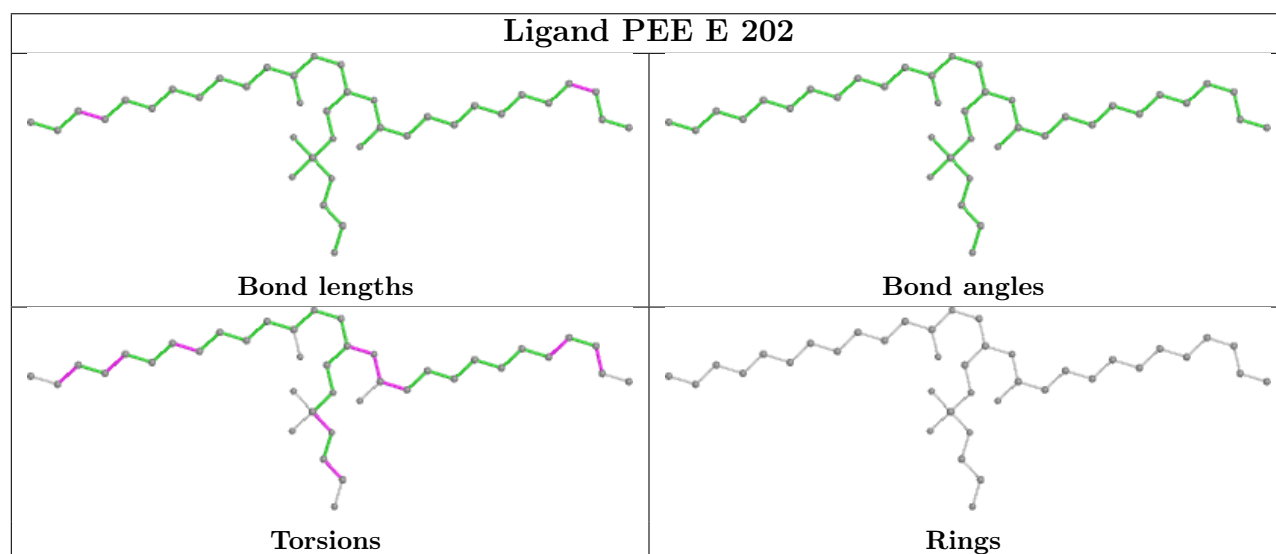
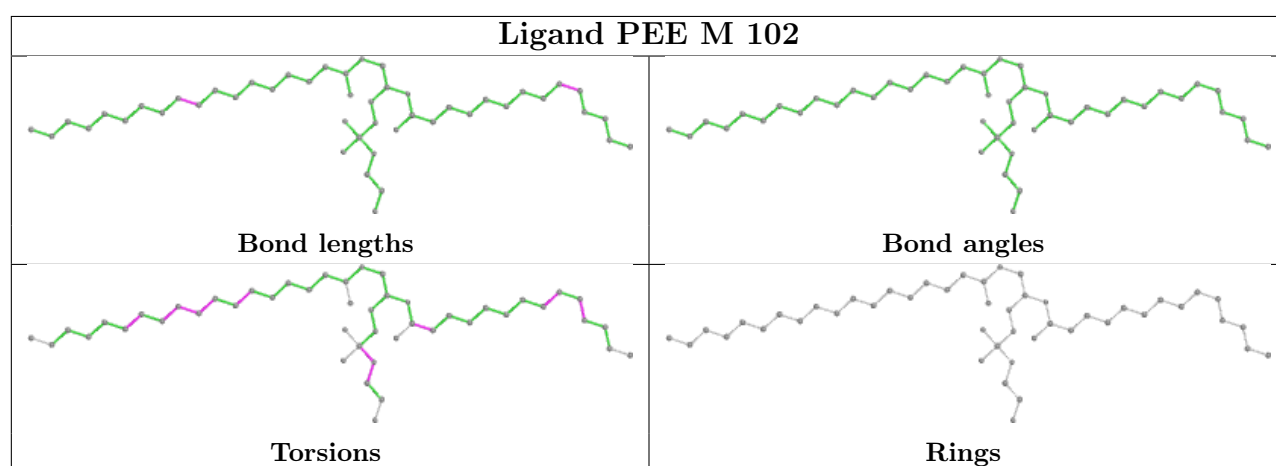
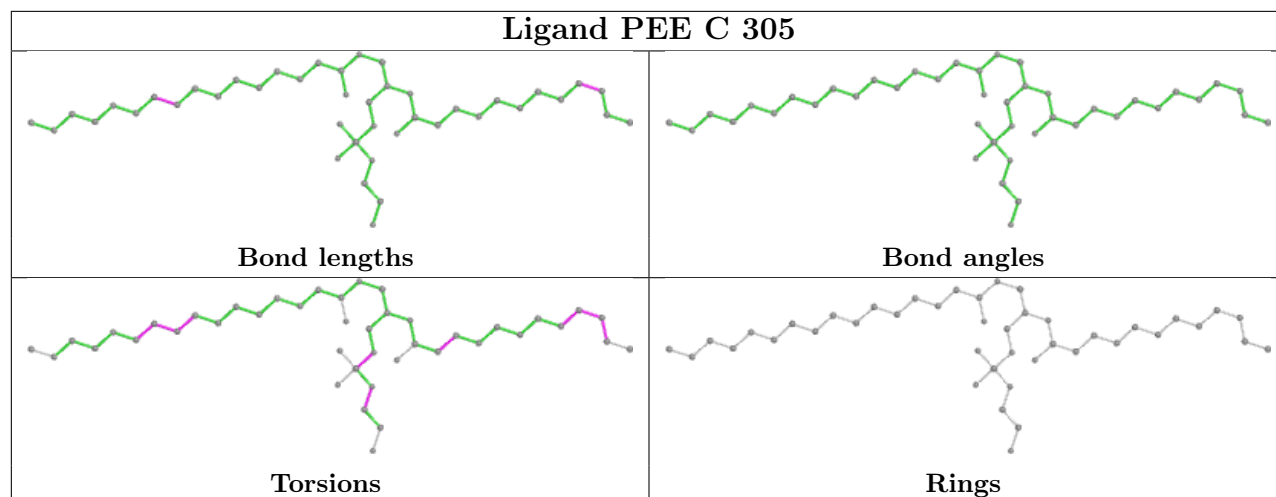
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

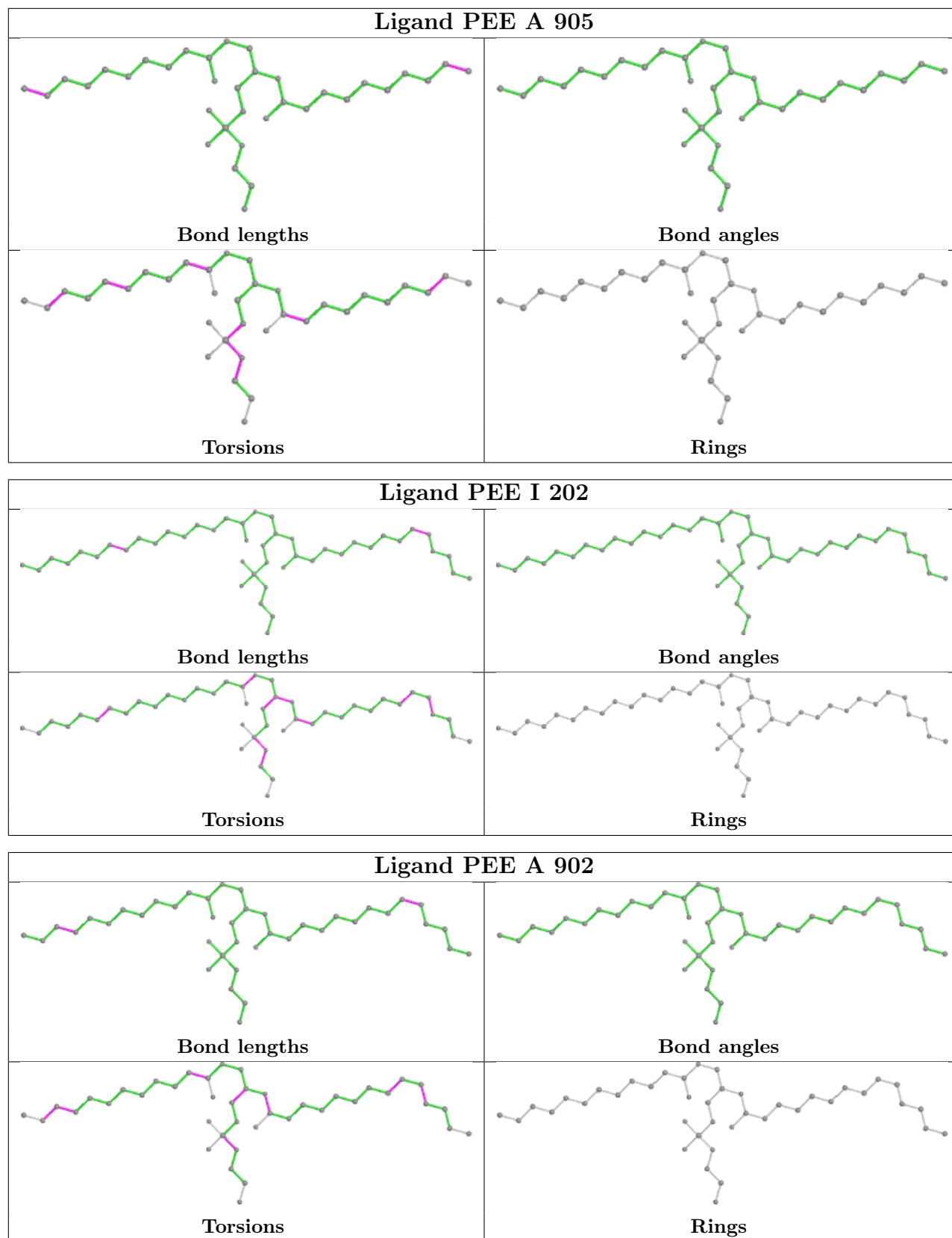


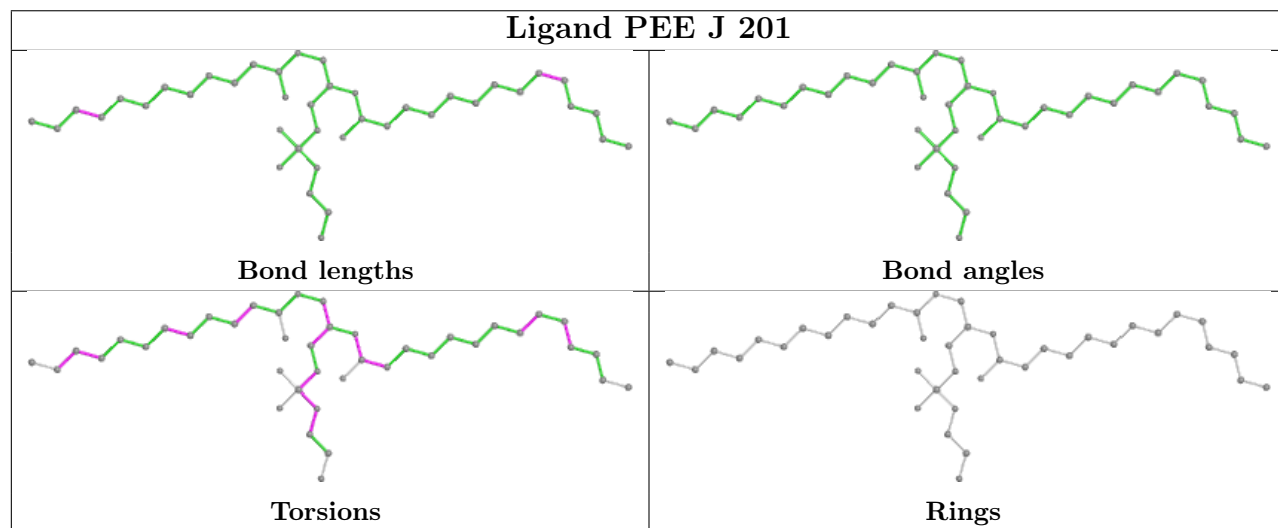
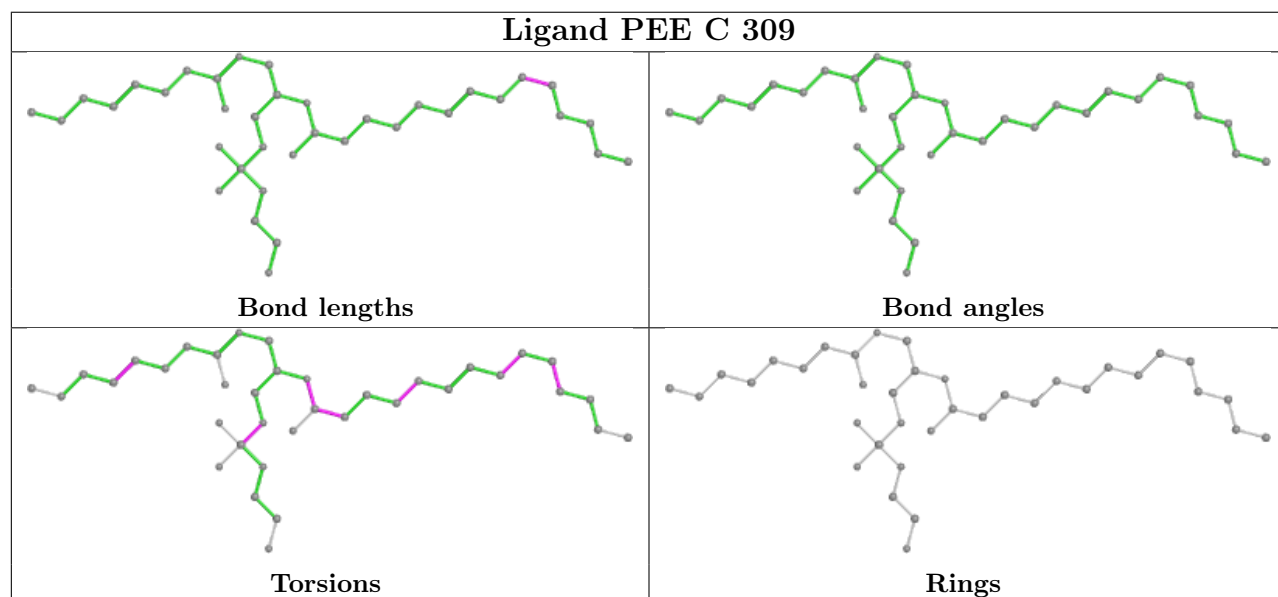
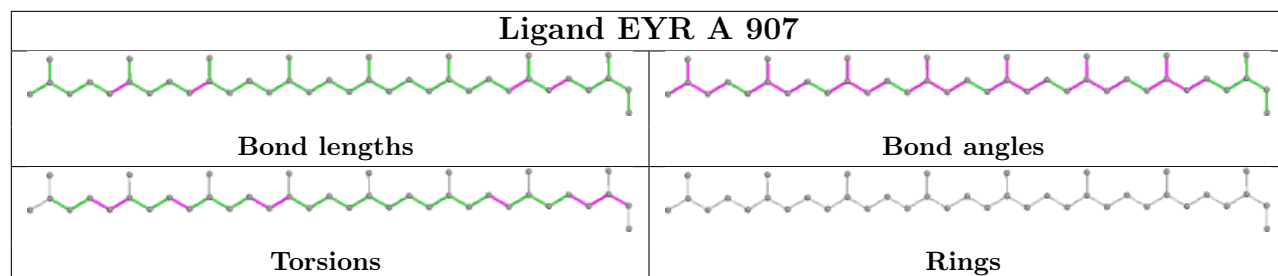


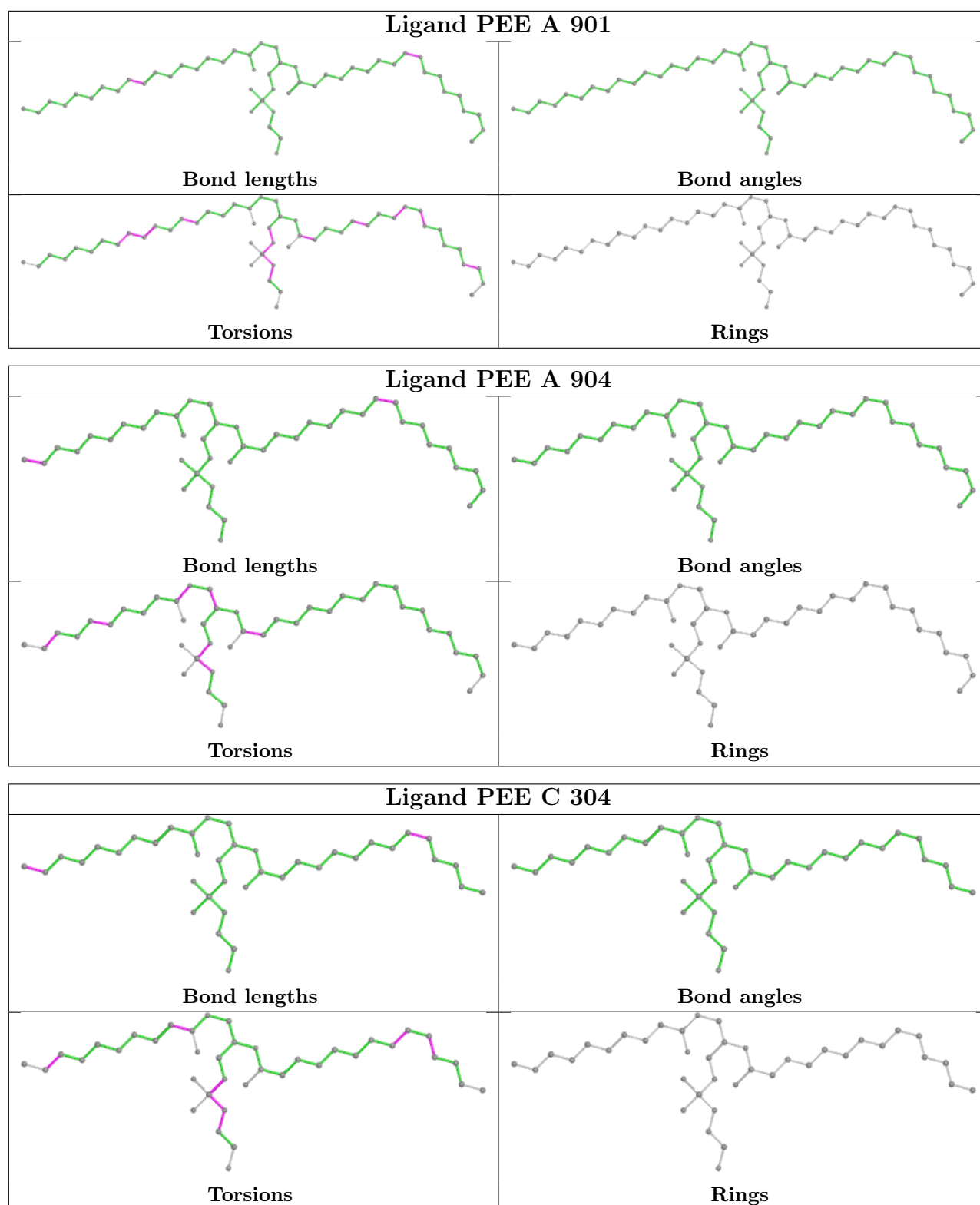


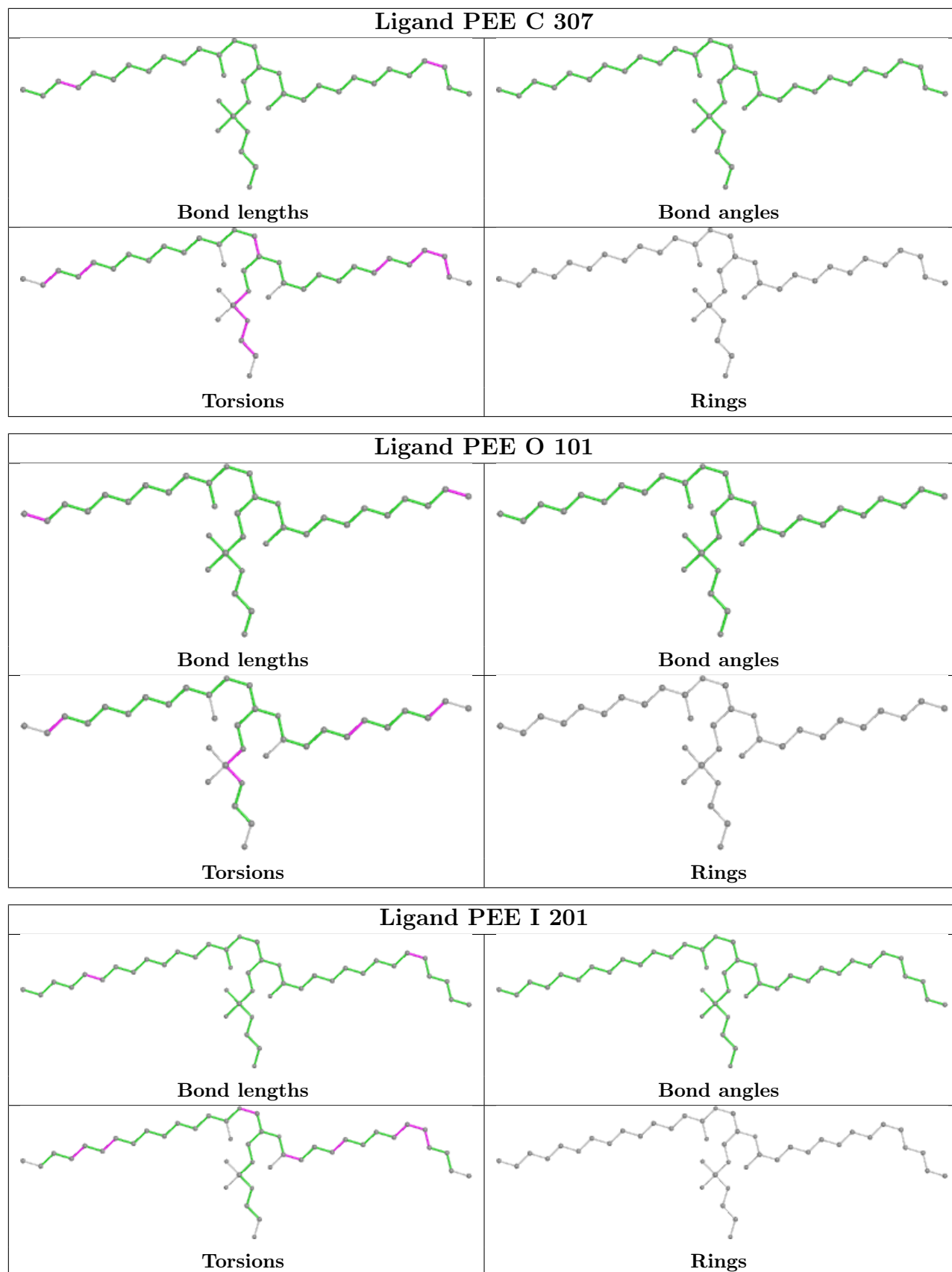


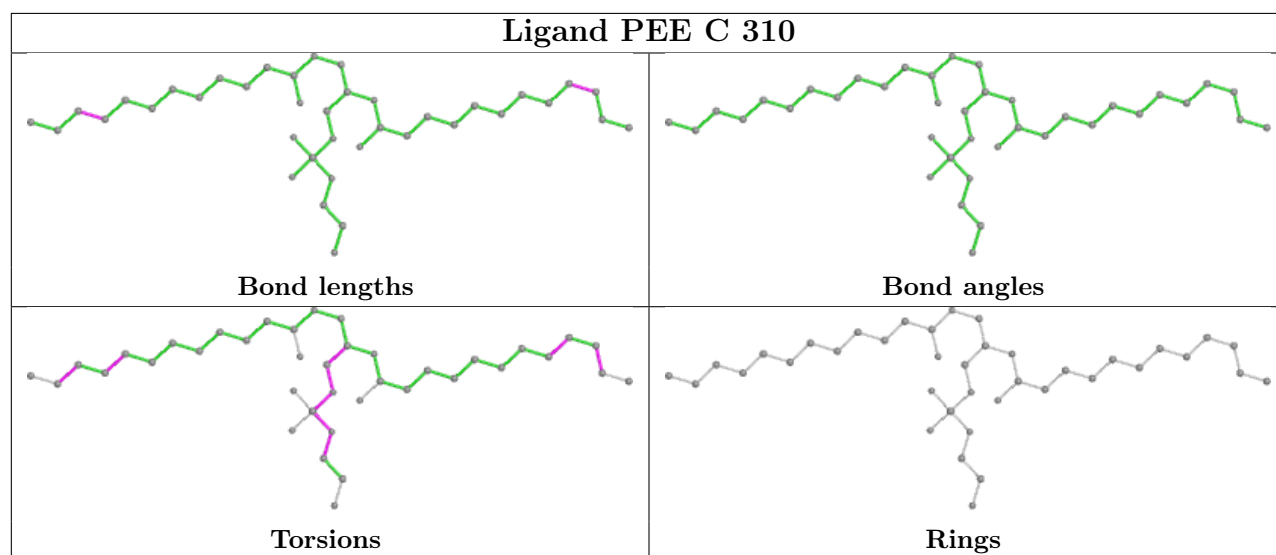
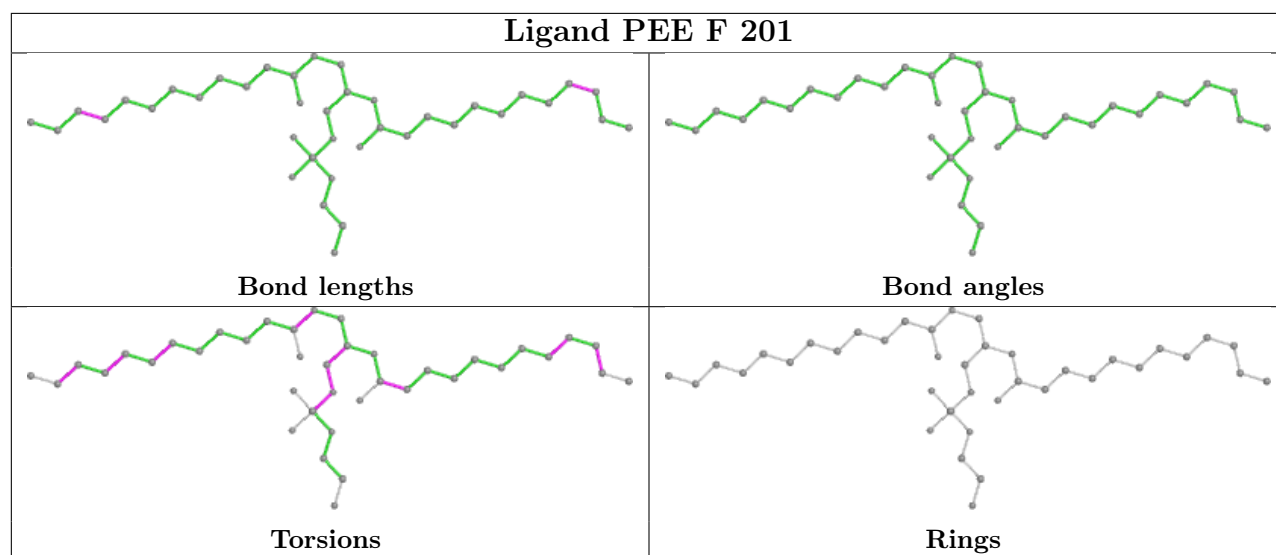
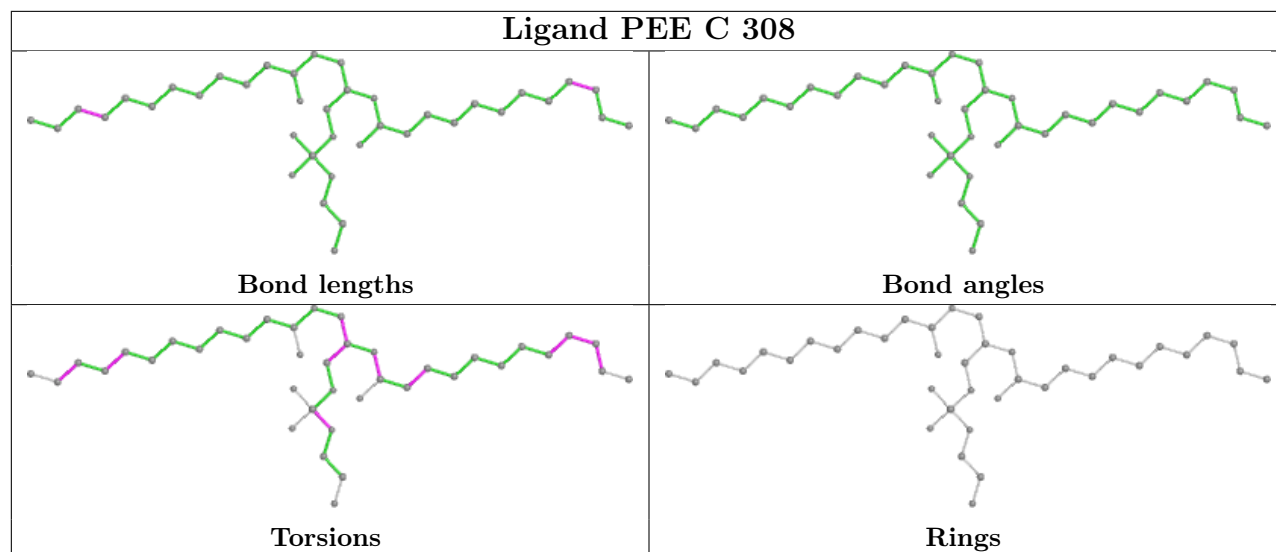


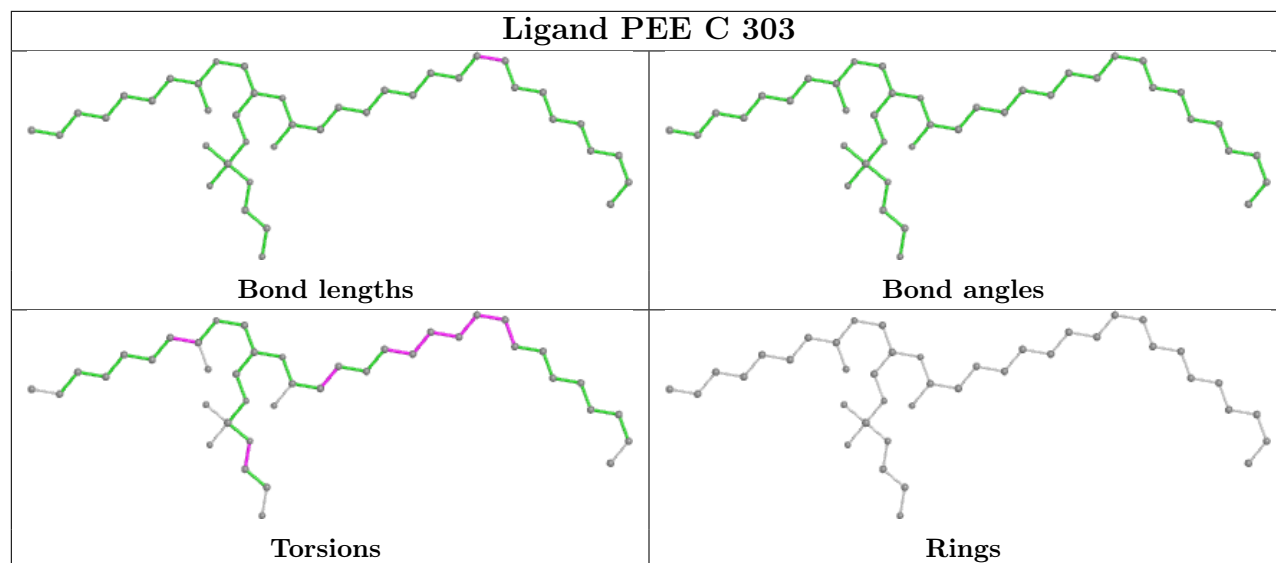












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

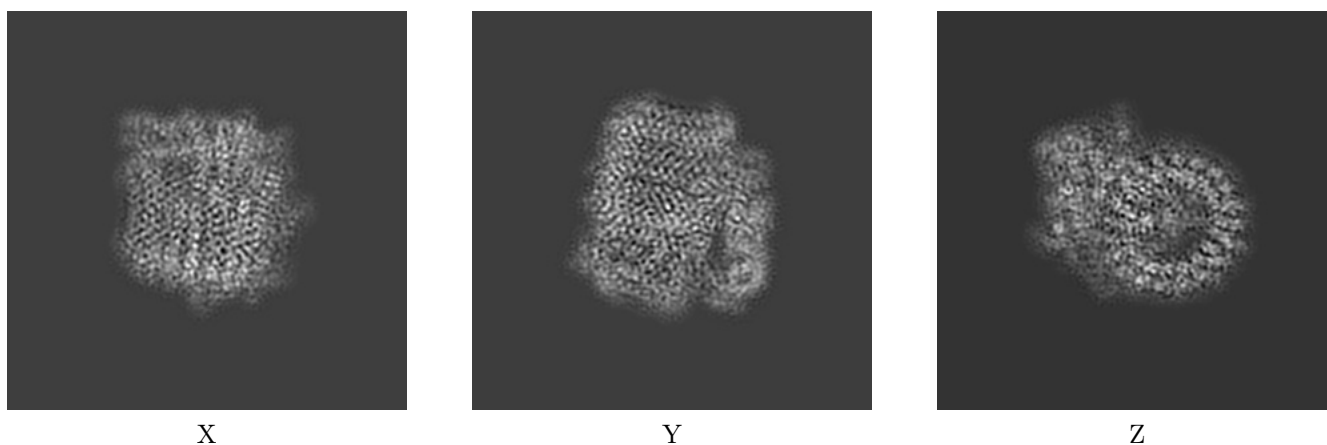
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30034. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

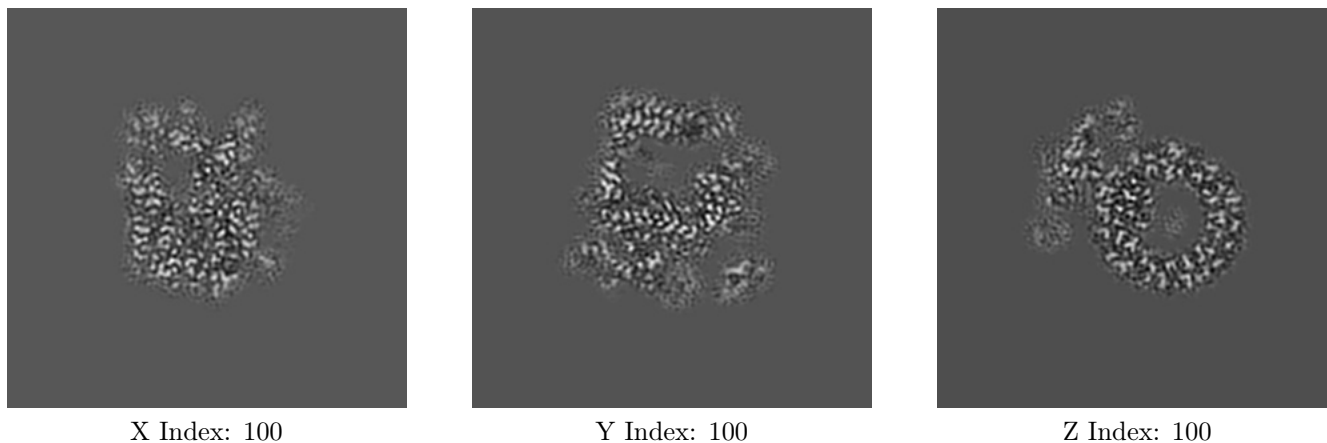
6.1.1 Primary map



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

6.2 Central slices [i](#)

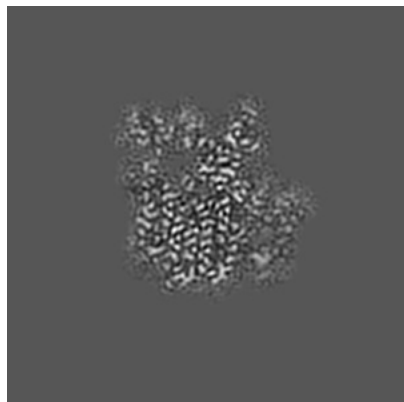
6.2.1 Primary map



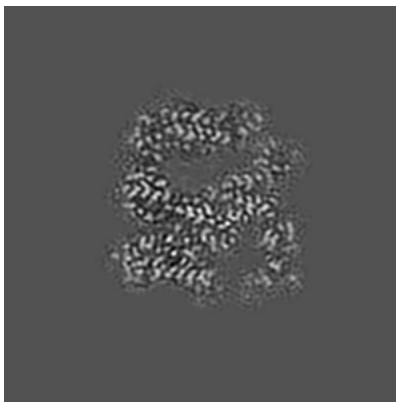
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

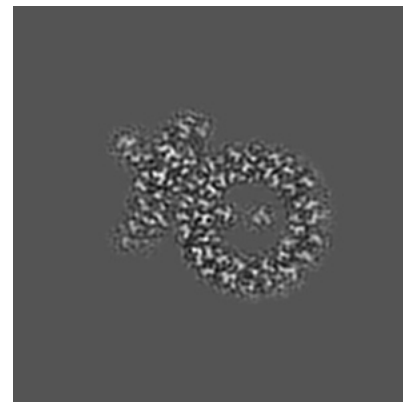
6.3.1 Primary map



X Index: 96



Y Index: 109

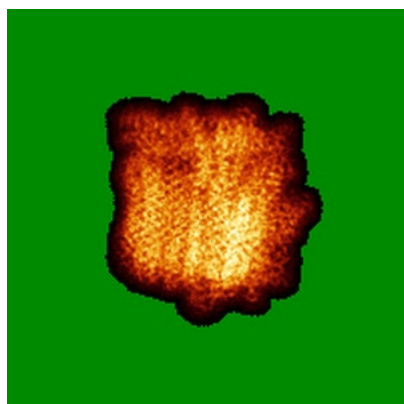


Z Index: 87

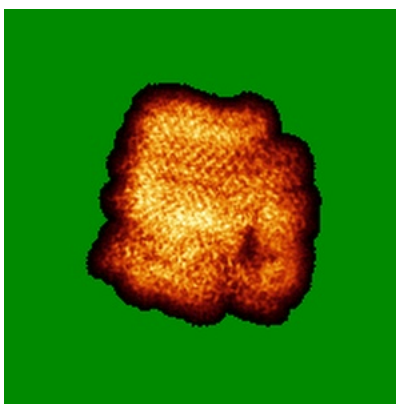
The images above show the largest variance slices of the map in three orthogonal directions.

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

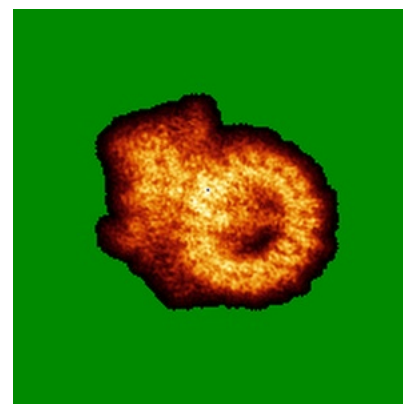
6.4.1 Primary map



X



Y

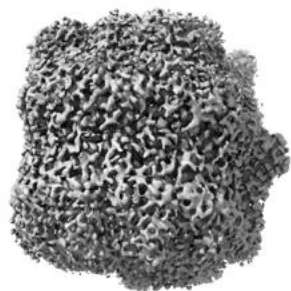


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

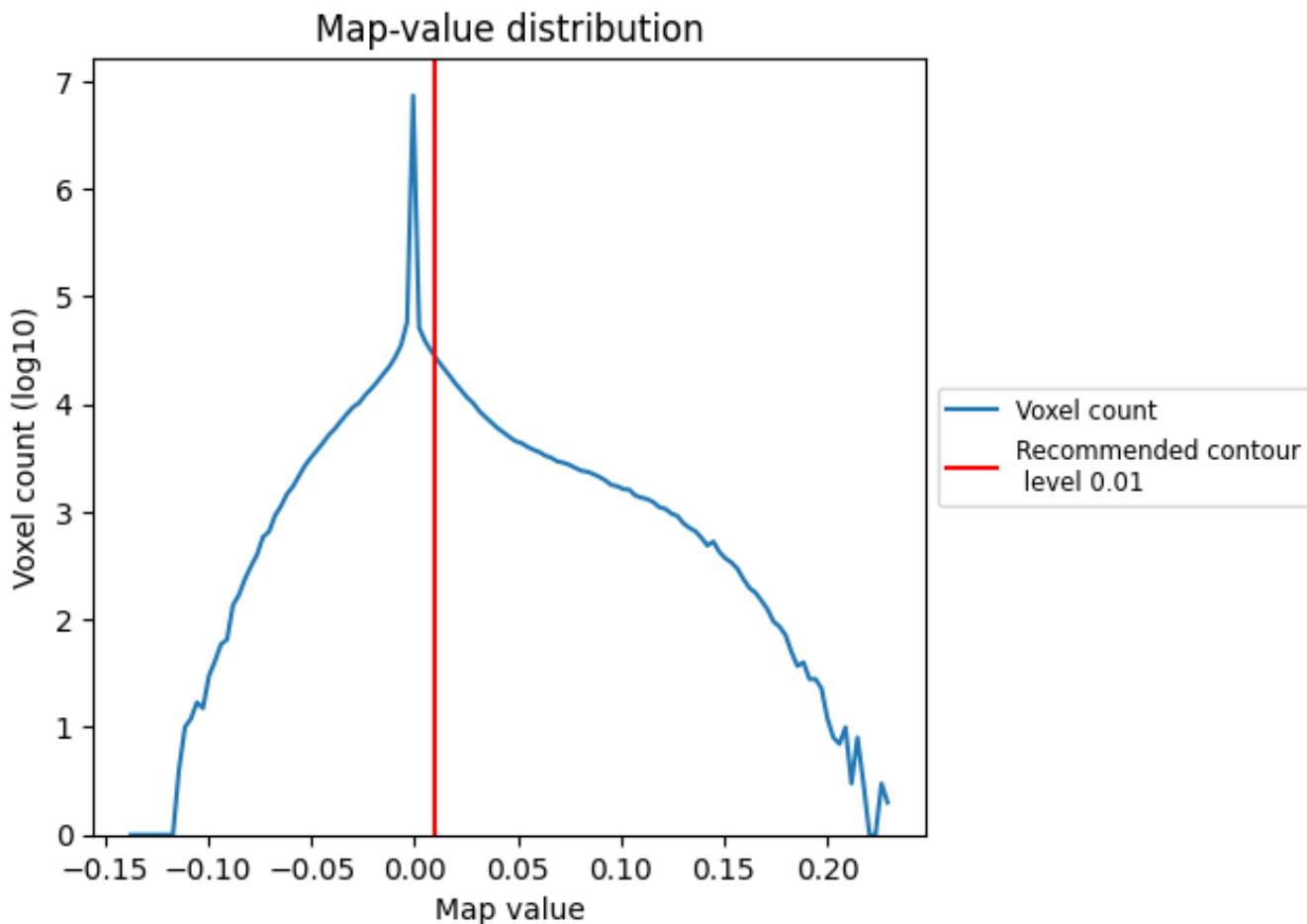
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

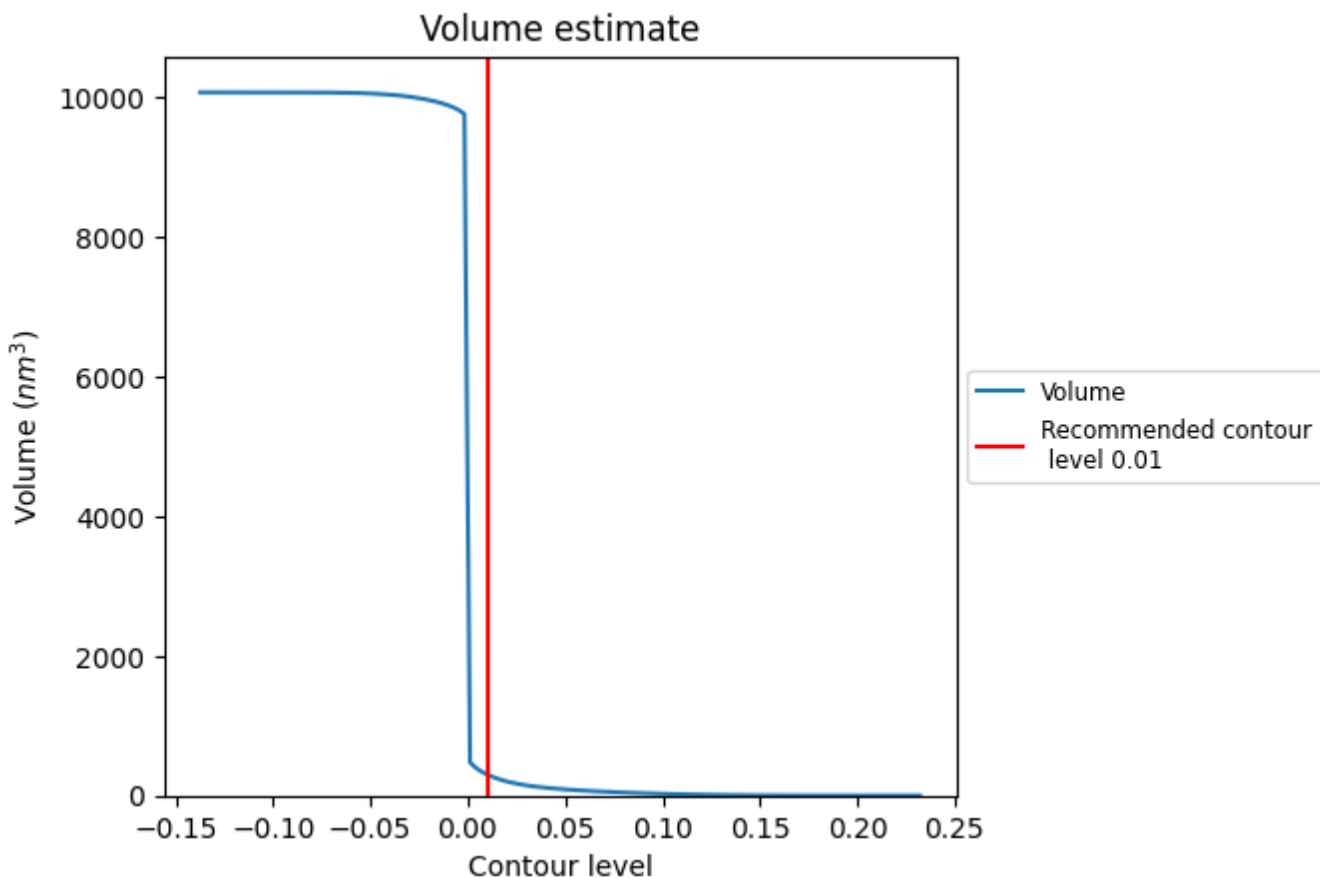
This section contains the results of statistical analysis of the map.

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.

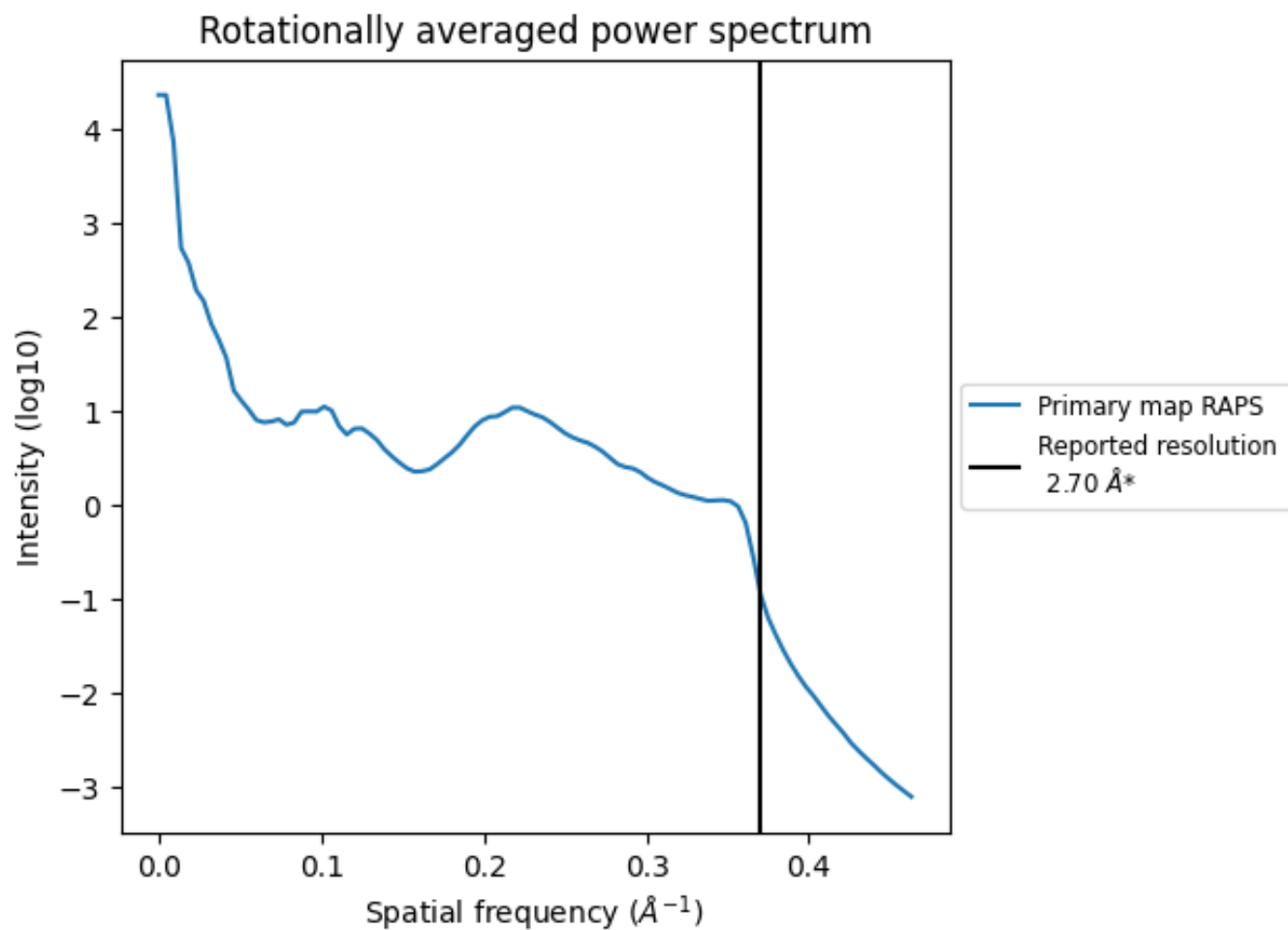
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 301 nm³; this corresponds to an approximate mass of 272 kDa.

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

7.3 Rotationally averaged power spectrum i

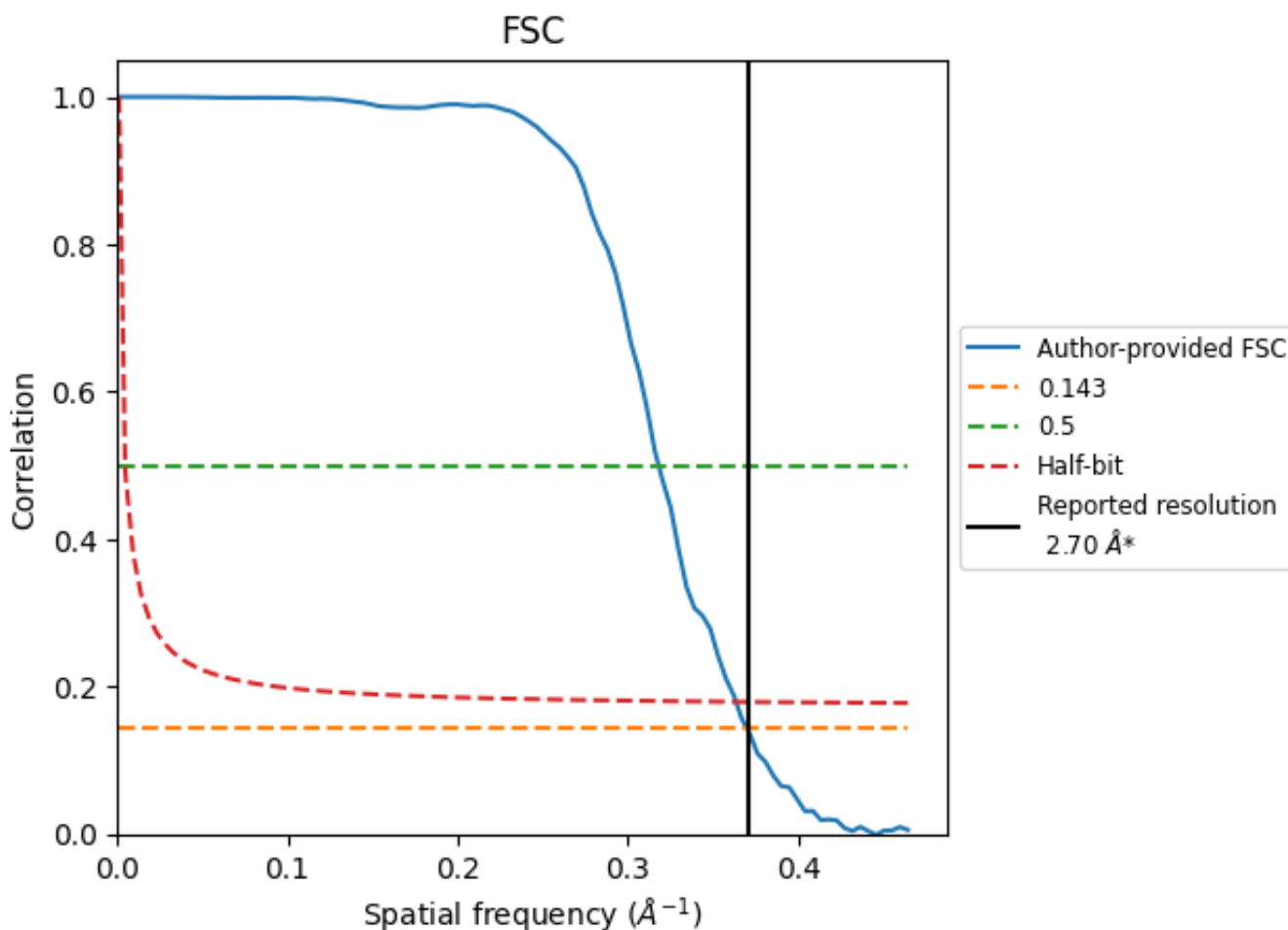


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

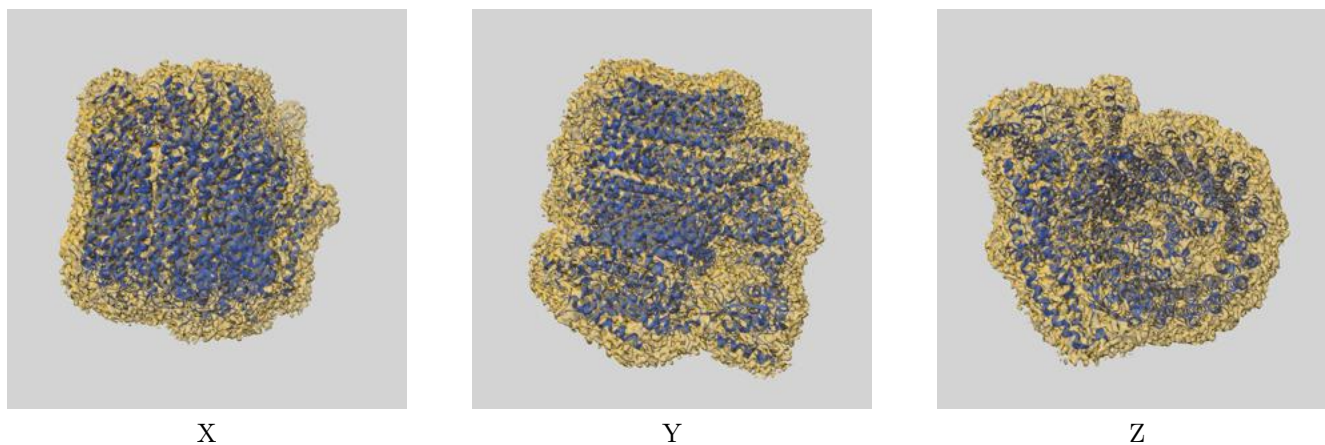
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.14	2.75
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

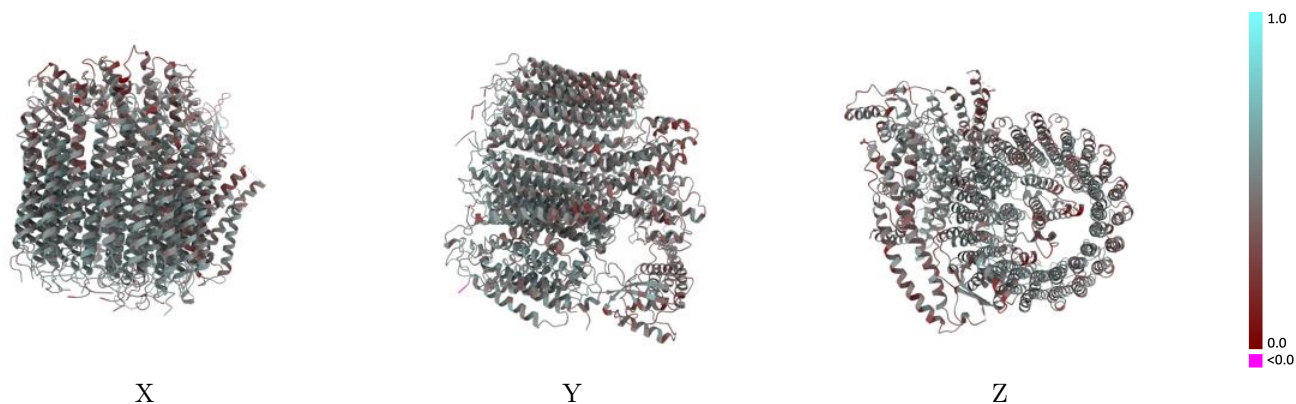
This section contains information regarding the fit between EMDB map EMD-30034 and PDB model 6M0R. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



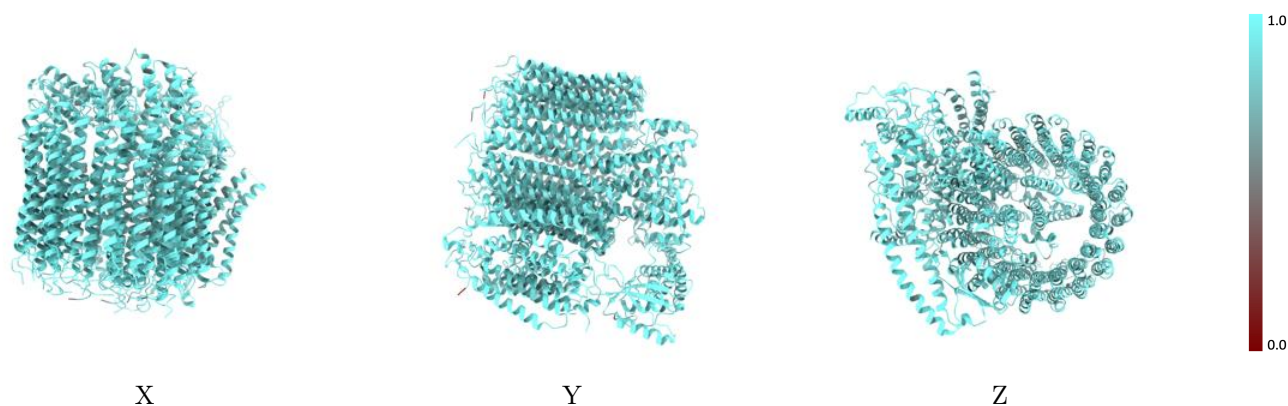
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



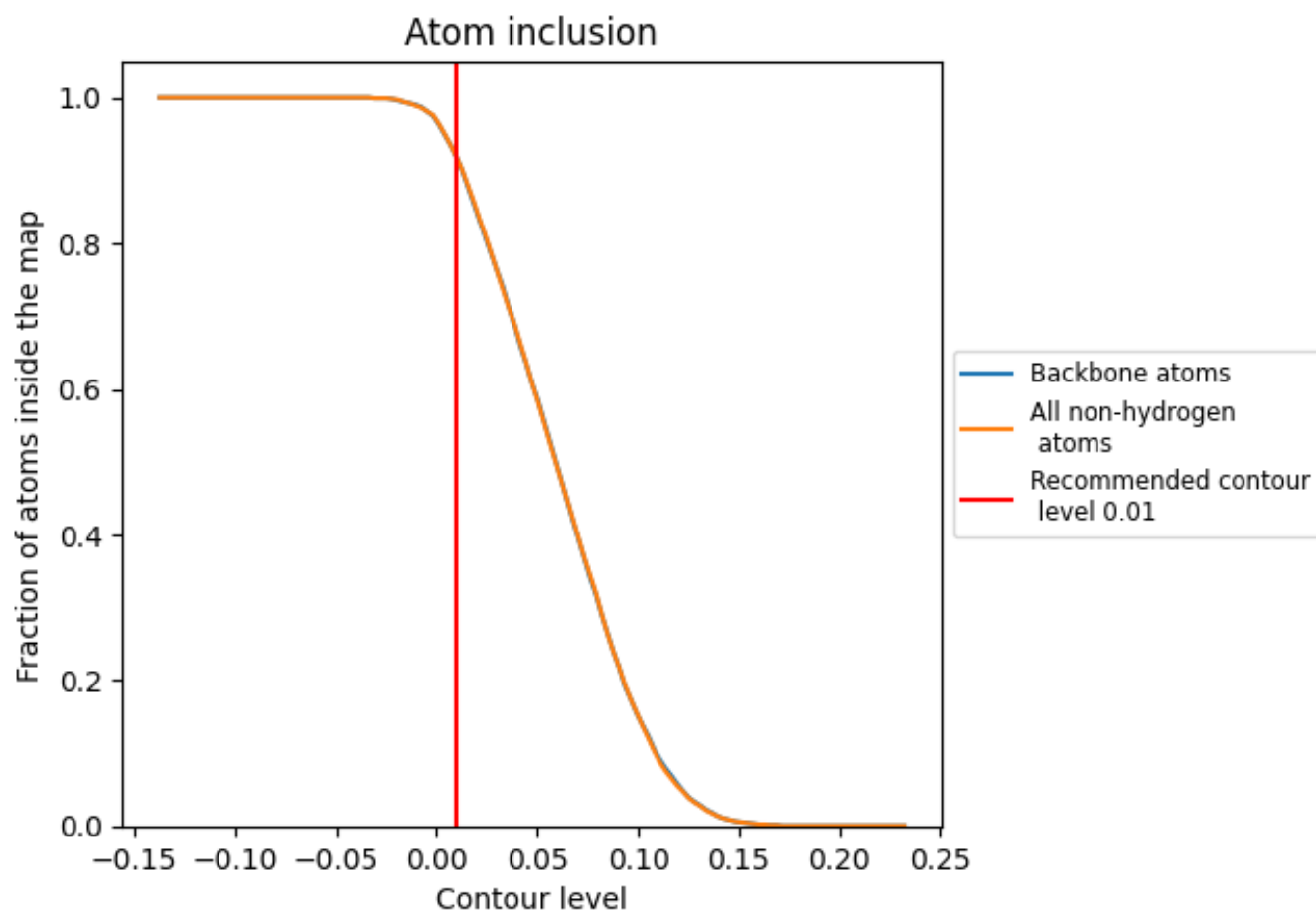
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.4670
A	 0.9230	 0.4520
B	 0.9210	 0.4320
C	 0.8700	 0.4690
D	 0.9400	 0.4790
E	 0.8860	 0.4590
F	 0.9080	 0.4600
G	 0.9150	 0.4580
H	 0.9250	 0.4700
I	 0.9220	 0.4910
J	 0.9390	 0.5120
K	 0.9290	 0.5160
L	 0.9440	 0.5260
M	 0.9110	 0.4900
N	 0.9170	 0.4740
O	 0.9430	 0.4590
P	 0.5480	 0.2730

