



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:58 AM UTC

PDB ID : 8TKP / pdb_00008tkp
EMDB ID : EMD-41356
Title : Structure of the *C. elegans* TMC-2 complex
Authors : Clark, S.; Jeong, H.; Goehring, A.; Posert, R.; Gouaux, E.
Deposited on : 2023-07-25
Resolution : 2.90 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:

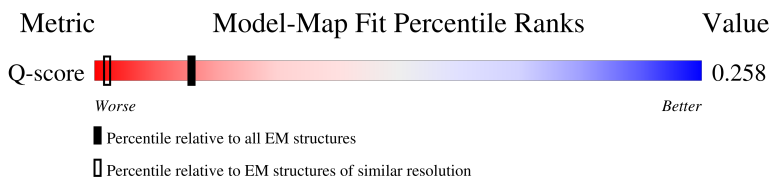
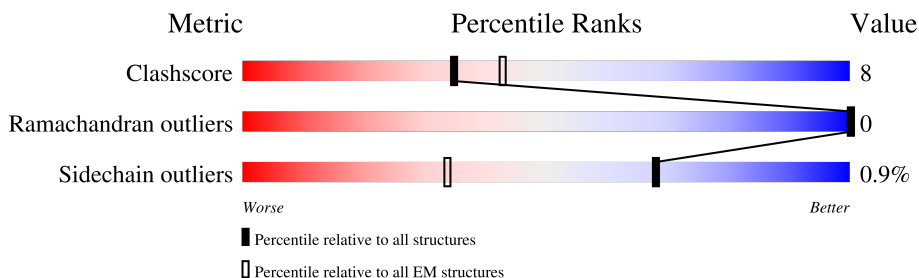
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.90 Å.

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



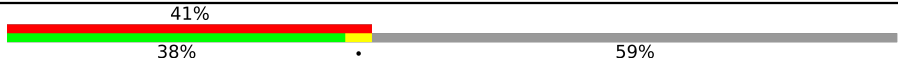



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	1203	<p>46% (Poor fit), 39% (0 outliers), 11% (1 outlier), 49% (Not modelled)</p>
1	D	1203	<p>42% (0 outliers), 9% (1 outlier), 49% (Not modelled)</p>
2	B	201	<p>93% (Poor fit), 81% (0 outliers), 11% (1 outlier), 7% (Not modelled)</p>
2	E	201	<p>76% (0 outliers), 17% (1 outlier), 7% (Not modelled)</p>

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Mol	Chain	Length	Quality of chain
3	C	117	 41% 38% 59%
3	F	117	 31% 10% 59%
4	H	2	 50% 50%
5	G	2	 100% 100%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 14666 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 Transmembrane channel-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	614	Total	C	N	O	S	0	0
			4992	3289	839	839	25		
1	D	614	Total	C	N	O	S	0	0
			4992	3289	839	839	25		

- Molecule 2 is a protein called CALMyrin (Calcium and Integrin Binding protein) homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	187	Total	C	N	O	S	0	0
			1554	989	260	298	7		
2	E	187	Total	C	N	O	S	0	0
			1554	989	260	298	7		

- Molecule 3 is a protein called Transmembrane inner ear expressed protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	48	Total	C	N	O	S	0	0
			378	251	67	55	5		
3	F	48	Total	C	N	O	S	0	0
			378	251	67	55	5		

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



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

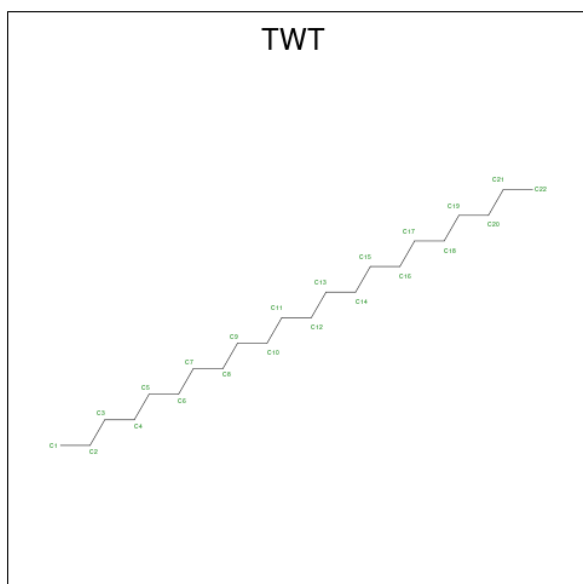
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



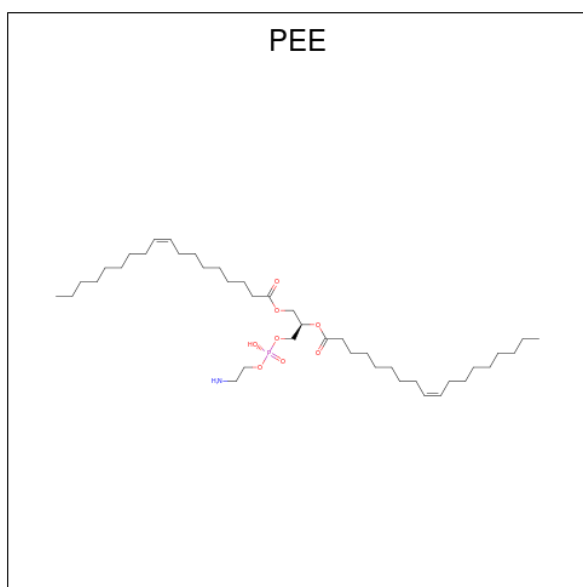
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	2	28	16	2	10	0	0

- Molecule 6 is DOCOSANE (CCD ID: TWT) (formula: C₂₂H₄₆).



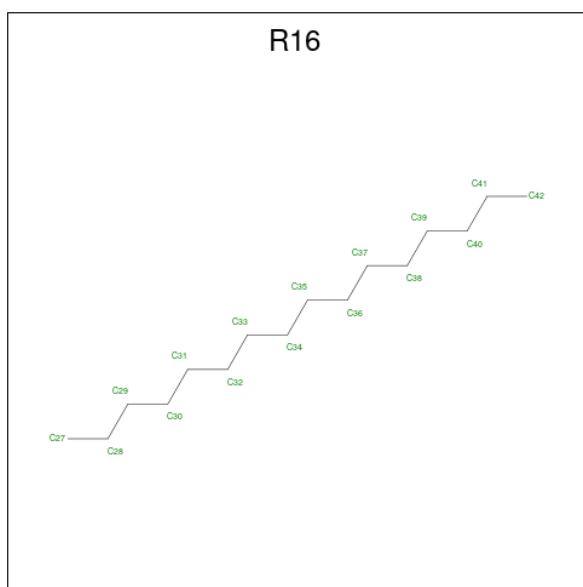
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C	0
			12	12	
6	A	1	Total	C	0
			19	19	
6	C	1	Total	C	0
			18	18	
6	D	1	Total	C	0
			17	17	
6	D	1	Total	C	0
			19	19	
6	F	1	Total	C	0
			19	19	

- Molecule 7 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	O	P		
7	A	1	29	20	8	1	0	
7	A	1	33	23	1	8	1	
7	A	1	27	17	1	8	1	
7	A	1	27	17	1	8	1	
7	C	1	25	15	1	8	1	
7	D	1	29	19	1	8	1	
7	D	1	33	23	1	8	1	
7	D	1	27	17	1	8	1	
7	D	1	27	17	1	8	1	
7	D	1	25	15	1	8	1	

- Molecule 8 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



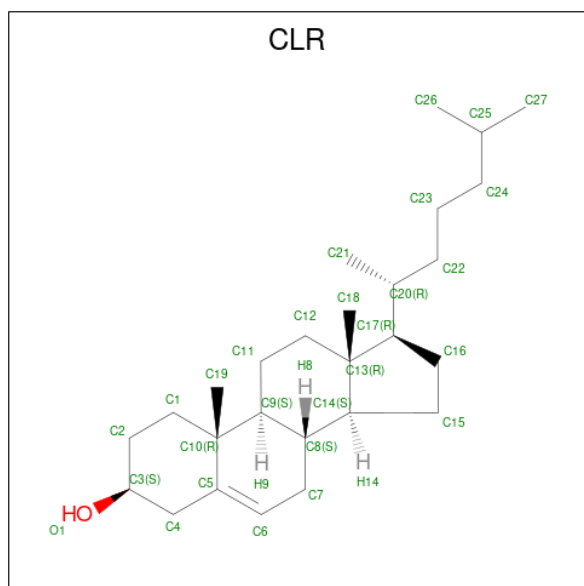
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C 16 16	0
8	A	1	Total C 10 10	0
8	A	1	Total C 10 10	0
8	A	1	Total C 15 15	0
8	A	1	Total C 10 10	0
8	A	1	Total C 11 11	0
8	A	1	Total C 10 10	0
8	A	1	Total C 10 10	0
8	A	1	Total C 10 10	0
8	C	1	Total C 12 12	0
8	C	1	Total C 11 11	0
8	D	1	Total C 16 16	0
8	D	1	Total C 10 10	0
8	D	1	Total C 6 6	0

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Mol	Chain	Residues	Atoms	AltConf
8	D	1	Total C 11 11	0
8	D	1	Total C 12 12	0
8	D	1	Total C 13 13	0
8	D	1	Total C 13 13	0
8	D	1	Total C 10 10	0
8	D	1	Total C 10 10	0
8	F	1	Total C 16 16	0
8	F	1	Total C 12 12	0

- Molecule 9 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C O 28 27 1	0
9	D	1	Total C O 28 27 1	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

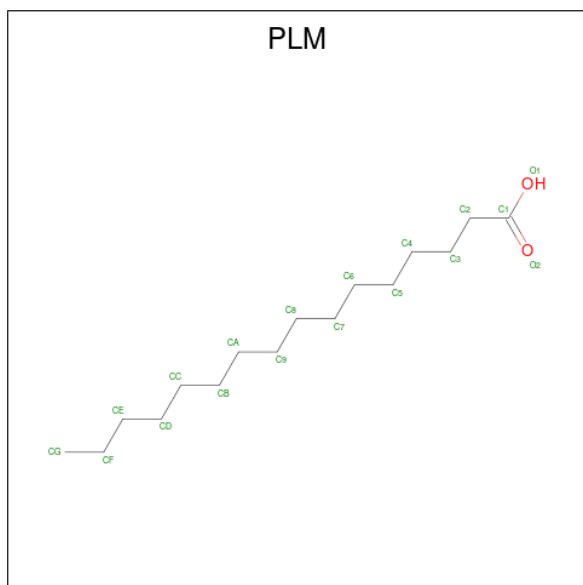


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	A	1	14	8	1	5	0
10	D	1	14	8	1	5	0

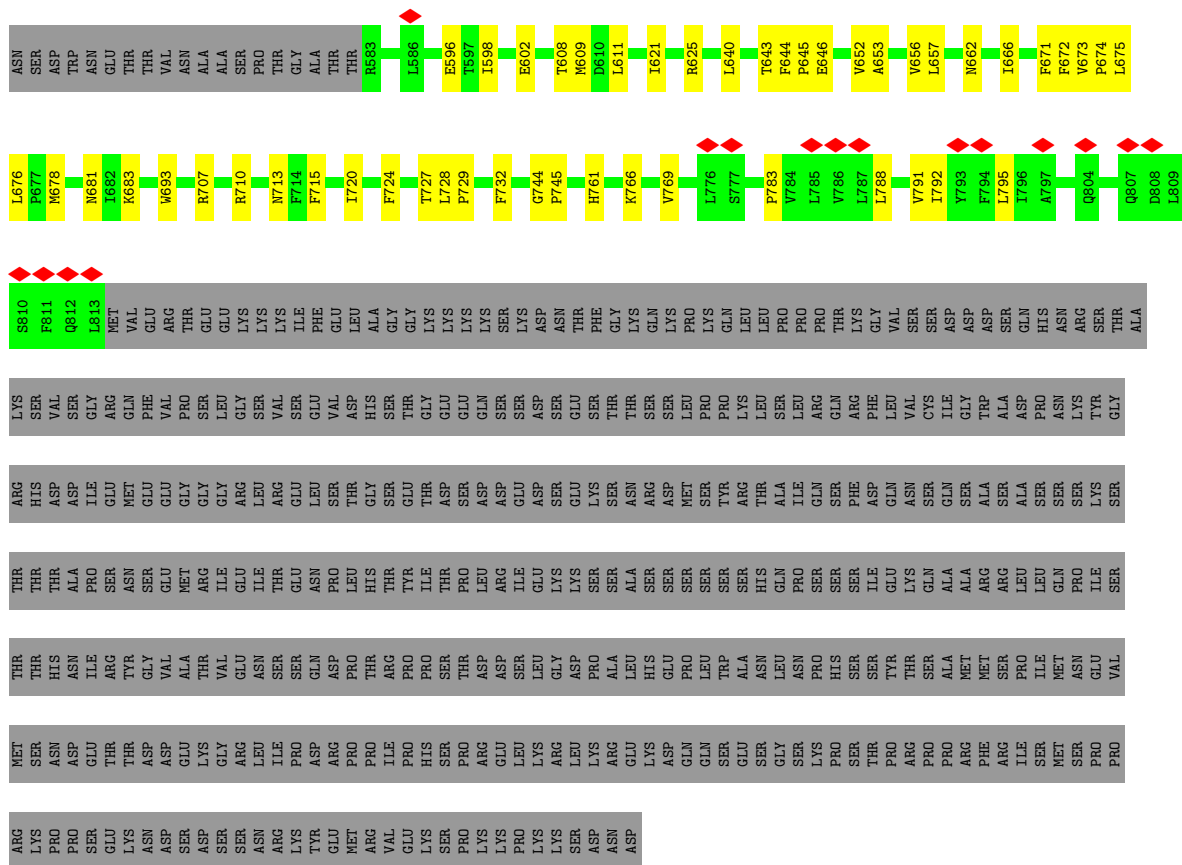
- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
11	B	2	2	2	0
11	E	2	2	2	0

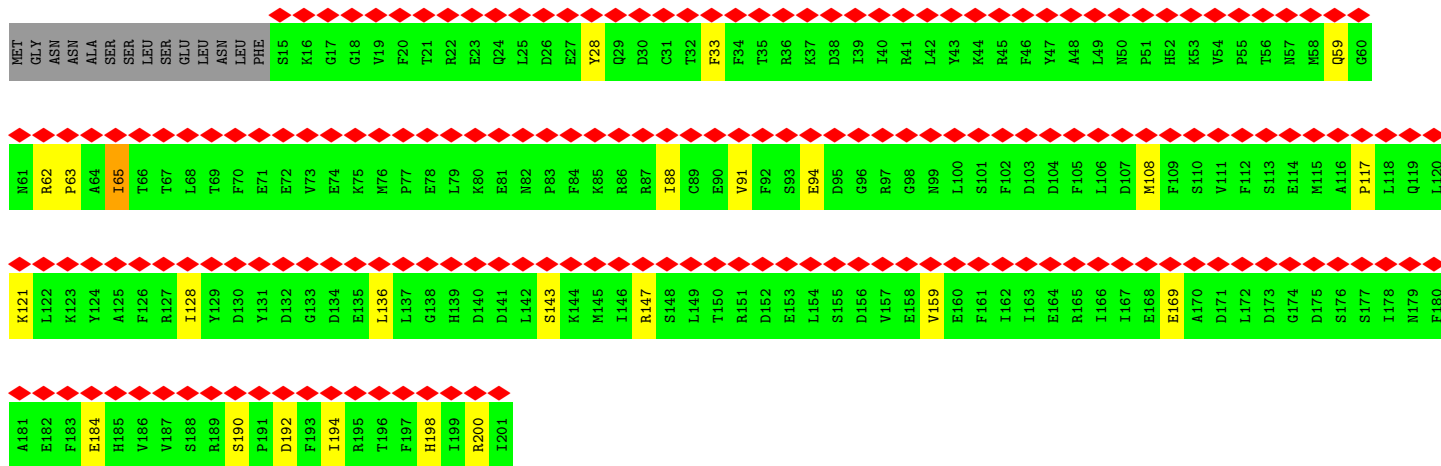
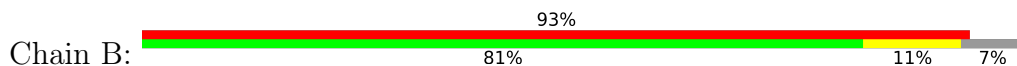
- Molecule 12 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



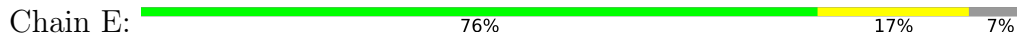
Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			11	10	1	
12	C	1	Total	C	O	0
			5	4	1	
12	F	1	Total	C	O	0
			12	11	1	
12	F	1	Total	C	O	0
			6	5	1	



● Molecule 2: CALMyrin (Calcium and Integrin Binding protein) homolog



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	207726	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.536	Depositor
Minimum map value	-0.244	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.075	Depositor
Map size (\AA)	373.94998, 373.94998, 373.94998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.831, 0.831, 0.831	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R16, CA, CLR, PEE, TWT, PLM, 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	A	0.34	2/5121 (0.0%)	0.45	4/6933 (0.1%)
1	D	0.12	0/5121	0.29	0/6933
2	B	0.11	0/1587	0.26	0/2135
2	E	0.10	0/1587	0.26	0/2135
3	C	0.12	0/383	0.28	0/517
3	F	0.12	0/383	0.38	0/517
All	All	0.23	2/14182 (0.0%)	0.35	4/19170 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	775	SER	CA-C	-5.71	1.45	1.52
1	A	770	ASN	C-O	-5.40	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	774	TYR	N-CA-C	-6.27	104.44	111.28
1	A	769	VAL	CB-CA-C	-5.89	104.18	112.14
1	A	807	GLN	N-CA-C	-5.74	104.02	111.02
1	A	806	ASN	O-C-N	5.50	127.96	122.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4992	0	5092	127	0
1	D	4992	0	5093	82	0
2	B	1554	0	1505	16	0
2	E	1554	0	1505	20	0
3	C	378	0	424	2	0
3	F	378	0	424	10	0
4	H	28	0	25	0	0
5	G	28	0	25	0	0
6	A	31	0	60	2	0
6	C	18	0	35	0	0
6	D	36	0	70	0	0
6	F	19	0	37	0	0
7	A	116	0	125	2	0
7	C	25	0	24	1	0
7	D	141	0	152	2	0
8	A	102	0	186	4	0
8	C	23	0	38	0	0
8	D	101	0	187	1	0
8	F	28	0	54	0	0
9	A	28	0	46	2	0
9	D	28	0	46	0	0
10	A	14	0	13	0	0
10	D	14	0	13	0	0
11	B	2	0	0	0	0
11	E	2	0	0	0	0
12	C	16	0	20	0	0
12	F	18	0	24	0	0
All	All	14666	0	15223	239	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 8.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:SER:O	1:A:807:GLN:HG3	1.15	1.32
1:A:764:LEU:CD2	1:A:768:LEU:HD22	1.60	1.29
1:A:803:SER:O	1:A:807:GLN:CG	1.88	1.20
1:A:797:ALA:O	1:A:800:THR:OG1	1.62	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:LEU:HD21	1:A:768:LEU:HD22	1.21	1.07
1:A:764:LEU:CD1	1:A:766:LYS:HG3	1.90	1.00
1:A:764:LEU:HD23	1:A:768:LEU:HD22	1.41	0.99
1:A:764:LEU:HD12	1:A:766:LYS:CG	1.91	0.99
1:A:764:LEU:CD1	1:A:766:LYS:CG	2.41	0.99
1:D:309:THR:HG22	1:D:310:LEU:H	1.30	0.97
1:A:764:LEU:HD12	1:A:766:LYS:HG2	1.43	0.96
1:A:764:LEU:HD11	1:A:766:LYS:HG3	1.45	0.96
1:D:643:THR:HG22	1:D:644:PHE:H	1.36	0.89
1:A:764:LEU:HD21	1:A:768:LEU:CD2	2.04	0.85
1:A:764:LEU:O	1:A:769:VAL:CG2	2.26	0.84
1:A:771:GLY:O	1:A:774:TYR:HB3	1.78	0.84
1:D:309:THR:HG22	1:D:310:LEU:N	1.91	0.82
1:A:764:LEU:CD2	1:A:768:LEU:CD2	2.54	0.81
1:D:309:THR:HG22	1:D:310:LEU:HD23	1.64	0.79
1:D:643:THR:HG22	1:D:644:PHE:N	1.95	0.79
1:D:309:THR:CG2	1:D:310:LEU:HD23	2.15	0.76
1:D:309:THR:CG2	1:D:310:LEU:H	1.98	0.76
1:A:795:LEU:HB3	1:D:795:LEU:CD2	2.17	0.74
1:A:768:LEU:C	1:A:768:LEU:HD23	2.14	0.73
1:D:643:THR:CG2	1:D:644:PHE:H	2.04	0.71
1:A:764:LEU:CD1	1:A:766:LYS:HG2	2.10	0.71
2:E:170:ALA:HB1	2:E:182:GLU:HB3	1.72	0.70
1:A:795:LEU:HB3	1:D:795:LEU:HD23	1.73	0.69
1:A:809:LEU:HD13	1:A:809:LEU:C	2.17	0.69
3:F:18:VAL:HG11	3:F:23:ARG:HH11	1.55	0.69
1:A:305:ASN:HB3	1:A:310:LEU:HD22	1.73	0.69
1:A:764:LEU:O	1:A:769:VAL:HG23	1.91	0.69
1:A:689:TYR:HB3	7:C:205:PEE:H7	1.77	0.67
1:A:804:GLN:O	1:A:807:GLN:HB2	1.96	0.66
1:A:673:VAL:HB	1:A:676:LEU:HB2	1.76	0.66
1:A:796:ILE:O	1:A:800:THR:HG23	1.96	0.65
1:A:803:SER:C	1:A:807:GLN:CG	2.70	0.65
1:D:213:ALA:HB2	1:D:270:PHE:HZ	1.62	0.64
1:A:764:LEU:HD23	1:A:768:LEU:CD2	2.22	0.63
1:D:282:TYR:OH	1:D:671:PHE:O	2.13	0.63
1:D:309:THR:CG2	1:D:310:LEU:N	2.59	0.63
3:C:23:ARG:HB3	3:C:26:MET:HG3	1.81	0.62
1:A:797:ALA:C	1:A:800:THR:HG1	2.01	0.62
1:D:693:TRP:HB2	7:D:1317:PEE:H3	1.80	0.61
1:A:611:LEU:HD13	1:A:683:LYS:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:ILE:HG12	1:D:609:MET:HE2	1.81	0.61
1:D:611:LEU:HD13	1:D:683:LYS:HG3	1.82	0.61
1:D:242:ASP:HB2	3:F:23:ARG:HE	1.64	0.61
1:A:198:ILE:HG23	1:A:289:ILE:HD13	1.82	0.60
1:D:673:VAL:HB	1:D:676:LEU:HB2	1.82	0.60
1:A:322:TRP:O	1:A:326:THR:OG1	2.19	0.60
1:A:93:ILE:HA	1:A:96:LYS:HE2	1.82	0.59
1:A:707:ARG:NH2	2:B:192:ASP:OD1	2.35	0.59
3:F:18:VAL:O	3:F:24:LEU:N	2.36	0.59
3:F:36:LEU:HD13	3:F:39:ILE:HD11	1.85	0.59
1:A:764:LEU:O	1:A:769:VAL:HG21	2.04	0.58
1:A:180:VAL:HG21	1:A:705:ILE:HG21	1.85	0.58
1:A:774:TYR:HE1	1:D:732:PHE:CZ	2.21	0.58
1:A:184:TYR:HB2	1:A:652:VAL:HG13	1.87	0.57
1:A:797:ALA:C	1:A:800:THR:OG1	2.45	0.57
1:A:223:ARG:NH2	1:A:267:GLU:O	2.38	0.57
1:D:203:CYS:HA	1:D:207:VAL:HB	1.86	0.57
1:D:129:GLN:OE1	1:D:130:GLN:NE2	2.37	0.56
1:A:195:ASN:ND2	1:A:681:ASN:OD1	2.36	0.56
1:A:766:LYS:O	1:A:769:VAL:HG23	2.04	0.56
1:A:804:GLN:O	1:A:807:GLN:CB	2.54	0.56
1:D:195:ASN:ND2	1:D:681:ASN:OD1	2.38	0.56
1:D:368:ARG:HE	1:D:430:LYS:HG3	1.72	0.55
1:D:184:TYR:HB2	1:D:652:VAL:HG13	1.89	0.55
1:A:809:LEU:HD13	1:A:809:LEU:O	2.06	0.55
1:A:387:ILE:HD11	1:A:450:LEU:HB3	1.87	0.55
1:D:328:TRP:HB2	2:E:149:LEU:HD21	1.89	0.54
1:A:764:LEU:HD21	1:A:768:LEU:HD13	1.90	0.54
2:B:59:GLN:H	2:B:62:ARG:HD2	1.71	0.54
1:A:774:TYR:CE1	1:D:732:PHE:CZ	2.96	0.54
1:A:164:ILE:HG12	7:A:1314:PEE:H14	1.90	0.54
2:B:88:ILE:HG22	2:B:108:MET:HE2	1.89	0.53
1:A:741:LYS:NZ	1:A:748:ASN:OD1	2.40	0.53
1:A:795:LEU:CB	1:D:795:LEU:HD23	2.38	0.53
1:D:264:TYR:CE1	1:D:674:PRO:HG2	2.43	0.53
1:A:203:CYS:HA	1:A:207:VAL:HB	1.88	0.53
1:A:603:ILE:HD11	1:A:665:MET:HE3	1.90	0.53
1:D:321:ASN:HD22	2:E:186:VAL:HG11	1.72	0.53
1:D:761:HIS:O	1:D:766:LYS:NZ	2.41	0.53
1:A:205:PHE:O	1:A:276:TYR:OH	2.25	0.53
1:A:707:ARG:HE	1:A:710:ARG:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ILE:HG23	1:D:289:ILE:HD13	1.90	0.53
1:D:213:ALA:HB2	1:D:270:PHE:CZ	2.43	0.52
2:E:122:LEU:HD13	2:E:184:GLU:HG2	1.90	0.52
1:A:694:ALA:O	1:A:699:ASN:ND2	2.30	0.52
1:D:441:LEU:HD11	1:D:653:ALA:HB1	1.91	0.52
1:A:792:ILE:HG22	1:D:792:ILE:HG22	1.91	0.52
1:A:764:LEU:C	1:A:766:LYS:H	2.17	0.52
1:D:233:MET:HG2	1:D:256:TYR:CG	2.46	0.51
1:D:761:HIS:HA	1:D:769:VAL:HG21	1.92	0.51
1:A:383:TYR:O	1:A:387:ILE:HG12	2.11	0.51
2:B:62:ARG:HG3	2:B:63:PRO:HD3	1.93	0.51
1:A:294:LEU:HD23	1:A:723:LEU:HD23	1.93	0.50
1:D:643:THR:CG2	1:D:644:PHE:N	2.63	0.50
1:A:409:ILE:HG12	1:A:609:MET:HE2	1.92	0.50
1:A:795:LEU:HB3	1:D:795:LEU:HD21	1.90	0.50
1:D:180:VAL:O	1:D:183:SER:OG	2.22	0.50
1:D:304:ASN:ND2	1:D:713:ASN:OD1	2.44	0.50
2:E:88:ILE:HG22	2:E:108:MET:HE2	1.94	0.50
2:E:100:LEU:HG	2:E:104:ASP:HB2	1.93	0.50
1:A:445:LEU:O	1:A:449:ILE:HG12	2.12	0.49
1:A:661:ASN:O	1:A:665:MET:HG2	2.11	0.49
1:D:598:ILE:O	1:D:602:GLU:HG2	2.12	0.49
1:A:767:THR:O	1:A:770:ASN:HB3	2.11	0.49
1:A:277:ARG:HH12	6:A:1315:TWT:H142	1.76	0.49
1:D:364:HIS:HB3	1:D:367:ILE:HD12	1.94	0.49
2:B:143:SER:O	2:B:147:ARG:HG2	2.12	0.49
1:A:180:VAL:O	1:A:183:SER:OG	2.24	0.48
1:D:310:LEU:H	1:D:310:LEU:HD23	1.78	0.48
1:A:764:LEU:HD11	1:A:766:LYS:CG	2.21	0.48
2:E:116:ALA:HB3	2:E:121:LYS:HE3	1.94	0.48
1:D:322:TRP:O	1:D:326:THR:OG1	2.24	0.48
1:A:764:LEU:C	1:A:766:LYS:N	2.69	0.48
1:A:766:LYS:C	1:A:768:LEU:N	2.70	0.48
1:A:621:ILE:O	1:A:625:ARG:NE	2.47	0.48
1:D:126:LYS:O	1:D:130:GLN:HG2	2.14	0.48
1:A:628:ALA:HA	1:A:632:LEU:HD23	1.95	0.47
7:A:1311:PEE:H67	1:D:783:PRO:HB3	1.96	0.47
1:D:662:ASN:O	1:D:666:ILE:HG12	2.14	0.47
1:A:804:GLN:O	1:A:807:GLN:CG	2.54	0.47
1:A:767:THR:O	1:A:770:ASN:N	2.47	0.47
1:D:621:ILE:O	1:D:625:ARG:NE	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:LYS:HD2	2:E:127:ARG:HH21	1.79	0.47
1:A:115:LYS:NZ	2:B:94:GLU:OE2	2.34	0.47
1:A:274:ILE:O	1:A:274:ILE:HG13	2.15	0.46
1:A:795:LEU:CB	1:D:795:LEU:CD2	2.89	0.46
1:A:807:GLN:HG3	1:A:807:GLN:H	1.36	0.46
2:E:198:HIS:HE1	2:E:200:ARG:HB2	1.80	0.46
1:A:630:ARG:NE	3:C:52:ARG:HE	2.14	0.46
1:D:441:LEU:HD13	1:D:657:LEU:HD11	1.97	0.46
1:A:717:ALA:O	1:A:720:ILE:HG13	2.15	0.46
1:A:774:TYR:CE1	1:D:732:PHE:CE1	3.04	0.46
2:E:175:ASP:OD1	2:E:175:ASP:N	2.46	0.46
1:D:213:ALA:O	1:D:217:THR:OG1	2.32	0.46
3:F:56:GLN:OE1	3:F:56:GLN:N	2.48	0.46
1:A:632:LEU:HD21	8:A:1310:R16:H392	1.97	0.46
2:B:62:ARG:HA	2:B:65:ILE:HG12	1.96	0.46
1:A:249:ASP:HA	1:A:605:LYS:HD3	1.98	0.46
2:E:15:SER:OG	2:E:16:LYS:N	2.48	0.46
1:D:319:LEU:HG	1:D:323:LYS:HE2	1.98	0.45
3:F:25:TRP:O	3:F:28:ILE:HG13	2.16	0.45
1:D:640:LEU:HD22	1:D:645:PRO:HD2	1.98	0.45
2:E:165:ARG:NE	2:E:168:GLU:OE2	2.45	0.45
1:A:787:LEU:O	1:A:791:VAL:HG23	2.16	0.45
1:D:678:MET:O	1:D:681:ASN:HB2	2.17	0.45
2:E:167:ILE:O	2:E:171:ASP:HB2	2.16	0.45
1:A:334:ASN:OD1	1:A:337:THR:N	2.42	0.45
1:A:783:PRO:HA	1:A:786:VAL:HG22	1.99	0.45
1:D:261:TYR:CZ	1:D:745:PRO:HD2	2.52	0.45
1:A:678:MET:O	1:A:681:ASN:HB2	2.16	0.45
1:A:166:TRP:H	6:A:1301:TWT:H2C1	1.82	0.45
1:A:456:ILE:O	1:A:459:LEU:HG	2.17	0.45
1:D:250:PHE:HZ	1:D:608:THR:HG21	1.82	0.44
3:F:18:VAL:HG11	3:F:23:ARG:NH1	2.26	0.44
1:A:372:ARG:HD3	1:A:431:LEU:HD21	2.00	0.44
1:D:254:PHE:O	1:D:257:SER:OG	2.32	0.44
1:A:809:LEU:C	1:A:809:LEU:CD1	2.85	0.44
1:A:158:ASN:O	1:A:161:ILE:HG22	2.17	0.44
1:A:662:ASN:O	1:A:666:ILE:HG12	2.17	0.44
1:D:297:ILE:HG21	1:D:720:ILE:HG13	2.00	0.44
1:A:283:PHE:HE2	1:A:753:TYR:HA	1.82	0.43
1:A:322:TRP:CD1	2:B:190:SER:HB2	2.53	0.43
1:D:425:LEU:O	1:D:428:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:LEU:HD22	1:A:809:LEU:HA	1.62	0.43
9:A:1305:CLR:H121	9:A:1305:CLR:H222	2.00	0.43
2:B:33:PHE:CZ	2:B:117:PRO:HD3	2.53	0.43
1:D:625:ARG:NH1	1:D:646:GLU:O	2.51	0.43
1:A:307:ARG:HD2	2:B:194:ILE:HG21	1.98	0.43
1:A:351:GLU:O	1:A:355:ASP:N	2.51	0.43
1:D:305:ASN:HB2	1:D:713:ASN:HD21	1.83	0.43
2:E:91:VAL:HG21	2:E:128:ILE:HA	2.01	0.43
2:E:33:PHE:CZ	2:E:117:PRO:HD3	2.52	0.43
3:F:36:LEU:HA	3:F:39:ILE:HG12	2.01	0.43
8:D:1304:R16:H362	8:D:1304:R16:H331	1.82	0.43
1:A:213:ALA:O	1:A:217:THR:OG1	2.37	0.43
3:F:28:ILE:HA	3:F:31:VAL:HG22	2.00	0.43
1:A:259:LEU:HD12	1:A:675:LEU:HB2	2.00	0.43
1:A:321:ASN:ND2	2:B:169:GLU:OE1	2.44	0.42
1:A:792:ILE:HG21	1:D:788:LEU:CD1	2.49	0.42
1:D:666:ILE:HD12	1:D:676:LEU:HG	1.99	0.42
2:B:117:PRO:O	2:B:121:LYS:HG3	2.18	0.42
1:A:97:ILE:HD11	1:A:131:GLN:HG3	2.01	0.42
1:A:415:THR:HG23	1:A:448:TYR:CE1	2.54	0.42
2:B:91:VAL:HG21	2:B:128:ILE:HA	2.01	0.42
8:A:1303:R16:H401	8:A:1303:R16:H372	1.82	0.42
2:E:104:ASP:OD1	2:E:104:ASP:N	2.51	0.42
1:A:261:TYR:CE2	1:A:745:PRO:HD2	2.54	0.42
1:A:639:ASP:HB2	8:A:1307:R16:H271	2.01	0.42
1:A:467:GLN:HA	1:A:593:LEU:HD11	2.01	0.42
1:A:644:PHE:HA	1:A:645:PRO:HA	1.86	0.42
1:A:768:LEU:HD23	1:A:768:LEU:O	2.19	0.42
1:A:429:GLU:OE2	1:A:443:ARG:NH2	2.40	0.42
1:A:293:SER:O	1:A:297:ILE:HG13	2.20	0.41
1:A:790:LEU:HD11	1:D:294:LEU:HD11	2.02	0.41
1:D:221:ASP:OD1	1:D:222:ASP:N	2.52	0.41
1:D:388:TRP:CE2	7:D:1312:PEE:H18	2.55	0.41
2:E:105:PHE:CZ	2:E:109:PHE:HE2	2.38	0.41
2:E:158:GLU:O	2:E:162:ILE:HG13	2.19	0.41
1:A:438:ARG:HG2	1:A:708:ALA:HB1	2.03	0.41
1:D:707:ARG:HH21	1:D:710:ARG:HA	1.85	0.41
1:D:724:PHE:HA	1:D:727:THR:HG22	2.01	0.41
2:E:92:PHE:CE1	2:E:108:MET:HA	2.56	0.41
1:A:118:ARG:NH2	2:B:28:TYR:OH	2.54	0.41
2:B:147:ARG:NH1	2:B:159:VAL:HG11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LYS:HE3	1:D:137:LYS:HB2	1.90	0.41
1:A:363:LYS:HB3	1:A:368:ARG:HD2	2.03	0.41
3:F:16:GLN:O	3:F:18:VAL:HG23	2.20	0.41
1:A:174:GLU:HG2	1:A:331:THR:HB	2.02	0.41
1:D:99:GLN:O	1:D:102:GLU:HG3	2.20	0.41
1:D:596:GLU:HB3	1:D:672:PHE:HD1	1.86	0.41
1:A:363:LYS:HD3	1:A:368:ARG:HD2	2.03	0.41
1:A:624:LEU:HD23	1:A:624:LEU:HA	1.89	0.41
1:A:649:GLU:OE1	1:A:649:GLU:N	2.54	0.41
1:A:768:LEU:CD2	1:A:768:LEU:C	2.85	0.41
9:A:1305:CLR:H212	9:A:1305:CLR:H162	1.78	0.41
1:D:158:ASN:O	1:D:161:ILE:HG22	2.21	0.41
1:D:261:TYR:CE1	1:D:744:GLY:HA3	2.56	0.41
1:D:656:VAL:HG11	1:D:715:PHE:CD1	2.55	0.41
1:D:728:LEU:HB3	1:D:729:PRO:HD3	2.02	0.41
1:A:195:ASN:O	1:A:199:THR:HG23	2.21	0.41
1:D:391:MET:HE1	1:D:461:LEU:HD12	2.03	0.41
1:D:788:LEU:HA	1:D:791:VAL:HG22	2.02	0.41
1:D:315:THR:OG1	1:D:316:GLN:N	2.54	0.40
1:A:596:GLU:HB3	1:A:672:PHE:HD1	1.85	0.40
1:A:638:TRP:CD1	8:A:1307:R16:H301	2.55	0.40
1:A:656:VAL:HG11	1:A:715:PHE:CD1	2.56	0.40
2:B:198:HIS:HE1	2:B:200:ARG:HB2	1.85	0.40
1:D:259:LEU:HD12	1:D:675:LEU:HB2	2.02	0.40
1:A:264:TYR:CE1	1:A:674:PRO:HG3	2.56	0.40
1:D:126:LYS:HD2	1:D:126:LYS:HA	1.92	0.40
1:A:432:HIS:CD2	1:A:434:ARG:HB3	2.57	0.40
1:A:724:PHE:O	1:A:727:THR:HG22	2.21	0.40
1:A:775:SER:O	1:A:777:SER:N	2.55	0.40
1:D:346:VAL:HG22	2:E:150:THR:HB	2.02	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	A	610/1203 (51%)	596 (98%)	14 (2%)	0	100	100
1	D	610/1203 (51%)	595 (98%)	15 (2%)	0	100	100
2	B	185/201 (92%)	185 (100%)	0	0	100	100
2	E	185/201 (92%)	184 (100%)	1 (0%)	0	100	100
3	C	46/117 (39%)	44 (96%)	2 (4%)	0	100	100
3	F	46/117 (39%)	42 (91%)	4 (9%)	0	100	100
All	All	1682/3042 (55%)	1646 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/1076 (50%)	528 (99%)	5 (1%)	70	90
1	D	533/1076 (50%)	531 (100%)	2 (0%)	84	94
2	B	173/185 (94%)	170 (98%)	3 (2%)	53	82
2	E	173/185 (94%)	172 (99%)	1 (1%)	78	93
3	C	41/96 (43%)	40 (98%)	1 (2%)	43	75
3	F	41/96 (43%)	39 (95%)	2 (5%)	22	54
All	All	1494/2714 (55%)	1480 (99%)	14 (1%)	68	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	LEU
1	A	455	LEU
1	A	743	CYS
1	A	770	ASN

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Mol	Chain	Res	Type
1	A	807	GLN
2	B	65	ILE
2	B	136	LEU
2	B	184	GLU
3	C	18	VAL
1	D	226	LYS
1	D	298	LEU
2	E	95	ASP
3	F	30	LEU
3	F	35	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	286	ASN
1	A	304	ASN
1	A	321	ASN
1	A	400	HIS
1	A	462	GLN
1	A	655	ASN
1	A	763	ASN
2	B	185	HIS
1	D	105	GLN
1	D	130	GLN
1	D	321	ASN
1	D	364	HIS
1	D	405	ASN
1	D	420	ASN
1	D	655	ASN
1	D	761	HIS
2	E	24	GLN
2	E	185	HIS

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

4 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
5	NAG	G	1	5,1	14,14,15	0.33	0	17,19,21	0.67	0
5	NAG	G	2	5	14,14,15	0.37	0	17,19,21	0.83	0
4	NAG	H	1	4,1	14,14,15	0.30	0	17,19,21	1.05	1 (5%)
4	NAG	H	2	4	14,14,15	0.33	0	17,19,21	0.62	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
5	NAG	G	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	H	1	NAG	C4-C3-C2	-2.42	107.48	111.02

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C1-C2-N2-C7
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2

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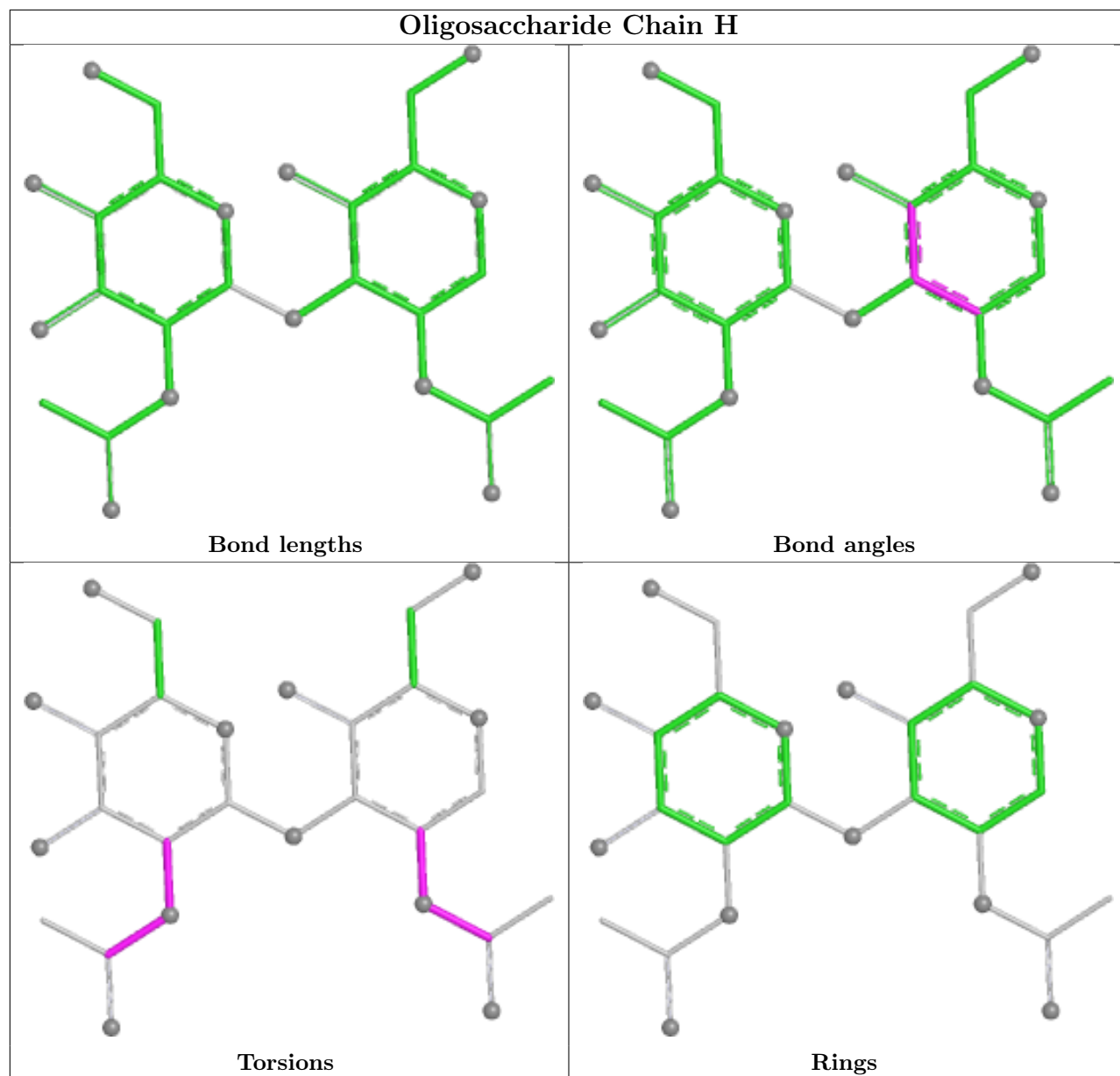
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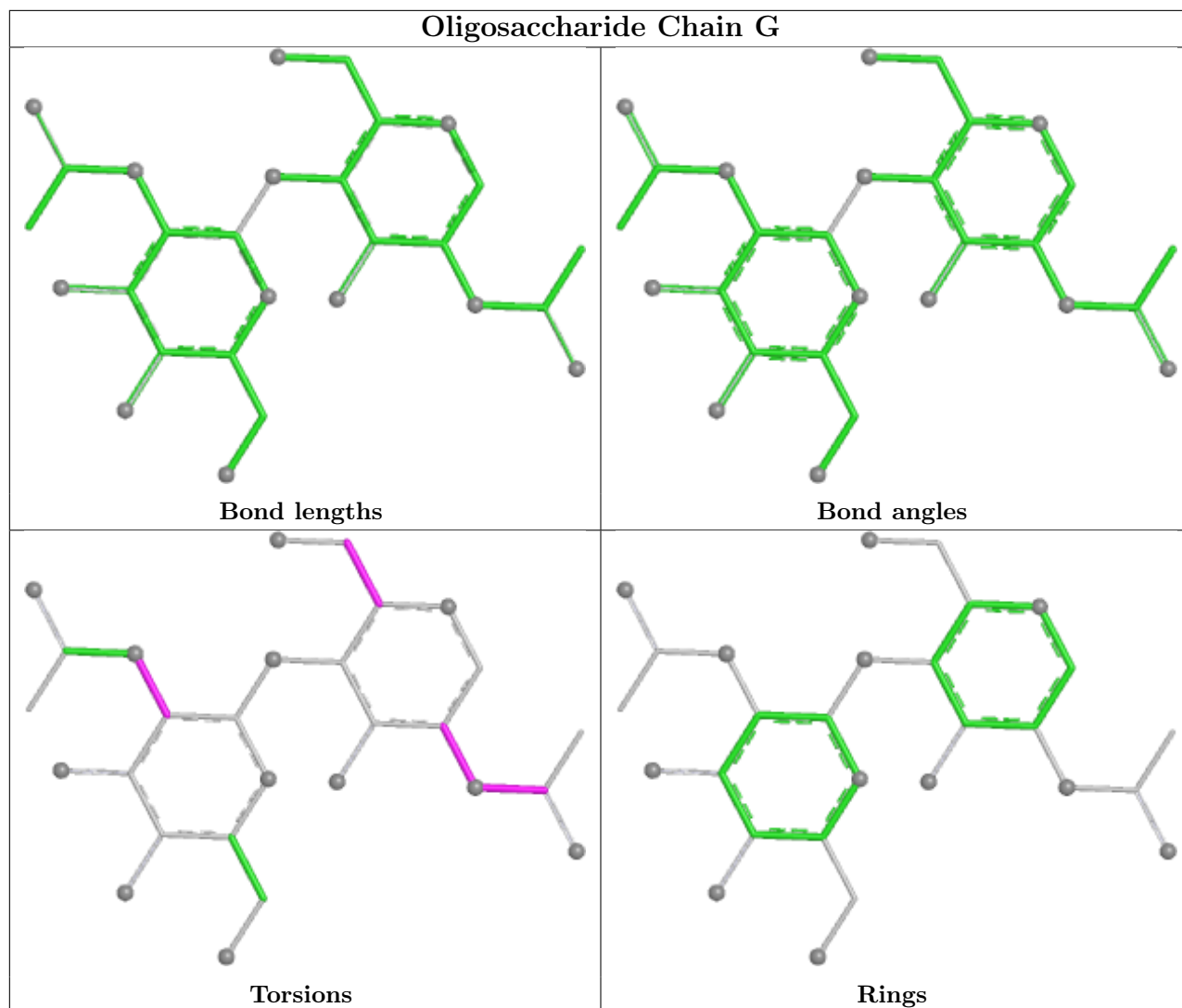
Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C3-C2-N2-C7
5	G	1	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	H	1	NAG	C3-C2-N2-C7
5	G	2	NAG	C1-C2-N2-C7
5	G	2	NAG	C3-C2-N2-C7
5	G	1	NAG	C4-C5-C6-O6

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](#)

Of 50 ligands modelled in this entry, 4 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PEE	A	1314	-	26,26,50	1.19	4 (15%)	29,31,55	1.20	2 (6%)
12	PLM	C	206	3	3,4,17	0.58	0	2,3,17	0.68	0
8	R16	A	1317	-	9,9,15	0.25	0	8,8,14	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	R16	A	1309	-	10,10,15	0.22	0	9,9,14	0.57	0
6	TWT	A	1315	-	18,18,21	0.23	0	17,17,20	0.63	0
8	R16	A	1310	-	9,9,15	0.22	0	8,8,14	0.58	0
9	CLR	D	1305	-	31,31,31	0.71	1 (3%)	48,48,48	1.16	7 (14%)
7	PEE	C	205	-	24,24,50	1.24	4 (16%)	27,29,55	1.23	2 (7%)
12	PLM	F	205	3	4,5,17	0.52	0	3,4,17	0.69	0
7	PEE	D	1314	-	26,26,50	1.16	4 (15%)	29,31,55	1.16	2 (6%)
8	R16	D	1308	-	11,11,15	0.22	0	10,10,14	0.58	0
8	R16	D	1307	-	10,10,15	0.22	0	9,9,14	0.57	0
6	TWT	A	1301	-	11,11,21	0.22	0	10,10,20	0.57	0
8	R16	D	1309	-	12,12,15	0.21	0	11,11,14	0.60	0
8	R16	D	1313	-	9,9,15	0.24	0	8,8,14	0.55	0
10	NAG	A	1316	1	14,14,15	0.29	0	17,19,21	0.60	0
10	NAG	D	1316	1	14,14,15	0.35	0	17,19,21	2.20	3 (17%)
7	PEE	A	1312	-	26,26,50	1.20	4 (15%)	29,31,55	1.17	2 (6%)
6	TWT	C	201	-	17,17,21	0.23	0	16,16,20	0.58	0
7	PEE	D	1302	-	28,28,50	1.14	4 (14%)	31,33,55	1.14	2 (6%)
8	R16	C	203	-	10,10,15	0.24	0	9,9,14	0.55	0
12	PLM	C	204	3	9,10,17	0.38	0	8,9,17	0.65	0
7	PEE	D	1312	-	26,26,50	1.19	4 (15%)	29,31,55	1.19	2 (6%)
8	R16	F	203	-	11,11,15	0.24	0	10,10,14	0.58	0
12	PLM	F	204	3	10,11,17	0.37	0	9,10,17	0.67	0
6	TWT	D	1301	-	16,16,21	0.22	0	15,15,20	0.59	0
7	PEE	D	1317	-	24,24,50	1.22	4 (16%)	27,29,55	1.12	2 (7%)
8	R16	A	1308	-	9,9,15	0.25	0	8,8,14	0.57	0
8	R16	A	1307	-	14,14,15	0.22	0	13,13,14	0.59	0
8	R16	D	1306	-	5,5,15	0.24	0	4,4,14	0.44	0
8	R16	A	1313	-	9,9,15	0.24	0	8,8,14	0.54	0
7	PEE	A	1311	-	32,32,50	1.27	5 (15%)	35,37,55	1.28	3 (8%)
8	R16	F	202	-	15,15,15	0.20	0	14,14,14	0.61	0
7	PEE	D	1311	-	32,32,50	1.27	5 (15%)	35,37,55	1.27	4 (11%)
8	R16	A	1303	-	15,15,15	0.20	0	14,14,14	0.63	0
8	R16	D	1318	-	9,9,15	0.25	0	8,8,14	0.56	0
8	R16	C	202	-	11,11,15	0.25	0	10,10,14	0.58	0
6	TWT	D	1315	-	18,18,21	0.23	0	17,17,20	0.61	0
8	R16	A	1306	-	9,9,15	0.23	0	8,8,14	0.56	0
8	R16	D	1304	-	9,9,15	0.25	0	8,8,14	0.57	0
7	PEE	A	1302	-	28,28,50	1.14	4 (14%)	31,33,55	1.12	2 (6%)
8	R16	D	1303	-	15,15,15	0.20	0	14,14,14	0.61	0
8	R16	A	1304	-	9,9,15	0.24	0	8,8,14	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLR	A	1305	-	31,31,31	0.63	0	48,48,48	1.06	2 (4%)
6	TWT	F	201	-	18,18,21	0.22	0	17,17,20	0.64	0
8	R16	D	1310	-	12,12,15	0.23	0	11,11,14	0.58	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	PEE	A	1314	-	-	15/30/30/54	-
12	PLM	C	206	3	-	1/2/2/15	-
8	R16	A	1317	-	-	0/7/7/13	-
8	R16	A	1309	-	-	0/8/8/13	-
6	TWT	A	1315	-	-	0/16/16/19	-
8	R16	A	1310	-	-	0/7/7/13	-
9	CLR	D	1305	-	-	6/10/68/68	0/4/4/4
7	PEE	C	205	-	-	9/28/28/54	-
12	PLM	F	205	3	-	1/3/3/15	-
7	PEE	D	1314	-	-	14/30/30/54	-
8	R16	D	1308	-	-	0/9/9/13	-
8	R16	D	1307	-	-	0/8/8/13	-
6	TWT	A	1301	-	-	4/9/9/19	-
8	R16	D	1309	-	-	0/10/10/13	-
8	R16	D	1313	-	-	0/7/7/13	-
10	NAG	A	1316	1	-	3/6/23/26	0/1/1/1
10	NAG	D	1316	1	-	3/6/23/26	0/1/1/1
7	PEE	A	1312	-	-	14/30/30/54	-
6	TWT	C	201	-	-	0/15/15/19	-
7	PEE	D	1302	-	-	15/32/32/54	-
8	R16	C	203	-	-	0/8/8/13	-
12	PLM	C	204	3	-	2/8/8/15	-
7	PEE	D	1312	-	-	9/30/30/54	-
8	R16	F	203	-	-	1/9/9/13	-
12	PLM	F	204	3	-	0/9/9/15	-
6	TWT	D	1301	-	-	1/14/14/19	-
7	PEE	D	1317	-	-	8/28/28/54	-
8	R16	A	1308	-	-	1/7/7/13	-
8	R16	A	1307	-	-	0/12/12/13	-
8	R16	D	1306	-	-	0/3/3/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	R16	A	1313	-	-	0/7/7/13	-
7	PEE	A	1311	-	-	15/36/36/54	-
8	R16	F	202	-	-	0/13/13/13	-
7	PEE	D	1311	-	-	19/36/36/54	-
8	R16	A	1303	-	-	3/13/13/13	-
8	R16	D	1318	-	-	0/7/7/13	-
8	R16	C	202	-	-	0/9/9/13	-
6	TWT	D	1315	-	-	4/16/16/19	-
8	R16	A	1306	-	-	0/7/7/13	-
8	R16	D	1304	-	-	1/7/7/13	-
7	PEE	A	1302	-	-	12/32/32/54	-
8	R16	D	1303	-	-	1/13/13/13	-
8	R16	A	1304	-	-	0/7/7/13	-
9	CLR	A	1305	-	-	8/10/68/68	0/4/4/4
6	TWT	F	201	-	-	0/16/16/19	-
8	R16	D	1310	-	-	0/10/10/13	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1311	PEE	C39-C38	3.77	1.53	1.31
7	D	1311	PEE	C39-C38	3.75	1.53	1.31
7	C	205	PEE	O2-C2	-2.73	1.40	1.46
7	D	1311	PEE	O2-C2	-2.65	1.40	1.46
7	A	1314	PEE	O2-C2	-2.64	1.40	1.46
7	D	1302	PEE	O2-C2	-2.60	1.40	1.46
7	D	1312	PEE	O2-C2	-2.58	1.40	1.46
7	A	1312	PEE	O2-C2	-2.57	1.40	1.46
7	A	1311	PEE	O2-C2	-2.55	1.40	1.46
7	A	1311	PEE	O3-C30	2.46	1.40	1.33
7	A	1302	PEE	O3-C30	2.44	1.40	1.33
7	D	1312	PEE	O3-C30	2.44	1.40	1.33
7	D	1317	PEE	O3-C30	2.43	1.40	1.33
7	A	1312	PEE	O3-C30	2.43	1.40	1.33
7	A	1314	PEE	O3-C30	2.42	1.40	1.33
7	D	1317	PEE	O2-C10	2.40	1.41	1.34
7	D	1302	PEE	O3-C30	2.39	1.40	1.33
7	A	1302	PEE	O2-C10	2.39	1.41	1.34
7	C	205	PEE	O3-C30	2.39	1.40	1.33
7	D	1314	PEE	O3-C30	2.38	1.40	1.33
7	D	1311	PEE	O3-C30	2.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1317	PEE	O2-C2	-2.30	1.41	1.46
7	D	1312	PEE	O2-C10	2.25	1.40	1.34
7	A	1312	PEE	O2-C10	2.25	1.40	1.34
7	A	1302	PEE	O2-C2	-2.25	1.41	1.46
7	D	1311	PEE	O3-C3	-2.24	1.40	1.45
7	D	1314	PEE	O2-C2	-2.22	1.41	1.46
7	D	1314	PEE	O2-C10	2.22	1.40	1.34
7	A	1314	PEE	O2-C10	2.20	1.40	1.34
7	D	1311	PEE	O2-C10	2.20	1.40	1.34
7	D	1302	PEE	O2-C10	2.20	1.40	1.34
7	A	1311	PEE	O2-C10	2.17	1.40	1.34
7	D	1302	PEE	O3-C3	-2.17	1.40	1.45
7	D	1314	PEE	O3-C3	-2.16	1.40	1.45
7	A	1311	PEE	O3-C3	-2.16	1.40	1.45
7	C	205	PEE	O3-C3	-2.16	1.40	1.45
7	D	1312	PEE	O3-C3	-2.15	1.40	1.45
7	A	1312	PEE	O3-C3	-2.15	1.40	1.45
7	D	1317	PEE	O3-C3	-2.15	1.40	1.45
7	C	205	PEE	O2-C10	2.14	1.40	1.34
7	A	1314	PEE	O3-C3	-2.12	1.40	1.45
7	A	1302	PEE	O3-C3	-2.11	1.40	1.45
9	D	1305	CLR	C10-C9	-2.03	1.52	1.56

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1316	NAG	C1-O5-C5	7.97	122.87	112.19
7	A	1311	PEE	O2-C10-C11	4.06	120.26	111.48
7	D	1312	PEE	O2-C10-C11	3.93	119.97	111.48
7	A	1314	PEE	O2-C10-C11	3.92	119.97	111.48
7	A	1312	PEE	O2-C10-C11	3.89	119.89	111.48
7	C	205	PEE	O2-C10-C11	3.88	119.87	111.48
7	D	1311	PEE	O2-C10-C11	3.85	119.82	111.48
7	D	1302	PEE	O2-C10-C11	3.81	119.72	111.48
7	D	1314	PEE	O2-C10-C11	3.72	119.54	111.48
7	A	1302	PEE	O2-C10-C11	3.57	119.21	111.48
7	D	1317	PEE	O2-C10-C11	3.47	119.00	111.48
9	D	1305	CLR	C4-C5-C10	3.02	120.29	116.42
7	D	1311	PEE	C40-C39-C38	-2.81	109.49	126.42
7	A	1314	PEE	O3-C30-C31	2.76	120.26	111.83
7	A	1311	PEE	O3-C30-C31	2.76	120.24	111.83
7	D	1314	PEE	O3-C30-C31	2.73	120.16	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1311	PEE	C40-C39-C38	-2.72	110.05	126.42
7	D	1312	PEE	O3-C30-C31	2.71	120.09	111.83
7	C	205	PEE	O3-C30-C31	2.70	120.06	111.83
7	D	1317	PEE	O3-C30-C31	2.68	119.99	111.83
9	D	1305	CLR	C13-C17-C20	-2.67	115.37	119.50
7	A	1312	PEE	O3-C30-C31	2.65	119.93	111.83
7	D	1302	PEE	O3-C30-C31	2.64	119.90	111.83
9	D	1305	CLR	C19-C10-C9	-2.60	108.74	111.66
7	D	1311	PEE	O3-C30-C31	2.60	119.78	111.83
9	A	1305	CLR	C22-C20-C17	2.58	115.69	110.33
7	A	1302	PEE	O3-C30-C31	2.55	119.62	111.83
9	D	1305	CLR	C4-C5-C6	-2.41	117.30	120.57
9	A	1305	CLR	C8-C7-C6	-2.34	109.53	112.76
10	D	1316	NAG	O5-C5-C4	2.24	116.27	110.83
9	D	1305	CLR	C17-C13-C14	2.20	102.62	100.10
10	D	1316	NAG	O5-C1-C2	2.19	114.68	111.29
9	D	1305	CLR	C11-C12-C13	-2.13	109.15	112.74
9	D	1305	CLR	C11-C9-C10	-2.10	110.49	113.08
7	D	1311	PEE	C37-C38-C39	-2.04	109.51	124.83

There are no chirality outliers.

All (170) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1311	PEE	C11-C10-O2-C2
7	A	1311	PEE	O4-C10-O2-C2
7	A	1311	PEE	C4-O4P-P-O1P
7	A	1311	PEE	O4P-C4-C5-N
7	A	1312	PEE	C1-O3P-P-O4P
7	A	1312	PEE	C4-O4P-P-O3P
7	A	1312	PEE	C4-O4P-P-O1P
7	A	1314	PEE	C1-O3P-P-O2P
7	A	1314	PEE	C1-O3P-P-O4P
7	A	1314	PEE	O4P-C4-C5-N
7	C	205	PEE	C4-O4P-P-O3P
7	C	205	PEE	C4-O4P-P-O2P
7	C	205	PEE	C4-O4P-P-O1P
7	C	205	PEE	O4P-C4-C5-N
7	D	1302	PEE	O2-C2-C3-O3
7	D	1302	PEE	C1-O3P-P-O1P
7	D	1302	PEE	C4-O4P-P-O3P
7	D	1302	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
7	D	1302	PEE	O4P-C4-C5-N
7	D	1311	PEE	C11-C10-O2-C2
7	D	1311	PEE	C1-O3P-P-O1P
7	D	1311	PEE	C1-O3P-P-O4P
7	D	1311	PEE	O4P-C4-C5-N
7	D	1312	PEE	O2-C2-C3-O3
7	D	1312	PEE	O4P-C4-C5-N
7	D	1314	PEE	C11-C10-O2-C2
7	D	1314	PEE	C1-O3P-P-O1P
7	D	1314	PEE	C1-O3P-P-O4P
7	D	1314	PEE	O4P-C4-C5-N
7	D	1317	PEE	C11-C10-O2-C2
7	D	1317	PEE	C1-O3P-P-O1P
9	A	1305	CLR	C13-C17-C20-C22
10	A	1316	NAG	C1-C2-N2-C7
10	A	1316	NAG	C8-C7-N2-C2
10	A	1316	NAG	O7-C7-N2-C2
12	C	204	PLM	O2-C1-C2-C3
12	C	206	PLM	O2-C1-C2-C3
12	F	205	PLM	O2-C1-C2-C3
7	D	1311	PEE	O5-C30-O3-C3
7	D	1311	PEE	C31-C30-O3-C3
7	A	1311	PEE	O5-C30-O3-C3
7	D	1311	PEE	O4-C10-O2-C2
7	D	1314	PEE	O4-C10-O2-C2
7	D	1317	PEE	O4-C10-O2-C2
7	A	1311	PEE	C31-C30-O3-C3
9	A	1305	CLR	C17-C20-C22-C23
10	D	1316	NAG	C8-C7-N2-C2
9	A	1305	CLR	C16-C17-C20-C21
7	A	1302	PEE	O3P-C1-C2-O2
9	A	1305	CLR	C21-C20-C22-C23
10	D	1316	NAG	O7-C7-N2-C2
7	D	1311	PEE	C30-C31-C32-C33
9	D	1305	CLR	C20-C22-C23-C24
7	A	1314	PEE	C10-C11-C12-C13
9	A	1305	CLR	C16-C17-C20-C22
7	D	1302	PEE	C10-C11-C12-C13
9	A	1305	CLR	C22-C23-C24-C25
7	A	1311	PEE	C37-C38-C39-C40
7	D	1314	PEE	C3-C2-O2-C10
7	A	1302	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
7	A	1311	PEE	C30-C31-C32-C33
7	D	1312	PEE	C31-C30-O3-C3
7	A	1302	PEE	C12-C13-C14-C15
7	A	1302	PEE	O4-C10-O2-C2
7	A	1312	PEE	C11-C12-C13-C14
7	D	1312	PEE	O5-C30-O3-C3
9	A	1305	CLR	C13-C17-C20-C21
6	D	1315	TWT	C10-C11-C12-C13
8	A	1303	R16	C36-C37-C38-C39
7	A	1311	PEE	C38-C39-C40-C41
7	D	1302	PEE	C12-C13-C14-C15
7	D	1302	PEE	C31-C30-O3-C3
7	D	1314	PEE	C10-C11-C12-C13
6	D	1301	TWT	C6-C7-C8-C9
7	A	1314	PEE	O2-C2-C3-O3
7	A	1314	PEE	C11-C12-C13-C14
7	D	1314	PEE	O3P-C1-C2-C3
9	D	1305	CLR	C23-C24-C25-C27
10	D	1316	NAG	O5-C5-C6-O6
7	A	1312	PEE	C11-C10-O2-C2
7	C	205	PEE	C1-C2-C3-O3
7	D	1302	PEE	O5-C30-O3-C3
7	A	1302	PEE	C4-O4P-P-O1P
7	C	205	PEE	O2-C2-C3-O3
7	A	1302	PEE	C13-C14-C15-C16
7	A	1302	PEE	O3P-C1-C2-C3
9	D	1305	CLR	C23-C24-C25-C26
12	C	204	PLM	C4-C5-C6-C7
7	D	1302	PEE	C13-C14-C15-C16
7	A	1314	PEE	C1-C2-C3-O3
7	D	1302	PEE	C1-C2-C3-O3
7	D	1312	PEE	C1-C2-C3-O3
8	A	1303	R16	C39-C40-C41-C42
7	A	1314	PEE	O3P-C1-C2-O2
7	D	1312	PEE	O3P-C1-C2-O2
7	A	1311	PEE	C12-C13-C14-C15
7	D	1311	PEE	C32-C33-C34-C35
6	D	1315	TWT	C9-C10-C11-C12
7	D	1317	PEE	C30-C31-C32-C33
7	A	1311	PEE	C11-C12-C13-C14
7	D	1311	PEE	C34-C35-C36-C37
7	A	1312	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	D	1312	PEE	O3P-C1-C2-C3
6	A	1301	TWT	C3-C4-C5-C6
7	A	1312	PEE	O4-C10-O2-C2
7	D	1317	PEE	C3-C2-O2-C10
7	D	1302	PEE	O3P-C1-C2-O2
7	D	1311	PEE	O3P-C1-C2-O2
7	D	1314	PEE	O3P-C1-C2-O2
7	D	1314	PEE	C12-C13-C14-C15
7	D	1311	PEE	C1-C2-C3-O3
7	D	1311	PEE	O2-C2-C3-O3
8	A	1303	R16	C37-C38-C39-C40
7	D	1302	PEE	O3P-C1-C2-C3
7	D	1311	PEE	O3P-C1-C2-C3
7	A	1314	PEE	C12-C13-C14-C15
7	A	1312	PEE	O3P-C1-C2-O2
7	A	1302	PEE	C32-C33-C34-C35
7	A	1311	PEE	O2-C2-C3-O3
7	A	1312	PEE	C1-O3P-P-O1P
7	A	1312	PEE	C4-O4P-P-O2P
7	A	1312	PEE	O4P-C4-C5-N
7	C	205	PEE	C1-O3P-P-O1P
7	D	1317	PEE	O4P-C4-C5-N
7	D	1317	PEE	C11-C12-C13-C14
8	A	1308	R16	C32-C33-C34-C35
7	A	1302	PEE	C3-C2-O2-C10
6	D	1315	TWT	C11-C12-C13-C14
7	D	1311	PEE	C38-C39-C40-C41
7	A	1302	PEE	O2-C10-C11-C12
7	A	1312	PEE	C2-C1-O3P-P
7	D	1311	PEE	C2-C1-O3P-P
7	D	1312	PEE	C2-C1-O3P-P
9	D	1305	CLR	C13-C17-C20-C21
8	D	1304	R16	C34-C35-C36-C37
7	A	1314	PEE	C32-C33-C34-C35
9	D	1305	CLR	C13-C17-C20-C22
9	A	1305	CLR	C20-C22-C23-C24
7	A	1312	PEE	C31-C32-C33-C34
7	D	1317	PEE	O2-C10-C11-C12
7	D	1312	PEE	C31-C32-C33-C34
6	A	1301	TWT	C11-C10-C9-C8
7	D	1314	PEE	O5-C30-O3-C3
7	A	1314	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	A	1311	PEE	C36-C37-C38-C39
7	D	1311	PEE	C36-C37-C38-C39
8	F	203	R16	C34-C35-C36-C37
7	D	1314	PEE	C31-C30-O3-C3
7	A	1311	PEE	C1-C2-C3-O3
6	D	1315	TWT	C11-C10-C9-C8
8	D	1303	R16	C36-C37-C38-C39
7	D	1302	PEE	C11-C12-C13-C14
7	A	1302	PEE	O5-C30-O3-C3
7	D	1302	PEE	C31-C32-C33-C34
6	A	1301	TWT	C6-C7-C8-C9
9	D	1305	CLR	C16-C17-C20-C22
7	A	1314	PEE	O2-C10-C11-C12
7	C	205	PEE	O2-C10-C11-C12
7	D	1311	PEE	O2-C10-C11-C12
7	A	1312	PEE	C32-C33-C34-C35
7	A	1302	PEE	C31-C30-O3-C3
7	A	1311	PEE	C1-C2-O2-C10
6	A	1301	TWT	C4-C5-C6-C7
7	D	1314	PEE	C11-C12-C13-C14
7	D	1311	PEE	O4-C10-C11-C12
7	A	1314	PEE	O4-C10-C11-C12
7	A	1314	PEE	O4-C10-O2-C2
7	C	205	PEE	O4-C10-C11-C12
7	A	1314	PEE	C11-C10-O2-C2
7	D	1314	PEE	C30-C31-C32-C33

There are no ring outliers.

12 monomers are involved in 14 short contacts:

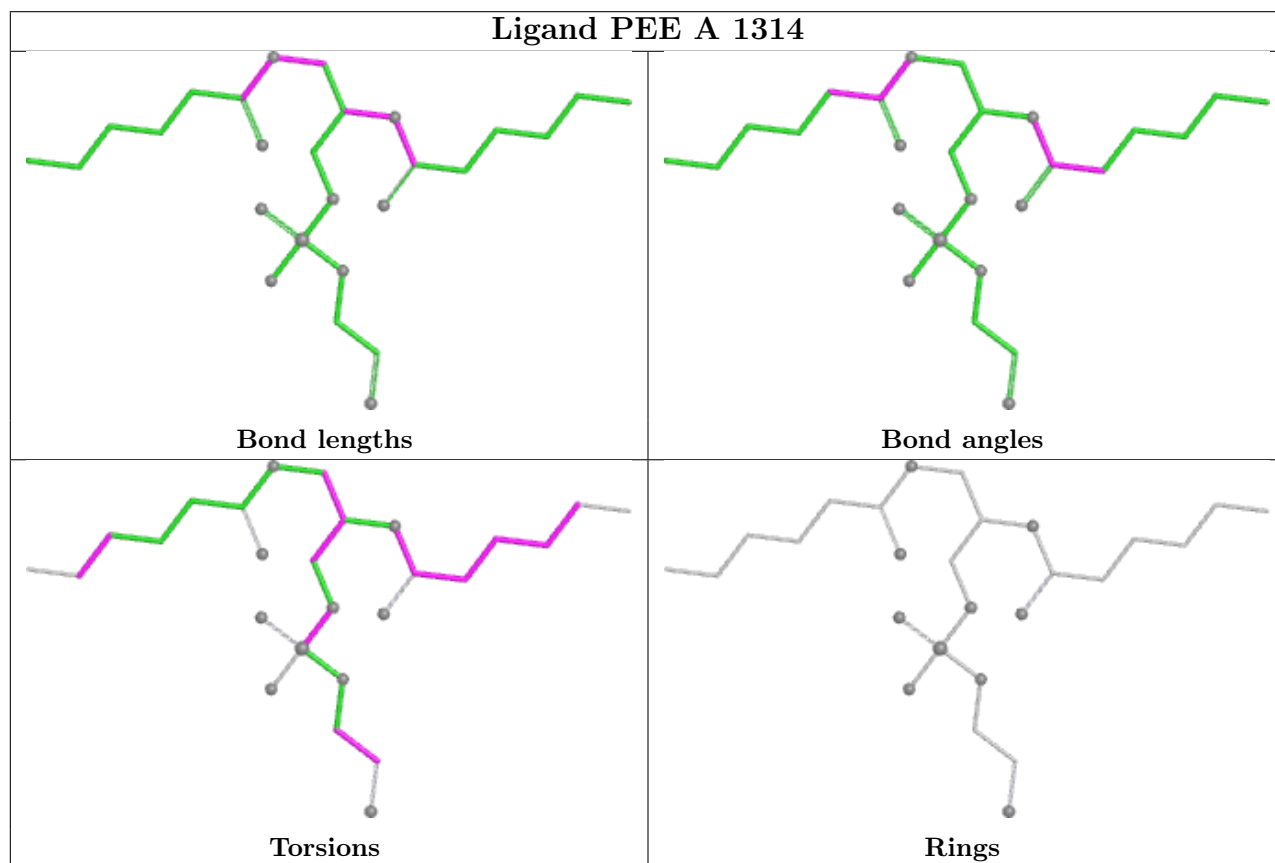
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1314	PEE	1	0
6	A	1315	TWT	1	0
8	A	1310	R16	1	0
7	C	205	PEE	1	0
6	A	1301	TWT	1	0
7	D	1312	PEE	1	0
7	D	1317	PEE	1	0
8	A	1307	R16	2	0
7	A	1311	PEE	1	0
8	A	1303	R16	1	0
8	D	1304	R16	1	0

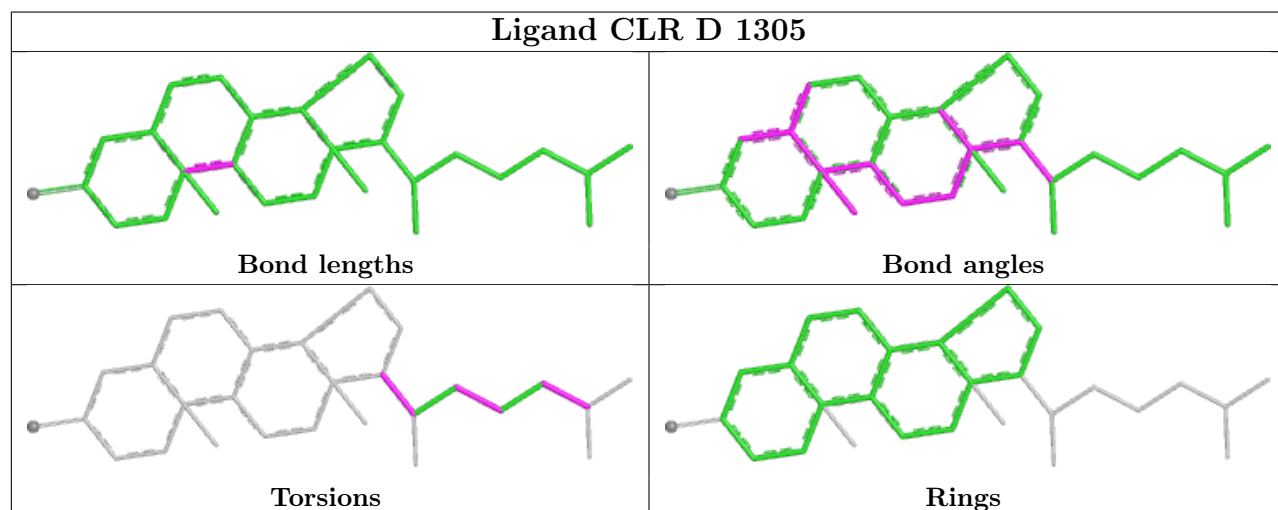
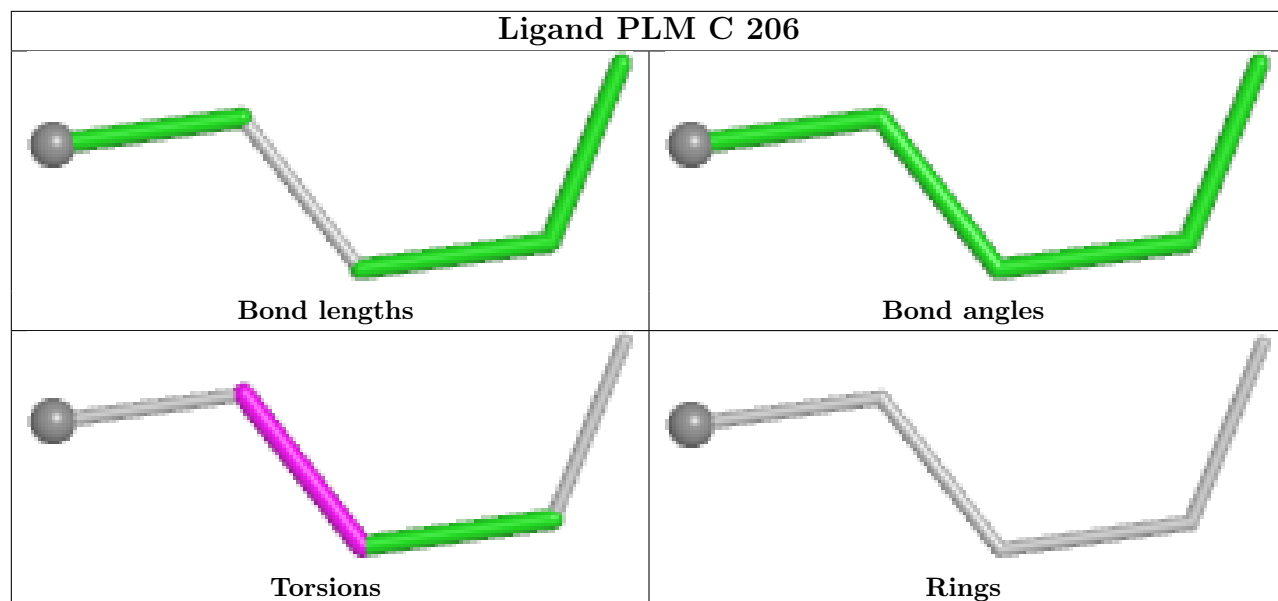
Continued on next page...

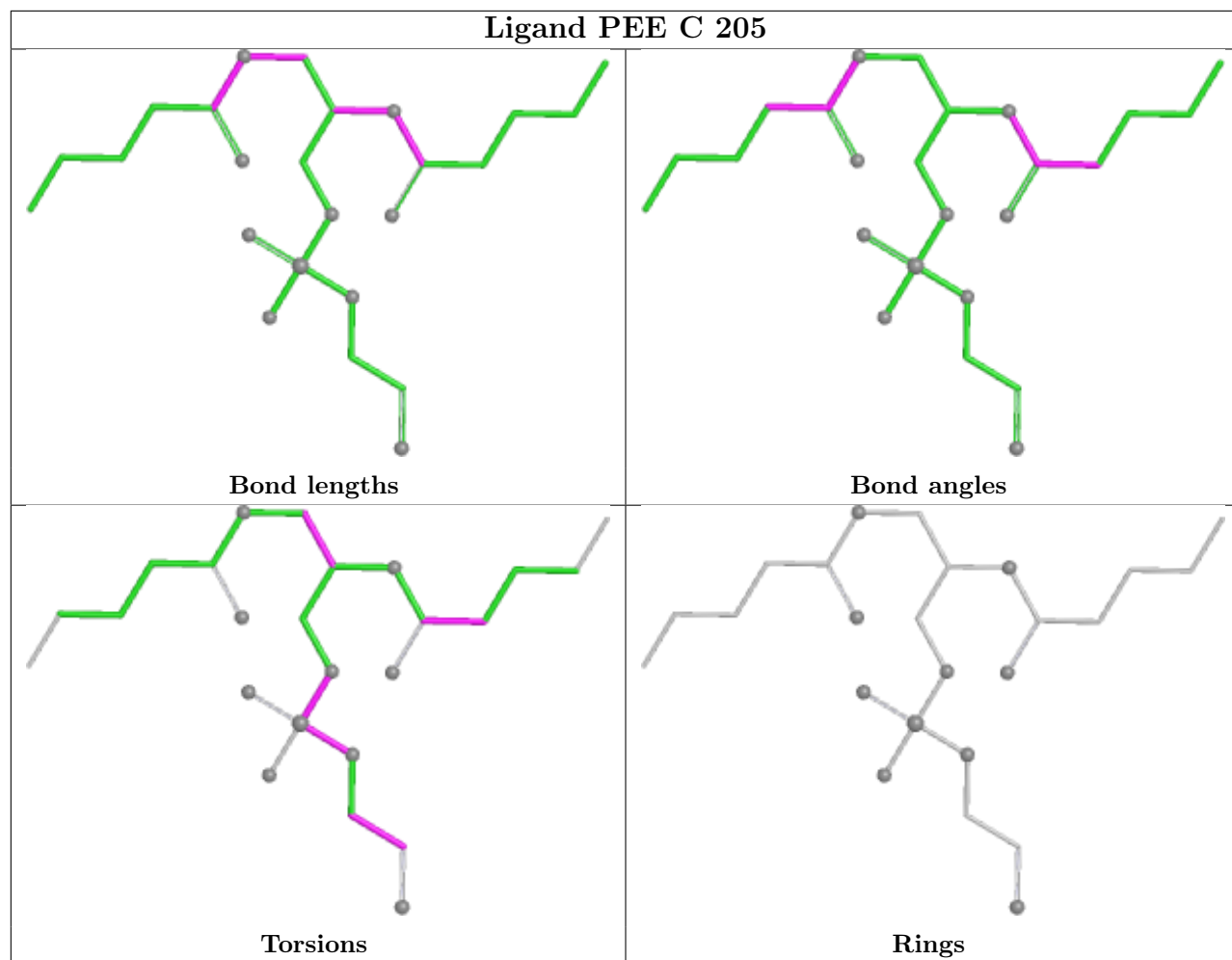
Continued from previous page...

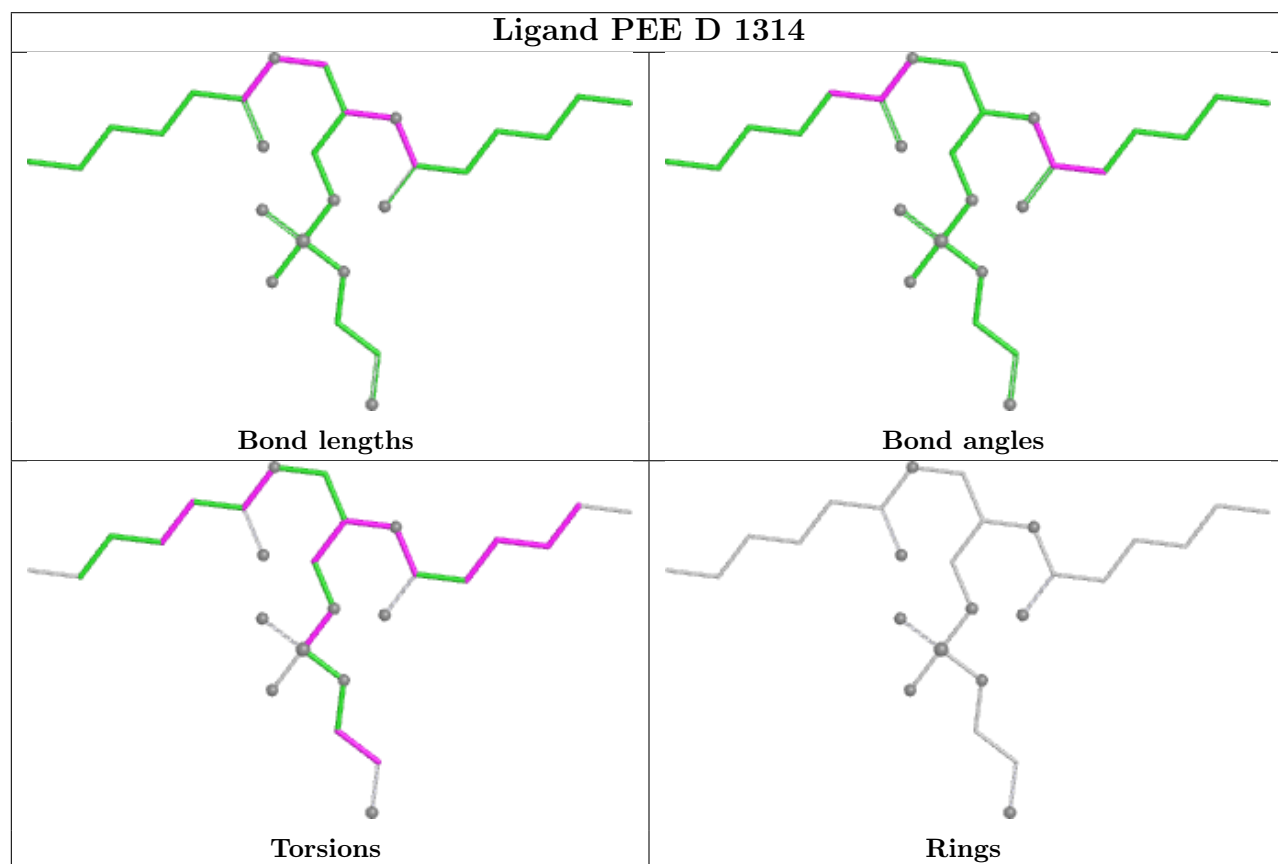
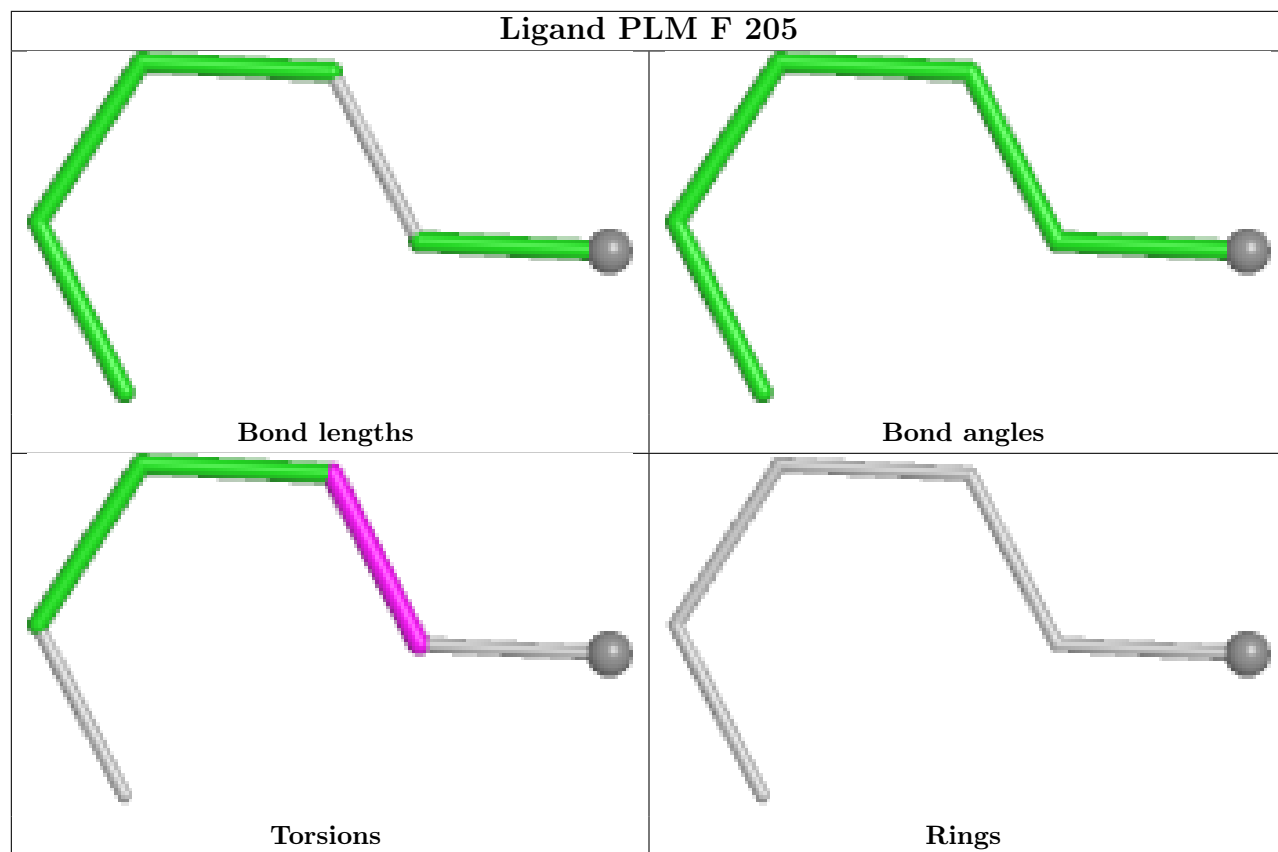
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1305	CLR	2	0

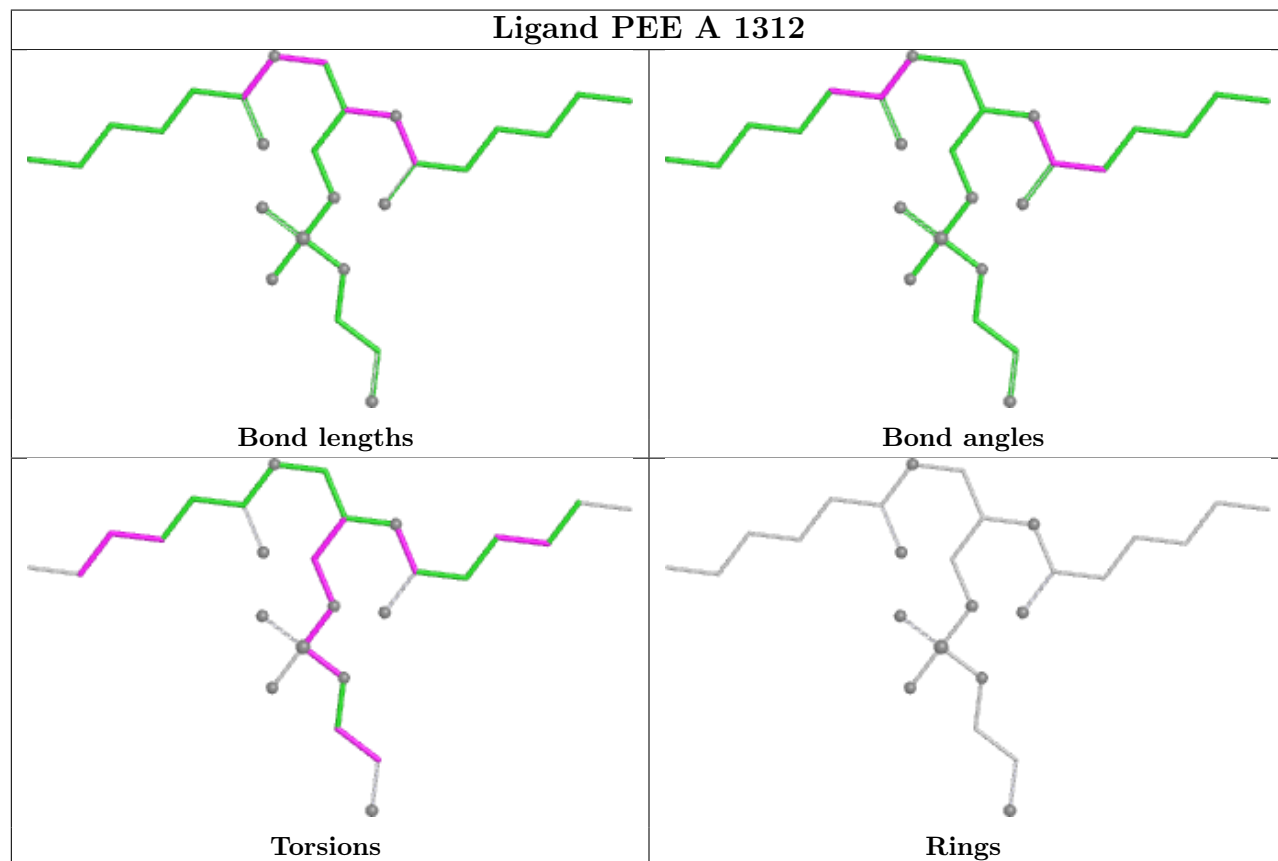
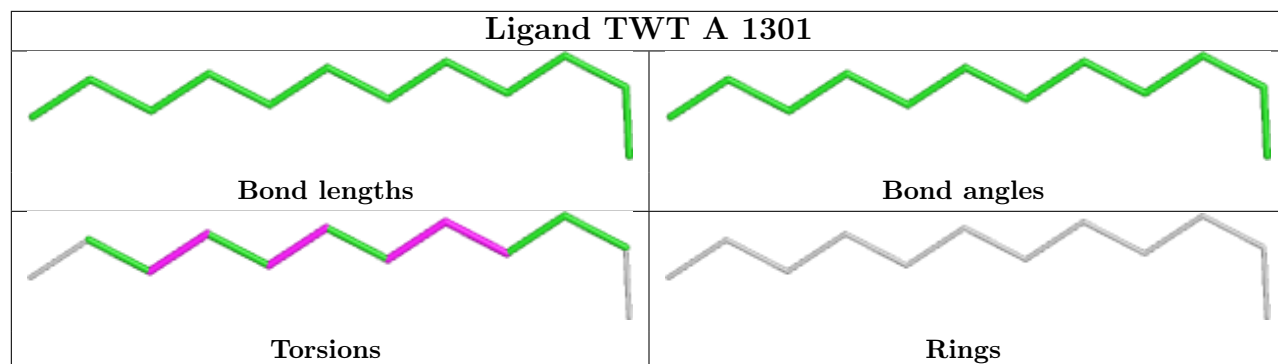
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

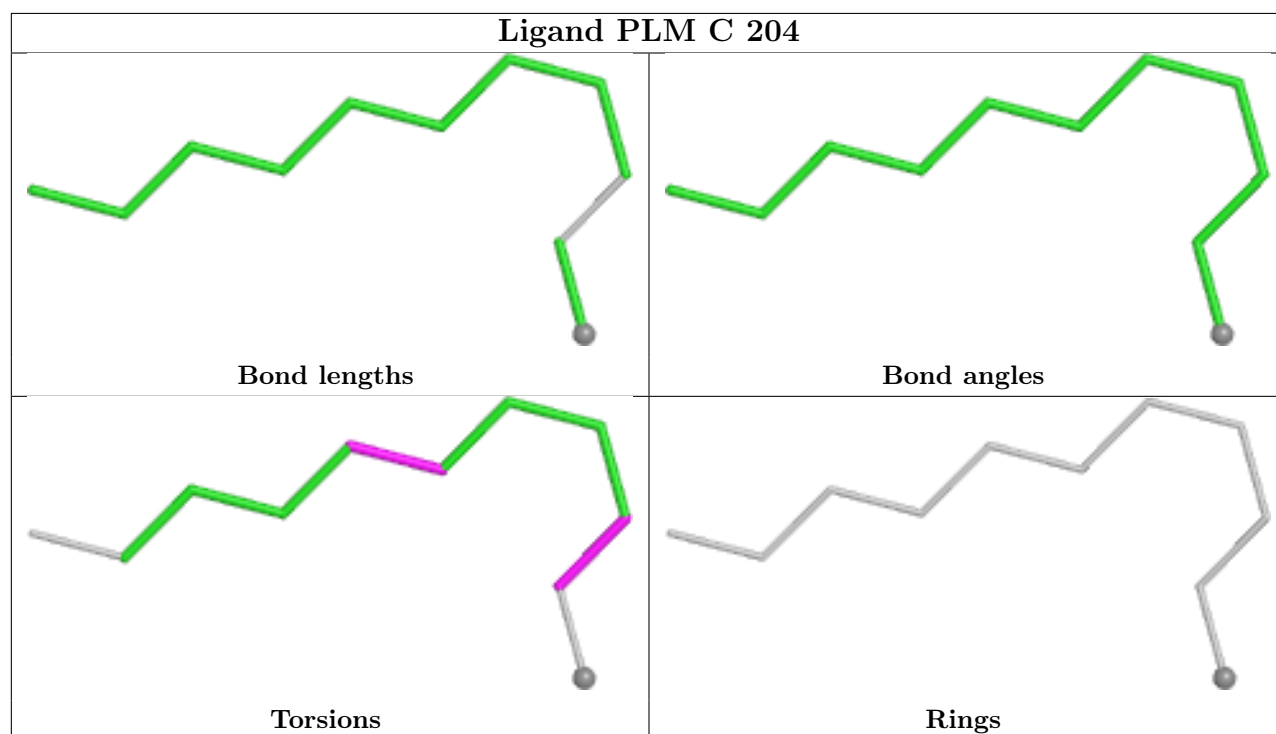
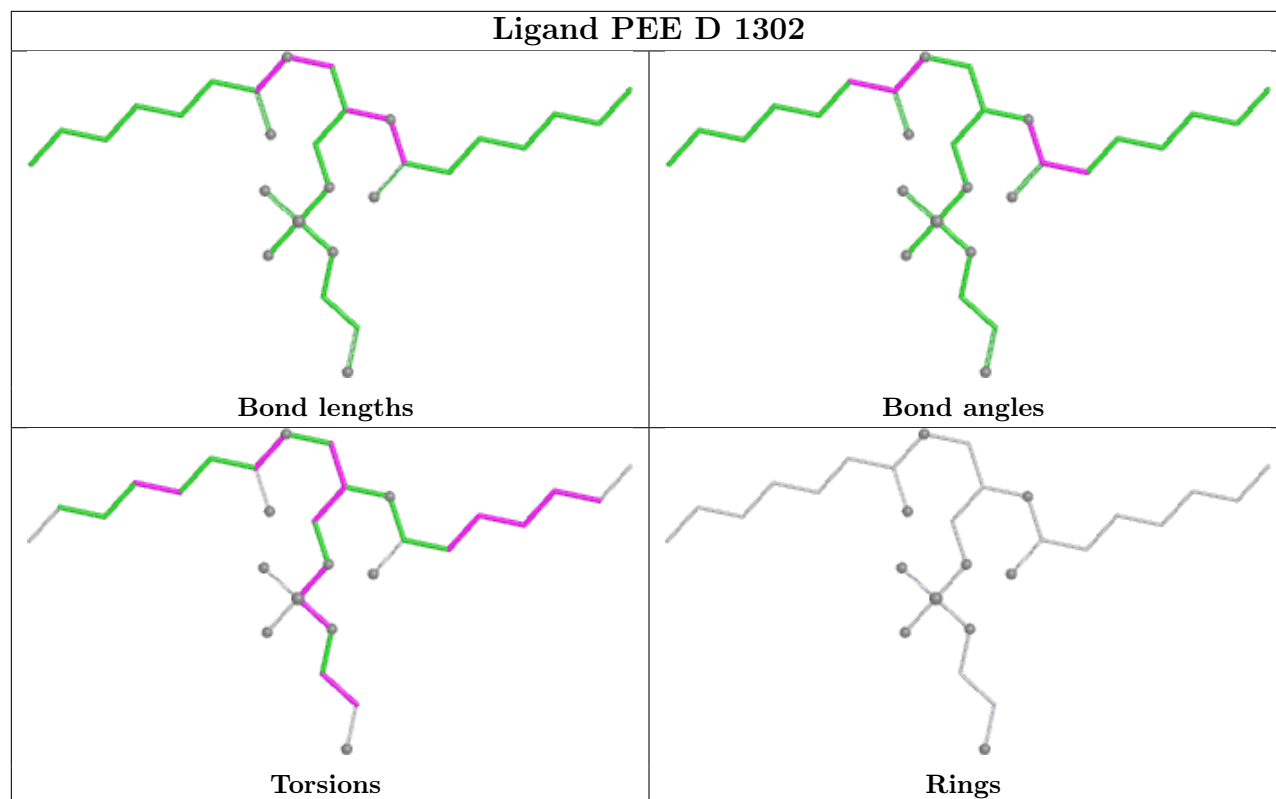


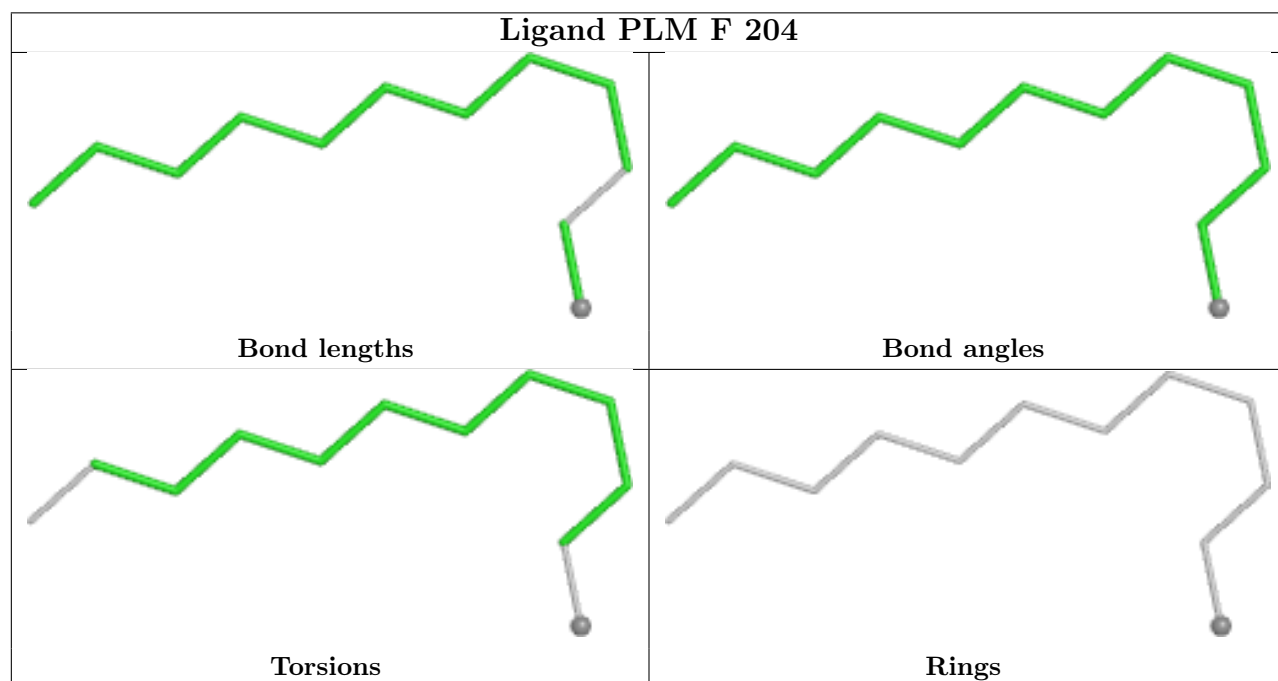
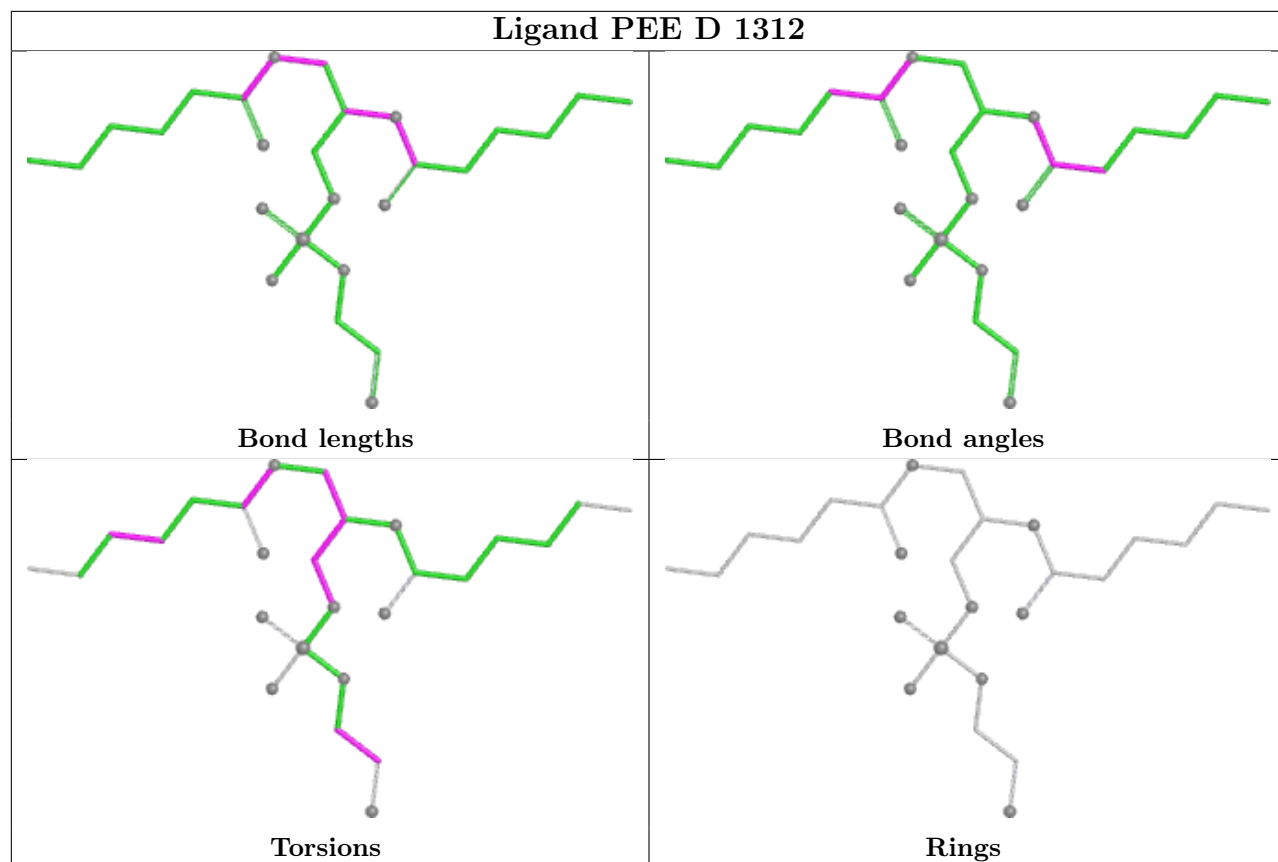


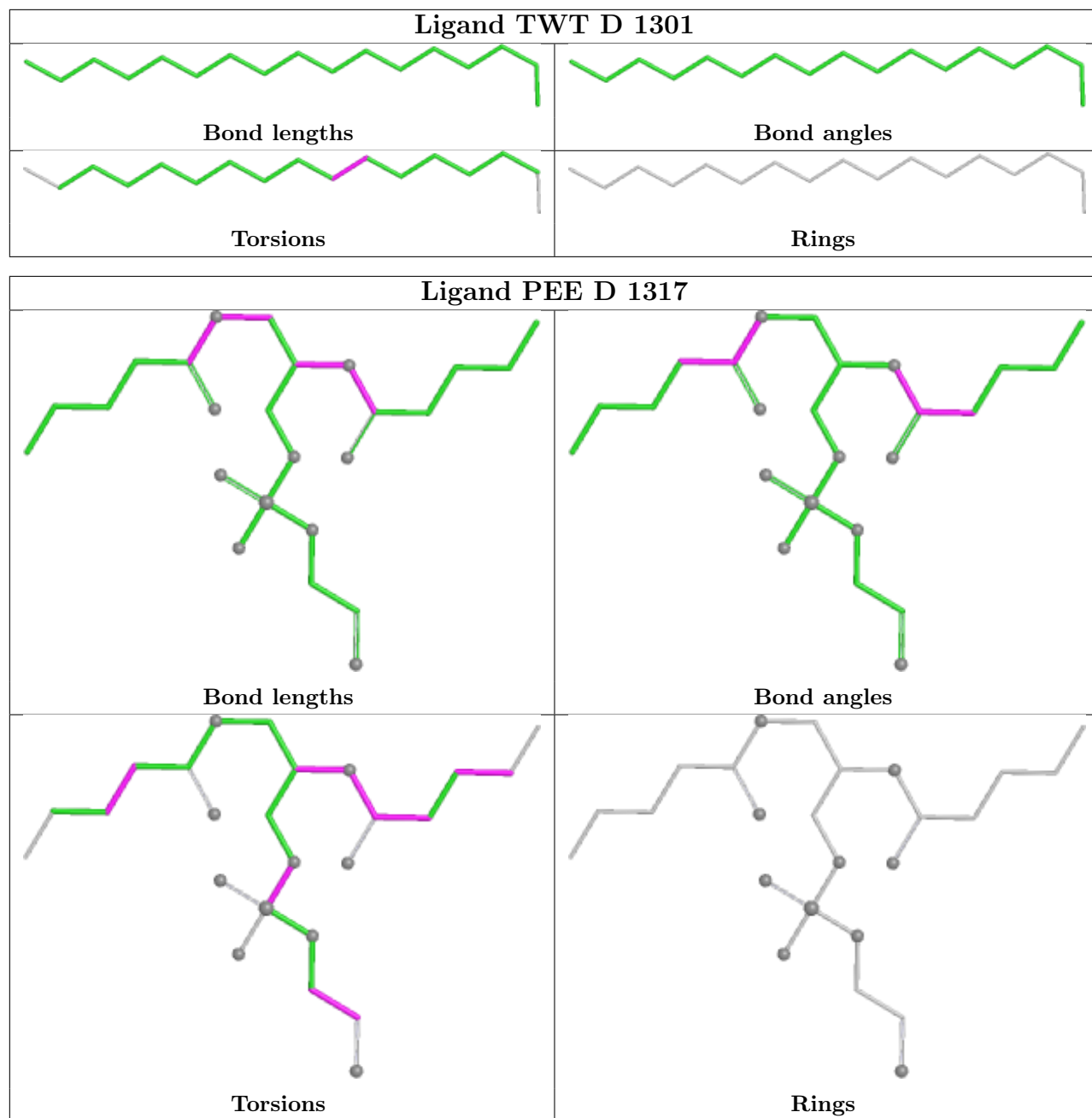


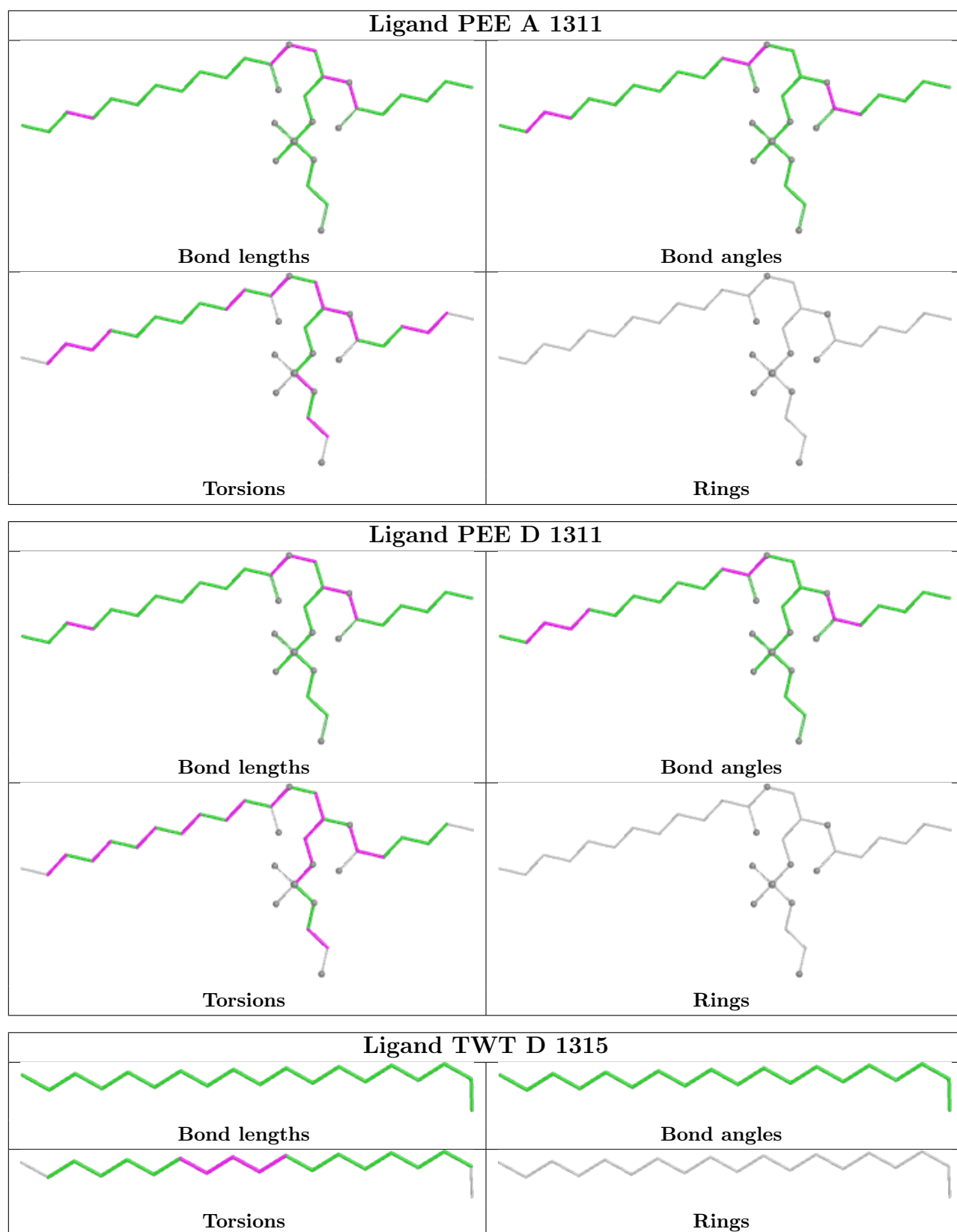


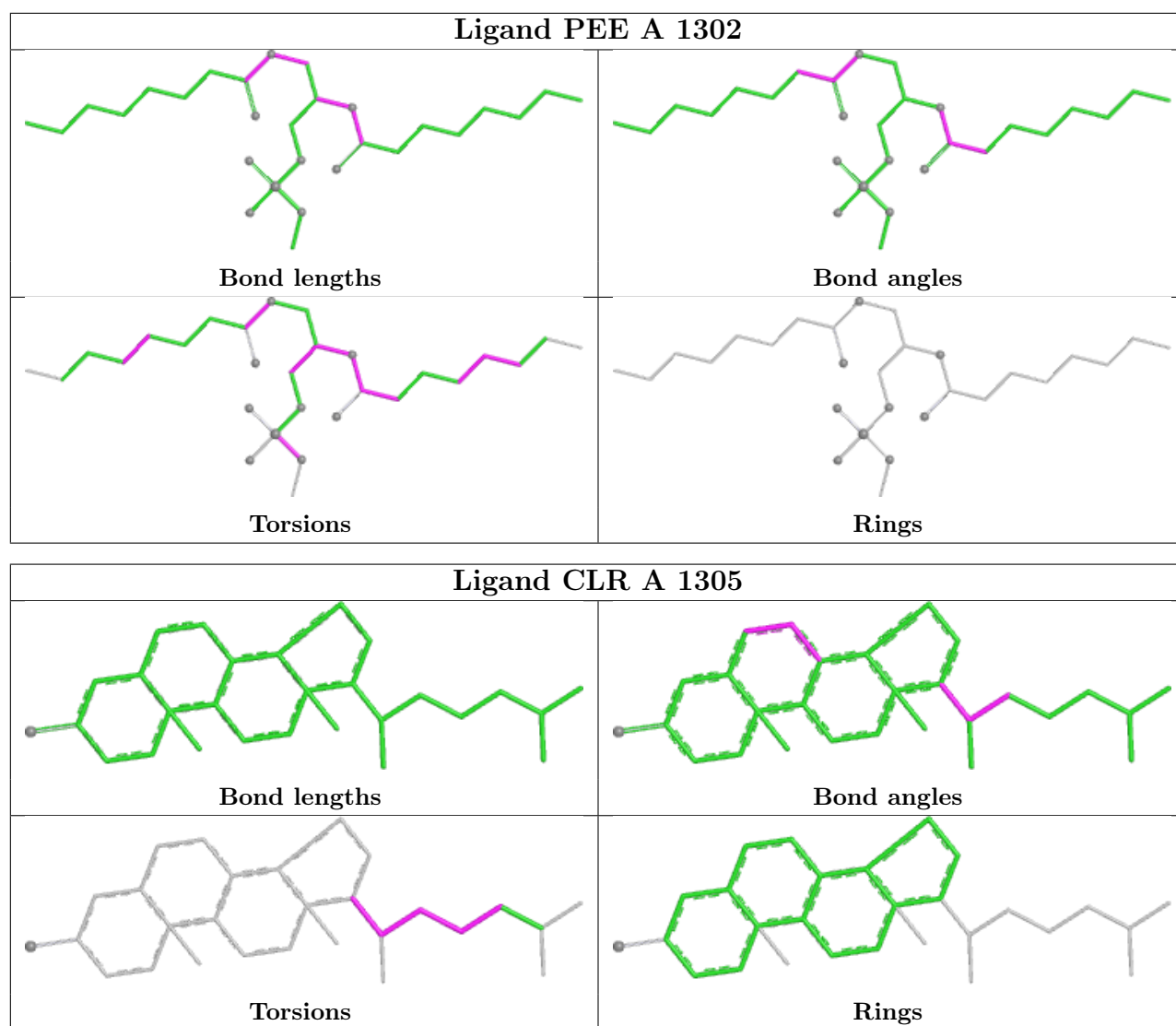












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

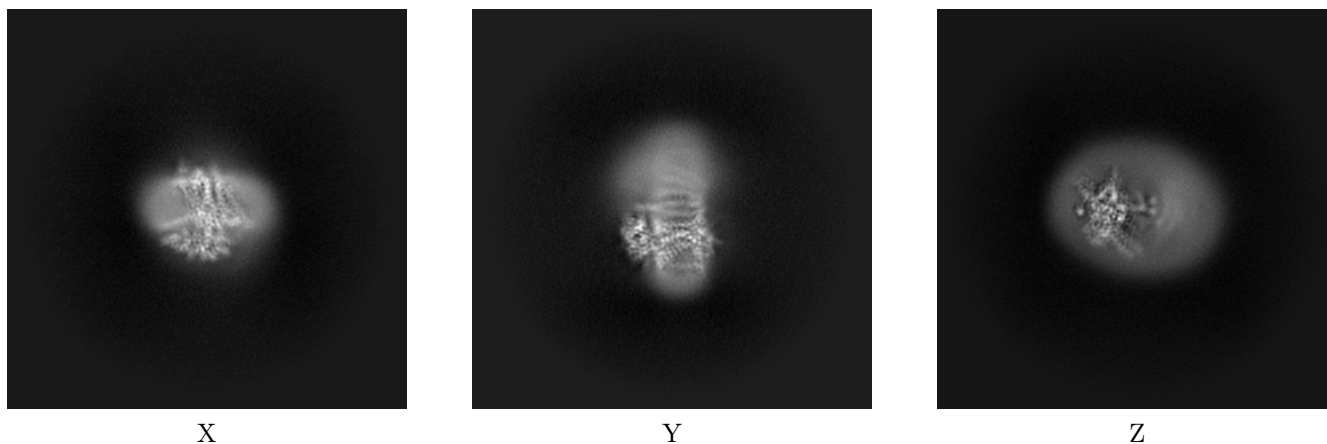
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41356. These allow visual inspection of the internal detail of the map and identification of artifacts.

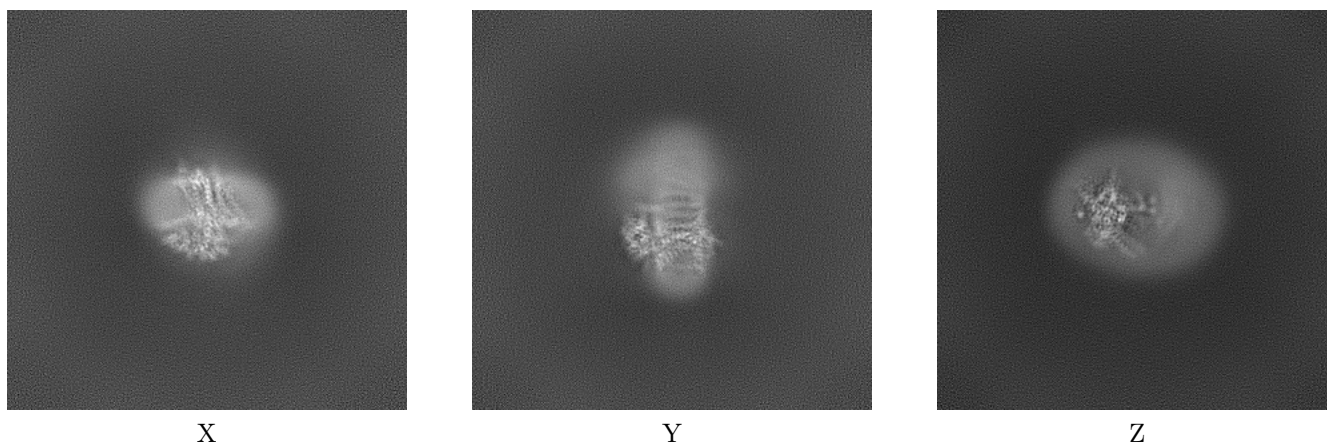
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



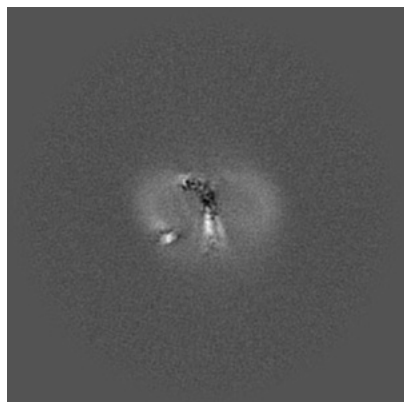
6.1.2 Raw map



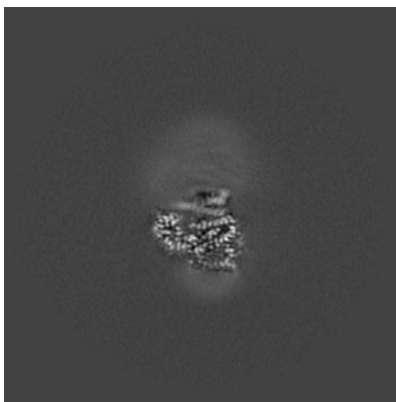
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

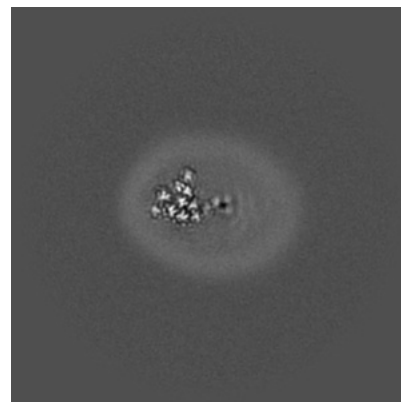
6.2.1 Primary map



X Index: 225

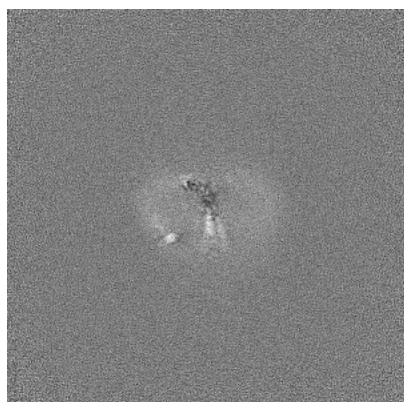


Y Index: 225

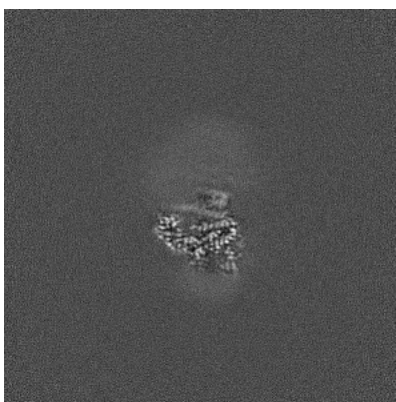


Z Index: 225

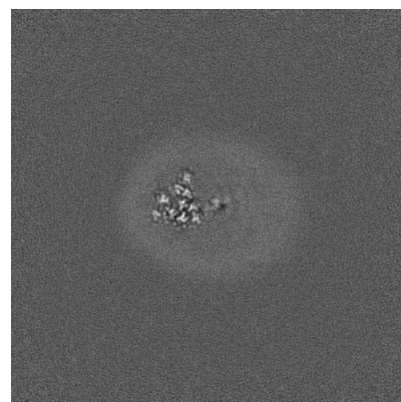
6.2.2 Raw map



X Index: 225



Y Index: 225

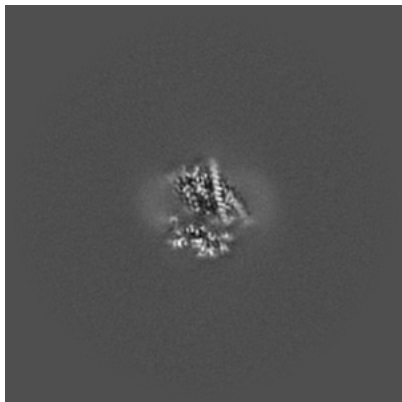


Z Index: 225

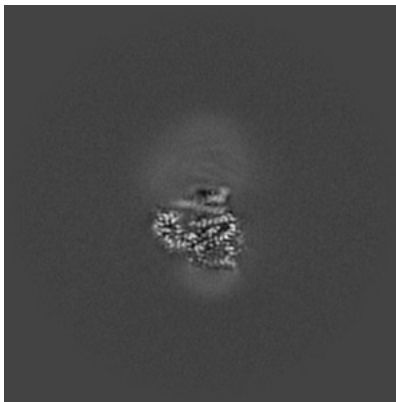
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

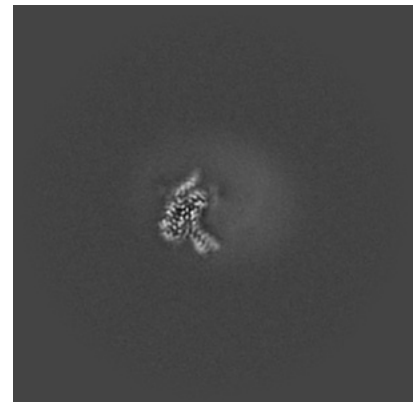
6.3.1 Primary map



X Index: 198

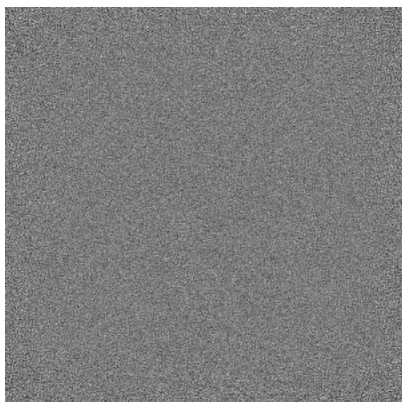


Y Index: 225

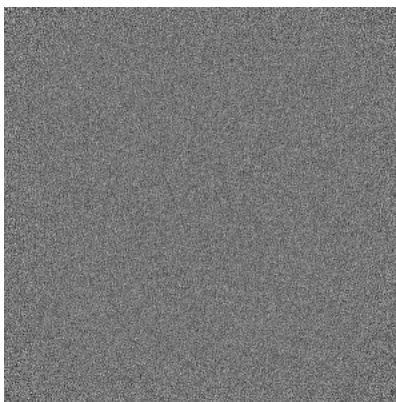


Z Index: 189

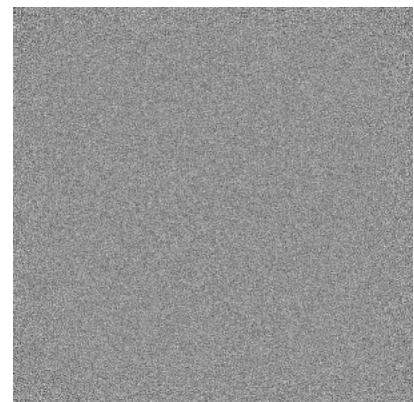
6.3.2 Raw map



X Index: 0



Y Index: 0

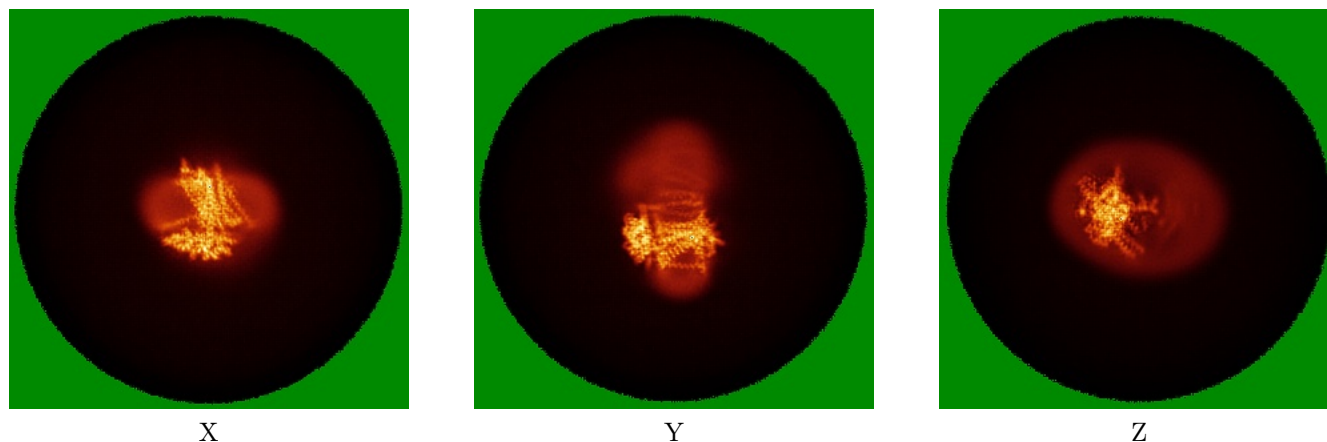


Z Index: 0

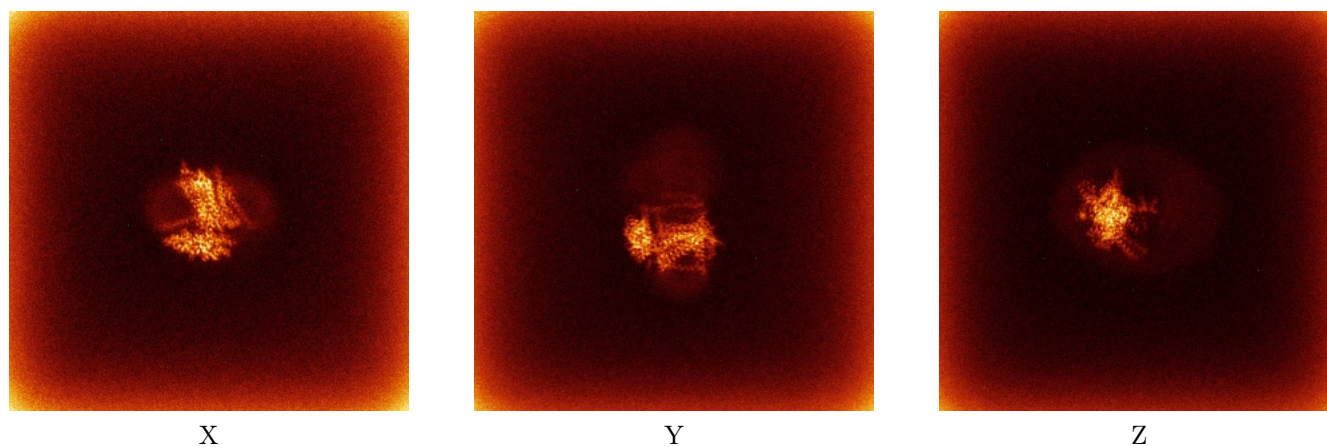
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



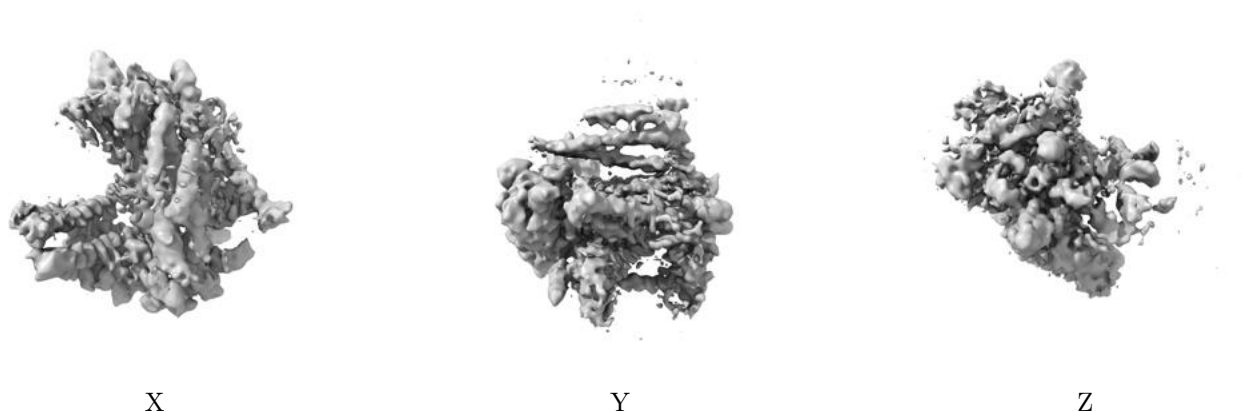
6.4.2 Raw map



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 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

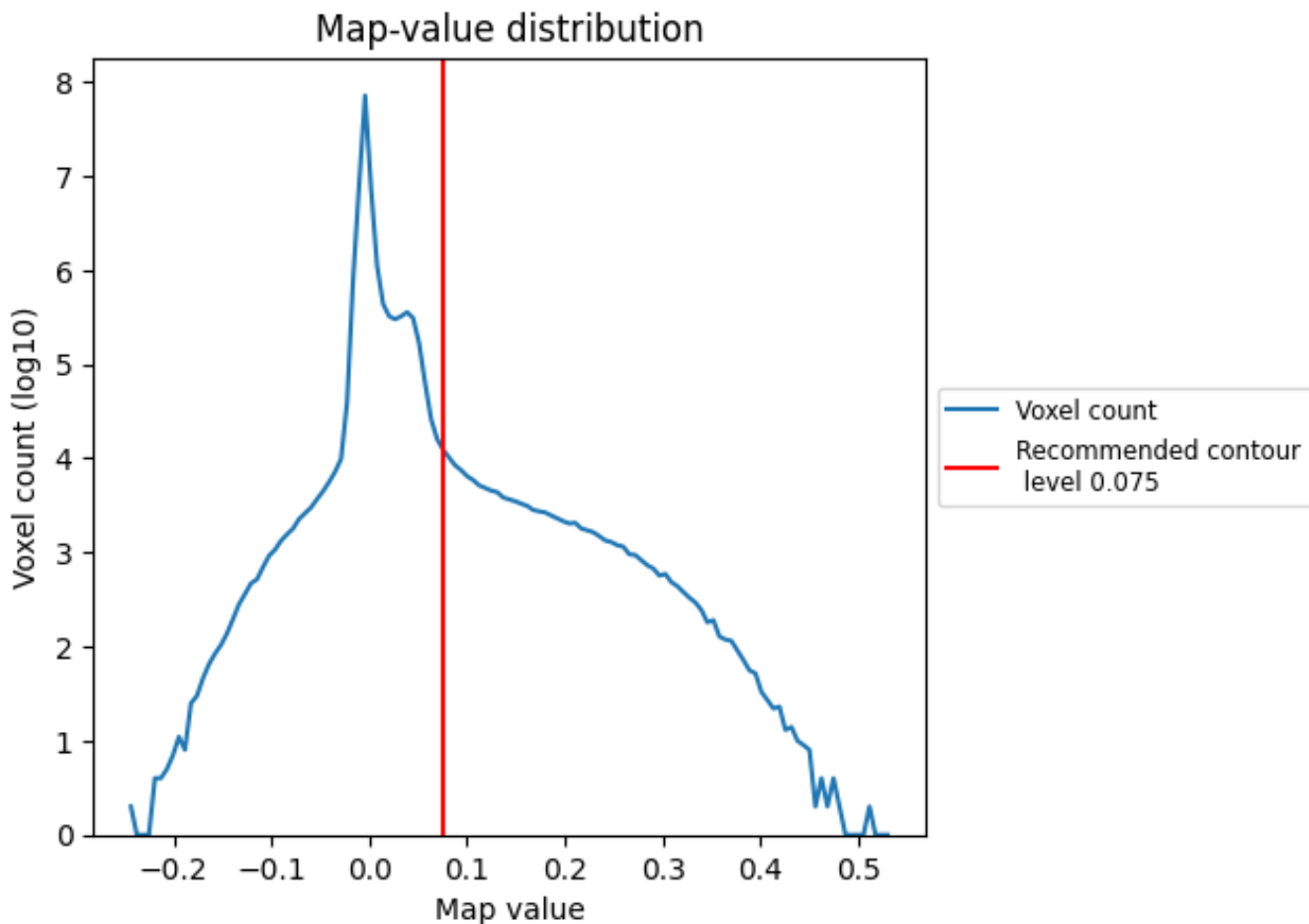
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

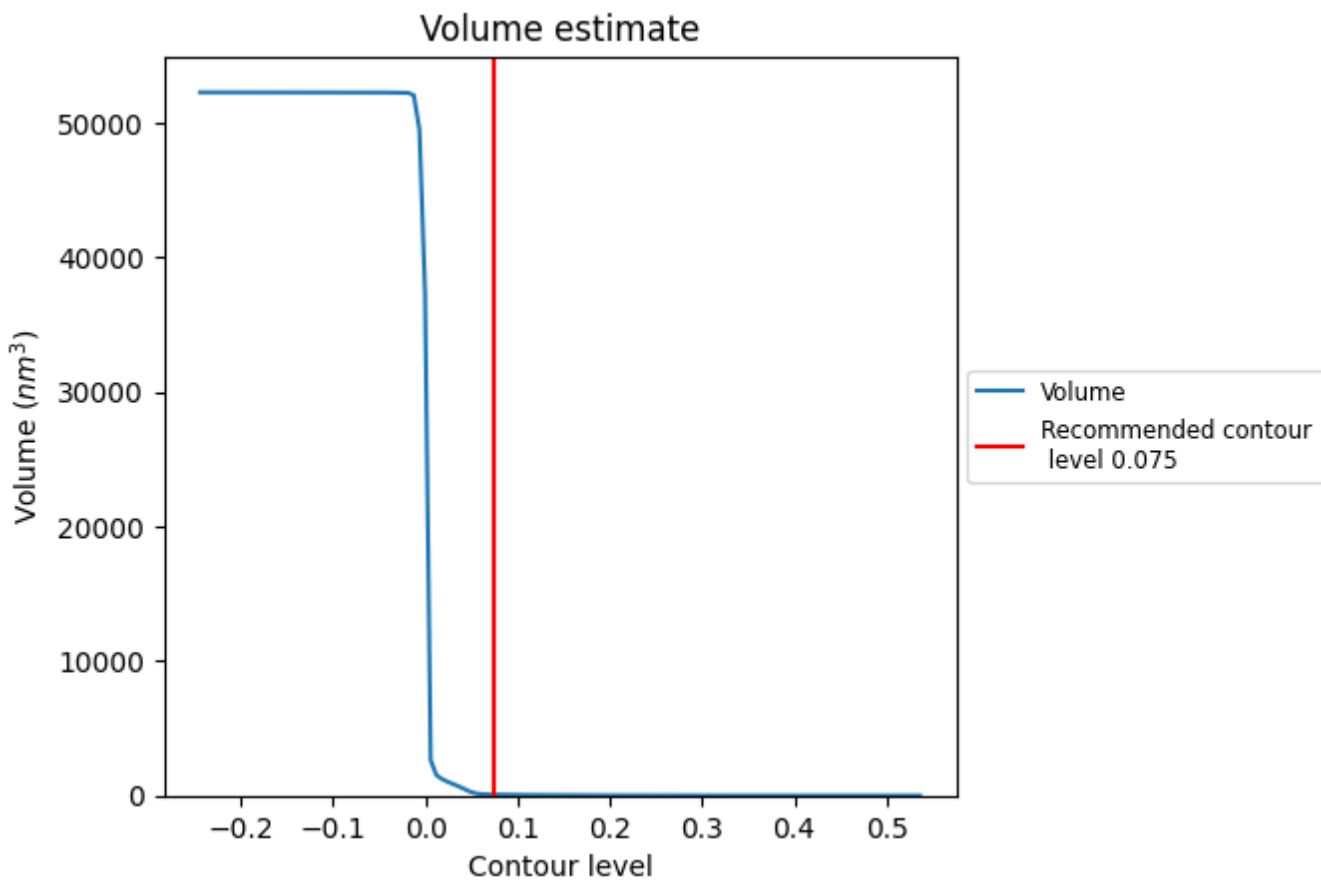
This section contains the results of statistical analysis of the map.

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.

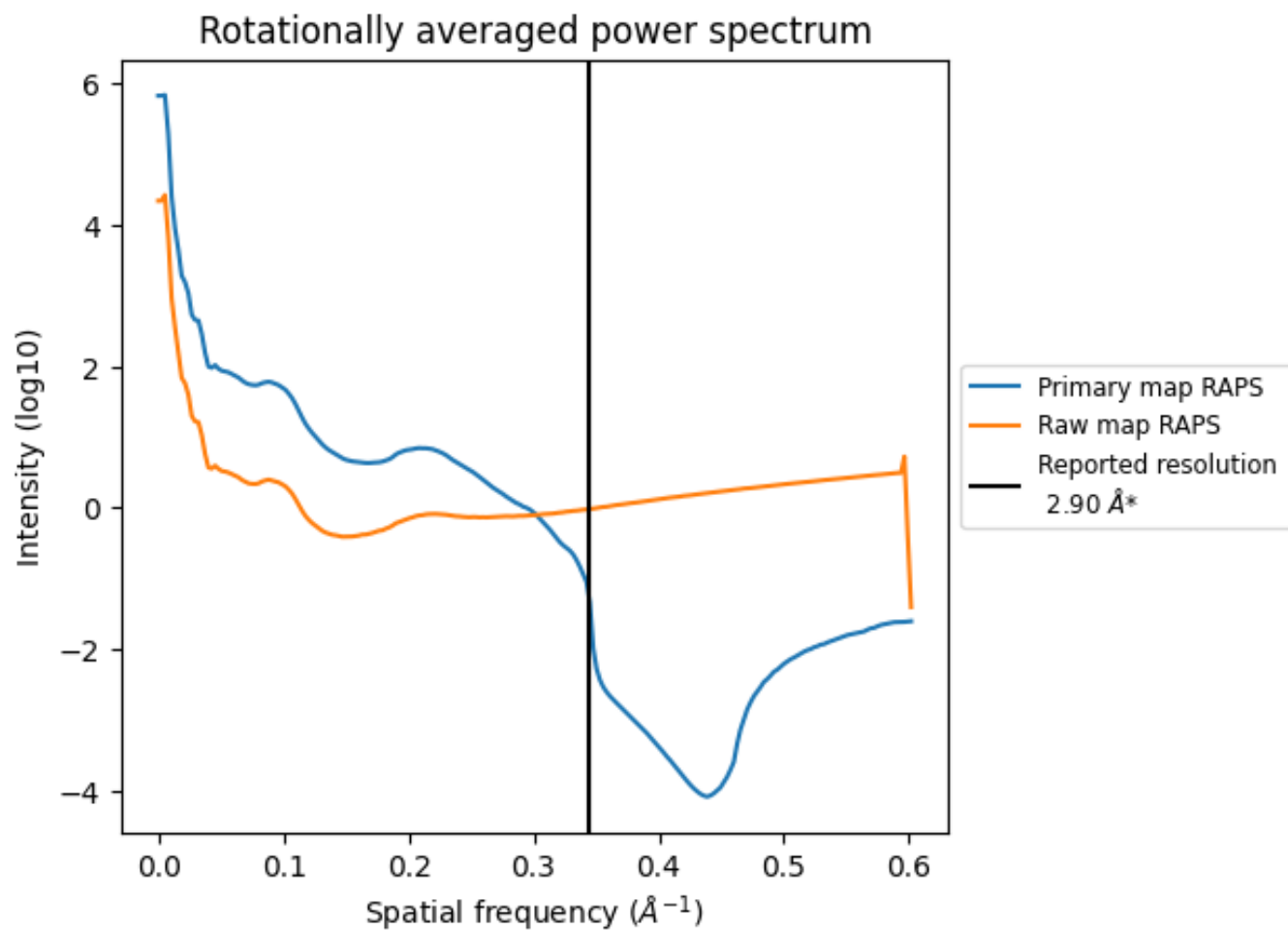
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 73 nm³; this corresponds to an approximate mass of 66 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

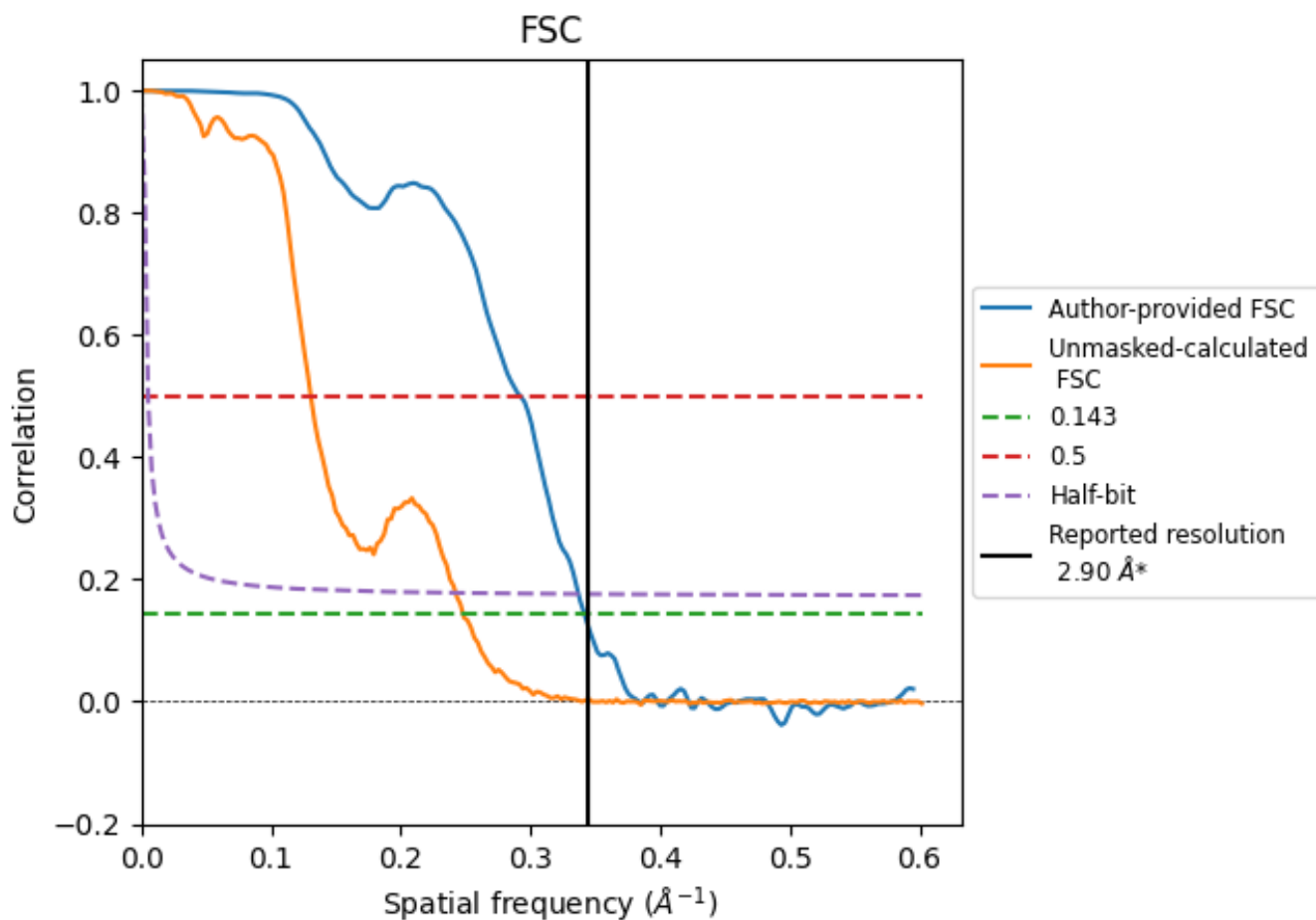


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

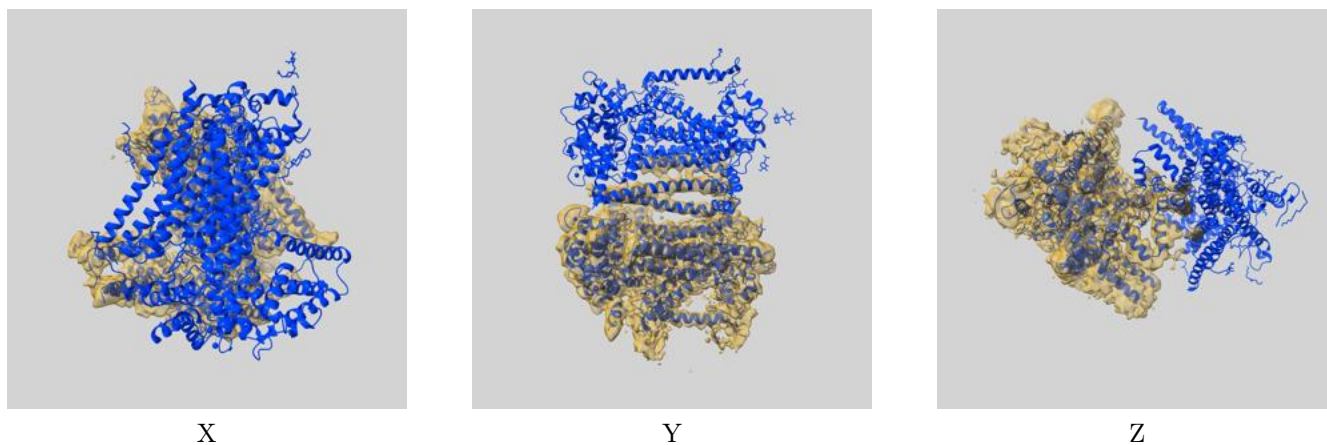
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.42	2.97
Unmasked-calculated*	4.03	7.65	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

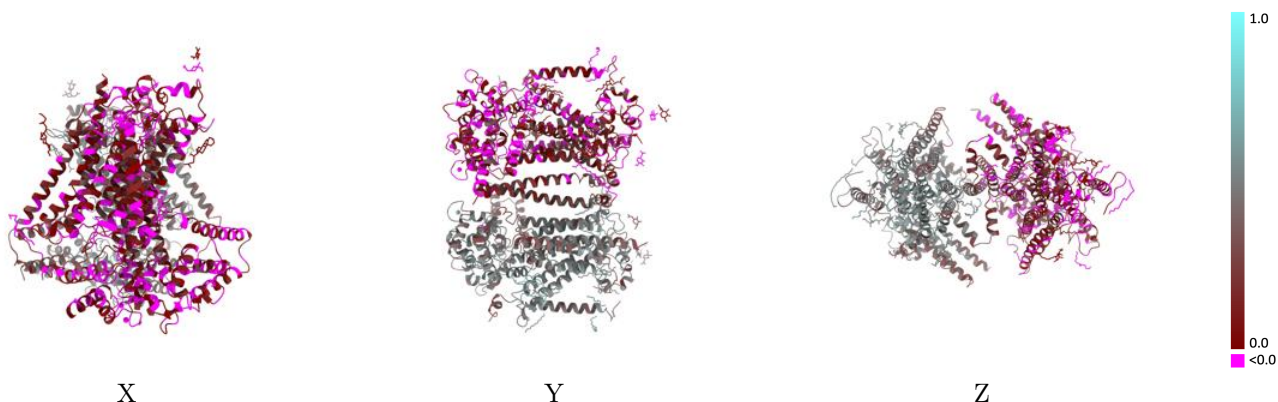
This section contains information regarding the fit between EMDB map EMD-41356 and PDB model 8TKP. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



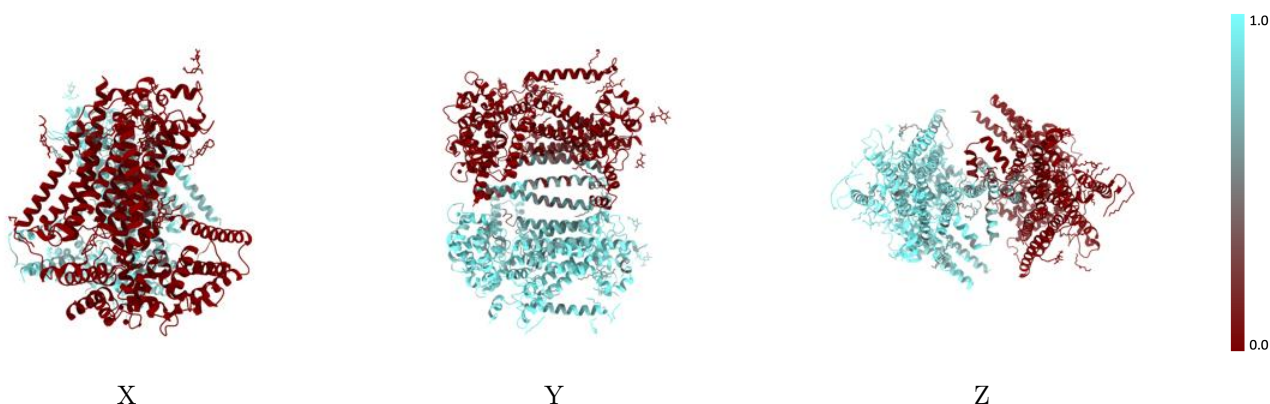
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



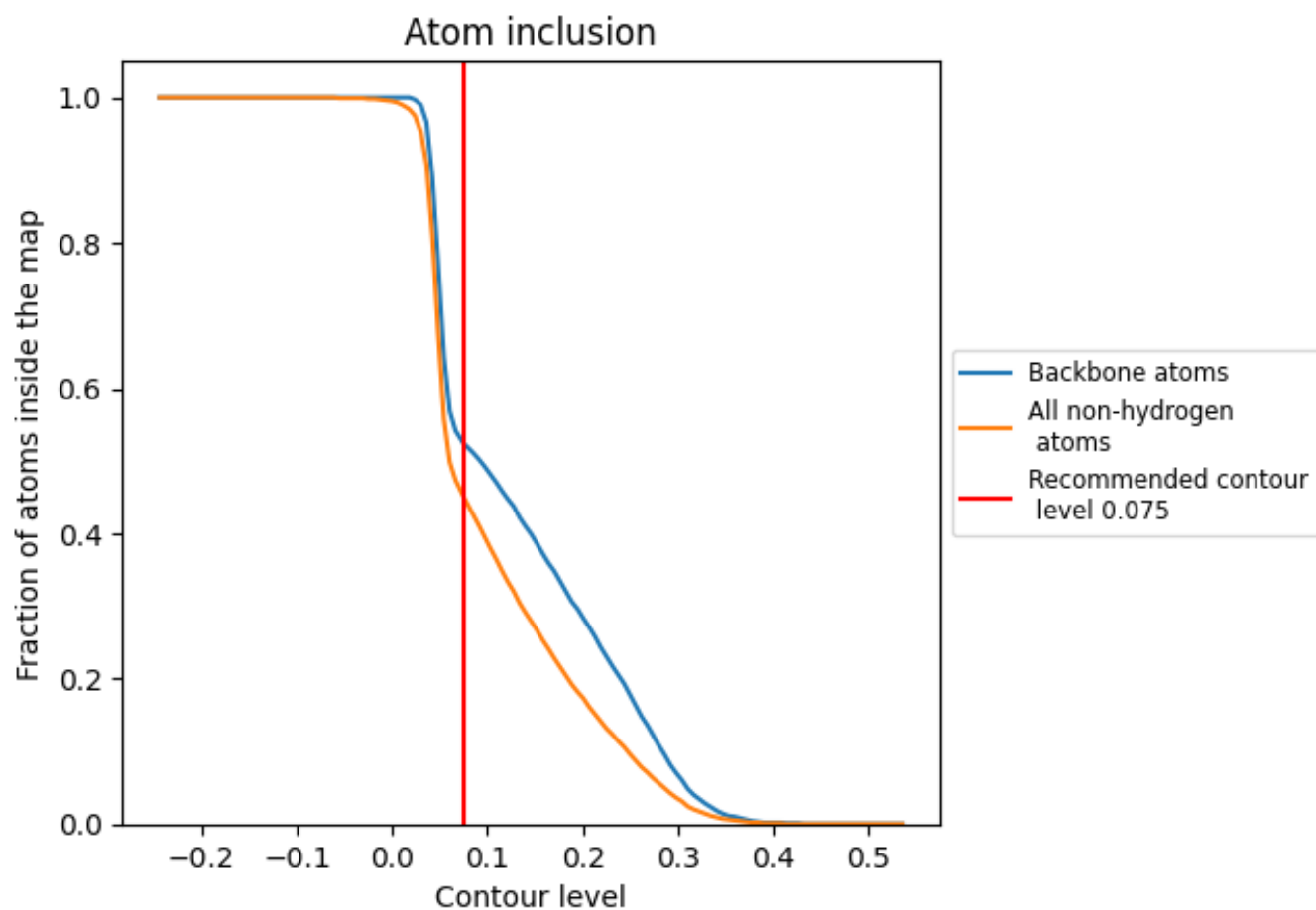
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 45% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4510	 0.2580
A	 0.0620	 0.0800
B	 0.0000	 0.0130
C	 0.0000	 0.0370
D	 0.8360	 0.4430
E	 0.9320	 0.4900
F	 0.8570	 0.4400
G	 0.0000	 0.0150
H	 0.8210	 0.3460

