



## Full wwPDB EM Validation Report ⓘ

Dec 2, 2025 – 10:14 AM JST

PDB ID : 9LAI / pdb\_00009lai  
EMDB ID : EMD-62929  
Title : Cryo-EM structure of nanodisc (PE:PS:PC) reconstituted GLIC at pH 4 in  
iiii conformation  
Authors : Li, Z.; Bharambe, N.; Basak, S.  
Deposited on : 2025-01-02  
Resolution : 3.08 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](mailto: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>.

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

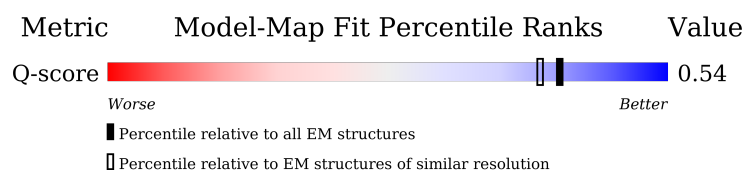
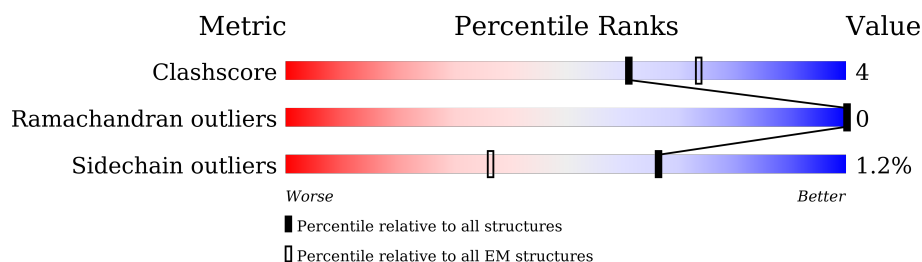
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.46

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.08 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14000 ( 2.58 - 3.58 )

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  $\geq 3$ , 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	312	<div> <div>6%</div> <div>85%</div> <div>14%</div> </div>
1	B	312	<div> <div>8%</div> <div>87%</div> <div>13%</div> </div>
1	C	312	<div> <div>9%</div> <div>87%</div> <div>13%</div> </div>
1	D	312	<div> <div>5%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	312	<div><div></div><div>90%</div><div>9% .</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13400 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.

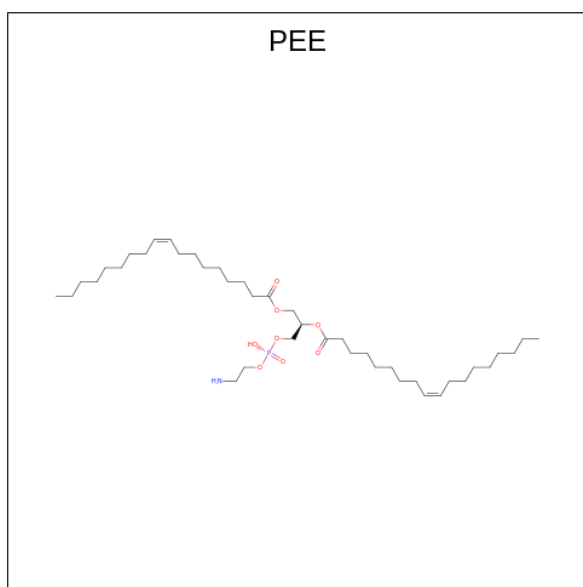
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	312	Total	C	N	O	S	0	0
			2529	1666	405	454	4		
1	B	312	Total	C	N	O	S	0	0
			2529	1666	405	454	4		
1	C	312	Total	C	N	O	S	0	0
			2529	1666	405	454	4		
1	E	312	Total	C	N	O	S	0	0
			2529	1666	405	454	4		
1	D	312	Total	C	N	O	S	1	0
			2540	1672	409	455	4		

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Cl	0
			1	1	
2	B	1	Total	Cl	0
			1	1	
2	C	1	Total	Cl	0
			1	1	
2	E	1	Total	Cl	0
			1	1	
2	D	1	Total	Cl	0
			1	1	

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			24	15	8	1	
3	A	1	Total	C	N	O	P
			39	29	1	8	1
3	A	1	Total	C			0
			15	15			
3	A	1	Total	C	N	O	P
			28	18	1	8	1
3	A	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C	O	P	0
			35	26	8	1	
3	B	1	Total	C	O	P	0
			28	19	8	1	
3	B	1	Total	C	O	P	0
			33	24	8	1	
3	B	1	Total	C			0
			15	15			
3	B	1	Total	C	N	O	P
			28	18	1	8	1
3	B	1	Total	C	N	O	P
			37	27	1	8	1
3	C	1	Total	C	O	P	0
			40	31	8	1	
3	C	1	Total	C	O	P	0
			24	15	8	1	
3	C	1	Total	C	O	P	0
			33	24	8	1	

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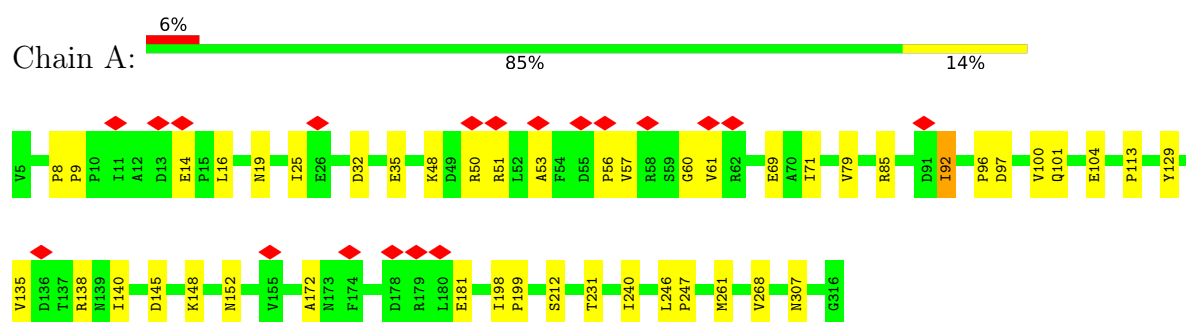
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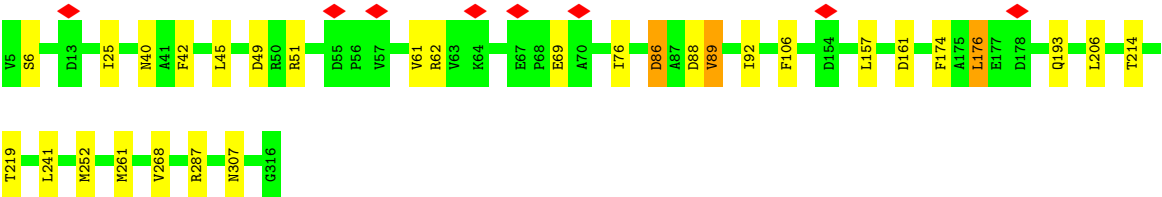
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C			0
			15	15			
3	E	1	Total	C	O	P	0
			27	18	8	1	
3	E	1	Total	C	O	P	0
			39	30	8	1	
3	E	1	Total	C	O	P	0
			41	32	8	1	
3	E	1	Total	C			0
			18	18			
3	E	1	Total	C	O	P	0
			28	19	8	1	
3	E	1	Total	C	O	P	0
			39	30	8	1	
3	D	1	Total	C	O	P	0
			36	27	8	1	
3	D	1	Total	C	N	O	P
			42	32	1	8	1
3	D	1	Total	C	O	P	0
			35	26	8	1	

### 3 Residue-property plots [i](#)

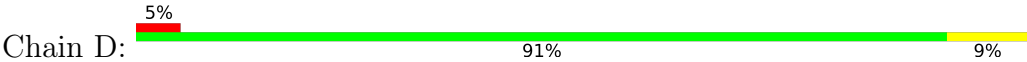
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Proton-gated ion channel





● Molecule 1: Proton-gated ion channel





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	71	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0023	Depositor
Map size (Å)	228.0, 228.0, 228.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	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: CL, PEE

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	0.14	0/2597	0.29	0/3550
1	B	0.13	0/2597	0.28	0/3550
1	C	0.14	0/2597	0.30	0/3550
1	D	0.13	0/2608	0.29	0/3564
1	E	0.14	0/2597	0.28	0/3550
All	All	0.14	0/12996	0.29	0/17764

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 [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	2529	0	2548	27	0
1	B	2529	0	2548	23	0
1	C	2529	0	2548	20	0
1	D	2540	0	2560	19	0
1	E	2529	0	2548	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	146	0	185	2	0
3	B	176	0	221	4	0
3	C	112	0	142	2	0
3	D	113	0	146	3	0
3	E	192	0	251	6	0
All	All	13400	0	13697	113	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 4.

All (113) 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:48:LYS:HE3	1:A:50:ARG:HB2	1.62	0.81
1:B:212:SER:HB2	1:B:231:THR:HG21	1.68	0.74
1:C:212:SER:HB2	1:C:231:THR:HG21	1.73	0.71
1:A:71:ILE:HD11	1:A:92:ILE:HD11	1.73	0.69
1:B:26:GLU:HB2	1:B:40:ASN:HB3	1.74	0.69
1:A:212:SER:HB3	1:A:231:THR:HG21	1.75	0.69
1:B:10:PRO:HA	1:B:138:ARG:HH11	1.60	0.66
1:B:19:ASN:HB2	1:B:46:SER:HB2	1.76	0.66
1:C:76:ILE:O	1:C:85:ARG:NH1	2.28	0.66
1:D:201:ILE:HD12	1:D:242:VAL:HG22	1.78	0.64
1:D:246:LEU:HD12	1:D:247:PRO:HD2	1.80	0.64
1:C:19:ASN:HB3	1:C:145:ASP:HB2	1.78	0.64
1:B:7:PRO:HG2	1:B:135:VAL:HG21	1.80	0.62
1:A:19:ASN:HB3	1:A:145:ASP:HB2	1.81	0.62
1:E:268:VAL:HG21	3:E:404:PEE:H43	1.81	0.61
1:B:198:ILE:HB	1:B:199:PRO:HD3	1.82	0.61
1:C:101:GLN:OE1	1:D:179:ARG:NH2	2.34	0.60
1:A:198:ILE:HB	1:A:199:PRO:HD3	1.82	0.60
1:B:163:GLU:OE2	1:B:189:ARG:NH1	2.34	0.60
1:C:198:ILE:HB	1:C:199:PRO:HD3	1.83	0.59
1:A:14:GLU:O	1:A:138:ARG:NE	2.34	0.59
1:B:25:ILE:HG22	1:B:26:GLU:HG2	1.85	0.58
1:D:6:SER:OG	1:D:51:ARG:NH1	2.36	0.58
1:A:85:ARG:NH1	1:A:104:GLU:OE2	2.37	0.57
1:A:101:GLN:OE1	1:A:148:LYS:NZ	2.37	0.57
1:E:49:ASP:OD2	1:E:51:ARG:NH2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:PEE:H58	3:A:403:PEE:H19	1.87	0.56
1:C:26:GLU:HB2	1:C:40:ASN:HB3	1.87	0.56
1:B:255:THR:O	1:B:259:ILE:HG12	2.06	0.55
1:E:206:LEU:HD21	3:E:403:PEE:H35	1.89	0.55
1:D:307:ASN:HD21	3:D:403:PEE:H32	1.72	0.54
1:C:25:ILE:HG22	1:C:26:GLU:HG2	1.88	0.54
1:D:26:GLU:HA	1:D:155:VAL:HG12	1.89	0.54
1:E:161:ASP:OD1	1:E:193:GLN:NE2	2.41	0.54
1:B:117:ARG:O	1:B:118:ARG:HG2	2.07	0.54
1:C:45:LEU:HD13	1:C:74:PRO:HG2	1.90	0.54
1:B:76:ILE:O	1:B:85:ARG:NH2	2.36	0.54
1:A:135:VAL:HG22	1:A:140:ILE:HD11	1.90	0.53
1:A:57:VAL:HG13	1:A:60:GLY:H	1.72	0.53
1:D:16:LEU:N	1:D:139:ASN:O	2.37	0.53
1:A:240:ILE:HG12	1:E:241:LEU:HD13	1.90	0.52
1:C:255:THR:O	1:C:259:ILE:HG12	2.10	0.52
1:D:139:ASN:HD21	1:D:180:LEU:HD23	1.75	0.52
1:A:172:ALA:HB3	1:A:181:GLU:HA	1.91	0.52
1:A:261:MET:HE1	1:A:307:ASN:OD1	2.11	0.51
1:B:66:TYR:HD2	1:B:70:ALA:HB1	1.76	0.50
1:C:126:LEU:HD12	1:C:188:LEU:HD23	1.94	0.50
1:D:88:ASP:N	1:D:88:ASP:OD1	2.43	0.50
1:C:284:GLN:OE1	1:C:287:ARG:NH1	2.45	0.49
1:C:36:THR:HG22	1:C:111:LEU:HD23	1.94	0.49
1:A:268:VAL:HG21	3:A:404:PEE:H47	1.95	0.49
1:B:19:ASN:HB3	1:B:145:ASP:HB2	1.92	0.49
1:E:69:GLU:OE1	1:E:69:GLU:N	2.46	0.49
1:E:287:ARG:NH2	3:E:404:PEE:O5	2.36	0.48
1:E:89:VAL:HG11	1:E:92:ILE:HD11	1.95	0.48
1:B:57:VAL:HG22	1:B:59:SER:H	1.79	0.47
1:A:181:GLU:OE1	1:A:181:GLU:N	2.41	0.47
3:D:403:PEE:H48	3:D:403:PEE:H19	1.95	0.47
3:B:404:PEE:H21	3:B:404:PEE:H55	1.96	0.47
3:C:404:PEE:H21	3:C:404:PEE:H59	1.97	0.46
1:D:261:MET:HE1	1:D:307:ASN:OD1	2.16	0.46
1:A:25:ILE:HD13	1:A:152:ASN:HB2	1.98	0.46
1:E:40:ASN:N	1:E:40:ASN:OD1	2.48	0.46
1:D:45:LEU:HB2	1:D:102:TYR:HB3	1.98	0.46
1:D:178:ASP:OD1	1:D:178:ASP:N	2.47	0.45
1:E:174:PHE:HE1	1:E:176:LEU:HD12	1.82	0.45
1:A:69:GLU:H	1:A:69:GLU:CD	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HB	1:A:129:TYR:HB2	1.99	0.44
1:B:261:MET:HE1	1:B:307:ASN:OD1	2.17	0.44
1:C:261:MET:HE1	1:C:307:ASN:OD1	2.18	0.44
1:D:75:GLU:H	1:D:75:GLU:CD	2.25	0.44
1:C:51:ARG:HA	1:C:51:ARG:HD2	1.82	0.44
1:E:6:SER:O	1:E:51:ARG:NH1	2.43	0.44
1:D:307:ASN:ND2	3:D:403:PEE:H32	2.31	0.44
1:A:53:ALA:HB1	1:A:97:ASP:HA	2.00	0.43
1:B:205:MET:HE3	1:B:238:PHE:HD2	1.83	0.43
1:D:48:LYS:HA	1:D:99:THR:HA	2.00	0.43
1:A:32:ASP:HB2	1:A:247:PRO:HG3	2.01	0.43
1:B:289:ALA:HA	1:B:292:THR:HG22	2.00	0.43
1:C:57:VAL:HG22	1:C:59:SER:H	1.82	0.43
1:B:147:GLU:N	1:B:147:GLU:OE1	2.52	0.43
1:D:55:ASP:OD1	1:D:55:ASP:N	2.49	0.43
1:A:97:ASP:N	1:A:97:ASP:OD1	2.51	0.43
1:C:76:ILE:HG21	1:C:130:LEU:HD23	2.01	0.42
3:E:403:PEE:H34	3:E:403:PEE:H28	1.75	0.42
1:A:56:PRO:HB3	1:A:97:ASP:HB3	2.01	0.42
1:B:62:ARG:H	1:B:62:ARG:HG3	1.53	0.42
1:B:83:ASN:N	1:B:83:ASN:OD1	2.53	0.42
1:A:51:ARG:HA	1:A:51:ARG:NH1	2.35	0.42
1:E:86:ASP:O	1:E:106:PHE:HA	2.20	0.42
1:E:88:ASP:OD1	1:E:88:ASP:N	2.52	0.42
1:D:86:ASP:OD2	1:D:86:ASP:N	2.39	0.42
1:A:16:LEU:HB2	1:A:138:ARG:NH2	2.35	0.42
1:A:8:PRO:HA	1:A:9:PRO:HD3	1.89	0.41
1:E:261:MET:HG3	3:E:405:PEE:H37	2.02	0.41
1:B:16:LEU:HB2	1:B:138:ARG:NH2	2.34	0.41
1:B:278:TYR:CD2	3:B:401:PEE:H8	2.54	0.41
3:B:407:PEE:H66	3:B:407:PEE:H61	1.95	0.41
3:E:405:PEE:H32	3:E:405:PEE:H38	1.76	0.41
1:D:14:GLU:HG2	1:D:15:PRO:O	2.20	0.41
1:D:91:ASP:OD1	1:D:92:ILE:N	2.53	0.41
1:B:252:MET:HG2	3:B:406:PEE:H10	2.03	0.41
1:E:45:LEU:HD21	1:E:76:ILE:HG13	2.03	0.41
1:A:61:VAL:HA	1:A:96:PRO:HG3	2.03	0.41
1:C:10:PRO:HB3	1:C:138:ARG:HG3	2.02	0.40
1:C:24:LEU:O	1:C:152:ASN:HB2	2.21	0.40
1:C:61:VAL:HA	1:C:96:PRO:HG3	2.04	0.40
1:C:205:MET:HE2	1:C:238:PHE:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:MET:HE1	1:E:307:ASN:OD1	2.19	0.40
1:A:35:GLU:CD	1:A:113:PRO:HA	2.46	0.40
1:E:61:VAL:O	1:E:62:ARG:NH1	2.48	0.40
3:C:404:PEE:H49	3:C:404:PEE:H54	1.95	0.40
1:E:25:ILE:HD11	1:E:42:PHE:CE2	2.57	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	310/312 (99%)	291 (94%)	19 (6%)	0	100	100
1	B	310/312 (99%)	299 (96%)	11 (4%)	0	100	100
1	C	310/312 (99%)	294 (95%)	16 (5%)	0	100	100
1	D	311/312 (100%)	299 (96%)	12 (4%)	0	100	100
1	E	310/312 (99%)	295 (95%)	15 (5%)	0	100	100
All	All	1551/1560 (99%)	1478 (95%)	73 (5%)	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	280/280 (100%)	277 (99%)	3 (1%)	70	83
1	B	280/280 (100%)	278 (99%)	2 (1%)	81	89
1	C	280/280 (100%)	276 (99%)	4 (1%)	62	79
1	D	281/280 (100%)	280 (100%)	1 (0%)	89	93
1	E	280/280 (100%)	273 (98%)	7 (2%)	42	66
All	All	1401/1400 (100%)	1384 (99%)	17 (1%)	66	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ILE
1	A	100	VAL
1	A	246	LEU
1	B	35	GLU
1	B	149	VAL
1	C	154	ASP
1	C	155	VAL
1	C	176	LEU
1	C	219	THR
1	E	86	ASP
1	E	89	VAL
1	E	157	LEU
1	E	176	LEU
1	E	214	THR
1	E	219	THR
1	E	252	MET
1	D	212	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	B	235	HIS
1	B	284	GLN
1	E	235	HIS
1	D	40	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 5 are monoatomic - leaving 24 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	$\# Z  > 2$
3	PEE	A	403	-	38,38,50	1.00	2 (5%)	41,43,55	0.66	0
3	PEE	B	407	-	36,36,50	0.83	1 (2%)	39,41,55	0.62	0
3	PEE	C	404	-	32,32,50	1.10	3 (9%)	36,37,55	1.27	3 (8%)
3	PEE	E	405	-	17,17,50	0.91	1 (5%)	16,16,55	0.56	0
3	PEE	A	404	-	14,14,50	1.00	1 (7%)	13,13,55	0.63	0
3	PEE	B	401	-	34,34,50	1.08	3 (8%)	37,39,55	1.19	3 (8%)
3	PEE	E	407	-	38,38,50	1.05	3 (7%)	42,43,55	1.13	2 (4%)
3	PEE	E	402	-	26,26,50	0.77	1 (3%)	30,31,55	1.18	2 (6%)
3	PEE	E	406	-	27,27,50	0.76	1 (3%)	31,32,55	1.20	2 (6%)
3	PEE	E	404	-	40,40,50	0.99	3 (7%)	44,45,55	1.08	3 (6%)
3	PEE	C	401	-	39,39,50	1.04	3 (7%)	43,44,55	1.10	2 (4%)
3	PEE	A	405	-	27,27,50	0.64	0	30,32,55	0.53	0
3	PEE	B	405	-	14,14,50	1.00	1 (7%)	13,13,55	0.63	0
3	PEE	B	404	-	32,32,50	1.10	3 (9%)	36,37,55	1.24	3 (8%)
3	PEE	D	403	-	41,41,50	0.96	2 (4%)	44,46,55	0.65	0
3	PEE	D	401	-	35,35,50	1.06	3 (8%)	39,40,55	1.13	3 (7%)
3	PEE	D	404	-	34,34,50	0.94	2 (5%)	38,39,55	1.14	2 (5%)
3	PEE	E	403	-	38,38,50	1.06	3 (7%)	41,43,55	1.10	3 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEE	B	403	-	27,27,50	0.77	1 (3%)	31,32,55	1.18	2 (6%)
3	PEE	B	406	-	27,27,50	0.64	0	30,32,55	0.55	0
3	PEE	A	402	-	23,23,50	0.83	1 (4%)	27,28,55	1.26	2 (7%)
3	PEE	C	405	-	14,14,50	1.00	1 (7%)	13,13,55	0.62	0
3	PEE	A	406	-	39,39,50	1.05	3 (7%)	43,44,55	1.09	2 (4%)
3	PEE	C	403	-	23,23,50	0.83	1 (4%)	27,28,55	1.25	2 (7%)

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
3	PEE	A	403	-	-	22/42/42/54	-
3	PEE	B	407	-	-	15/40/40/54	-
3	PEE	C	404	-	-	15/34/34/54	-
3	PEE	E	405	-	-	8/15/15/54	-
3	PEE	A	404	-	-	4/12/12/54	-
3	PEE	B	401	-	-	14/36/36/54	-
3	PEE	E	407	-	-	20/40/40/54	-
3	PEE	E	402	-	-	13/28/28/54	-
3	PEE	E	406	-	-	9/29/29/54	-
3	PEE	E	404	-	-	13/42/42/54	-
3	PEE	C	401	-	-	14/41/41/54	-
3	PEE	A	405	-	-	12/31/31/54	-
3	PEE	B	405	-	-	2/12/12/54	-
3	PEE	B	404	-	-	12/34/34/54	-
3	PEE	D	403	-	-	15/45/45/54	-
3	PEE	D	401	-	-	15/37/37/54	-
3	PEE	D	404	-	-	17/36/36/54	-
3	PEE	E	403	-	-	14/40/40/54	-
3	PEE	B	403	-	-	11/29/29/54	-
3	PEE	B	406	-	-	13/31/31/54	-
3	PEE	A	402	-	-	11/25/25/54	-
3	PEE	C	405	-	-	5/12/12/54	-
3	PEE	A	406	-	-	20/41/41/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEE	C	403	-	-	7/25/25/54	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	PEE	C18-C19	3.63	1.52	1.31
3	C	405	PEE	C18-C19	3.63	1.52	1.31
3	A	404	PEE	C18-C19	3.62	1.52	1.31
3	B	405	PEE	C18-C19	3.61	1.52	1.31
3	E	403	PEE	C39-C38	3.61	1.52	1.31
3	E	405	PEE	C18-C19	3.61	1.52	1.31
3	B	407	PEE	C39-C38	3.61	1.52	1.31
3	D	403	PEE	C39-C38	3.61	1.52	1.31
3	A	403	PEE	C39-C38	3.61	1.52	1.31
3	B	401	PEE	C18-C19	3.61	1.52	1.31
3	E	407	PEE	C18-C19	3.60	1.52	1.31
3	A	406	PEE	C39-C38	3.60	1.52	1.31
3	E	403	PEE	C18-C19	3.60	1.52	1.31
3	D	401	PEE	C18-C19	3.59	1.52	1.31
3	C	401	PEE	C39-C38	3.59	1.52	1.31
3	D	403	PEE	C18-C19	3.59	1.52	1.31
3	C	401	PEE	C18-C19	3.58	1.52	1.31
3	A	406	PEE	C18-C19	3.58	1.52	1.31
3	E	407	PEE	C39-C38	3.58	1.52	1.31
3	B	404	PEE	C19-C18	3.58	1.52	1.28
3	C	404	PEE	C19-C18	3.58	1.52	1.28
3	E	404	PEE	C18-C19	3.57	1.52	1.31
3	A	403	PEE	C19-C18	3.57	1.52	1.28
3	C	404	PEE	C38-C39	3.10	1.52	1.29
3	B	404	PEE	C38-C39	3.08	1.52	1.29
3	B	401	PEE	C38-C39	3.08	1.52	1.29
3	D	401	PEE	C38-C39	3.08	1.52	1.29
3	E	404	PEE	C38-C39	3.07	1.52	1.29
3	E	404	PEE	P-O4P	2.84	1.65	1.54
3	C	403	PEE	P-O4P	2.83	1.65	1.54
3	D	401	PEE	P-O4P	2.83	1.65	1.54
3	D	404	PEE	P-O4P	2.83	1.65	1.54
3	B	403	PEE	P-O4P	2.82	1.65	1.54
3	E	407	PEE	P-O4P	2.82	1.65	1.54
3	B	404	PEE	P-O4P	2.82	1.65	1.54
3	A	406	PEE	P-O4P	2.82	1.65	1.54
3	B	401	PEE	P-O4P	2.81	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	403	PEE	P-O4P	2.81	1.65	1.54
3	C	404	PEE	P-O4P	2.81	1.65	1.54
3	C	401	PEE	P-O4P	2.81	1.65	1.54
3	E	402	PEE	P-O4P	2.81	1.65	1.54
3	A	402	PEE	P-O4P	2.80	1.65	1.54
3	E	406	PEE	P-O4P	2.80	1.65	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	404	PEE	O4P-P-O3P	-5.34	92.53	106.73
3	D	404	PEE	O4P-P-O3P	-5.27	92.71	106.73
3	E	403	PEE	O4P-P-O3P	-5.26	92.75	106.73
3	B	403	PEE	O4P-P-O3P	-5.24	92.80	106.73
3	E	406	PEE	O4P-P-O3P	-5.22	92.84	106.73
3	A	402	PEE	O4P-P-O3P	-5.20	92.89	106.73
3	E	402	PEE	O4P-P-O3P	-5.19	92.91	106.73
3	B	401	PEE	O4P-P-O3P	-5.17	92.98	106.73
3	C	403	PEE	O4P-P-O3P	-5.17	92.98	106.73
3	A	406	PEE	O4P-P-O3P	-5.16	92.99	106.73
3	B	404	PEE	O4P-P-O3P	-5.16	93.00	106.73
3	C	401	PEE	O4P-P-O3P	-5.15	93.02	106.73
3	E	407	PEE	O4P-P-O3P	-5.15	93.02	106.73
3	E	404	PEE	O4P-P-O3P	-4.85	93.83	106.73
3	D	401	PEE	O4P-P-O3P	-4.75	94.09	106.73
3	A	406	PEE	O2P-P-O1P	2.30	119.69	110.68
3	E	407	PEE	O2P-P-O1P	2.29	119.65	110.68
3	C	401	PEE	O2P-P-O1P	2.28	119.61	110.68
3	E	406	PEE	O2P-P-O1P	2.28	119.59	110.68
3	C	403	PEE	O2P-P-O1P	2.27	119.56	110.68
3	A	402	PEE	O2P-P-O1P	2.26	119.51	110.68
3	B	403	PEE	O2P-P-O1P	2.25	119.51	110.68
3	C	404	PEE	O2P-P-O1P	2.25	119.50	110.68
3	E	403	PEE	O2P-P-O1P	2.23	119.43	110.68
3	B	404	PEE	O2P-P-O1P	2.23	119.40	110.68
3	D	404	PEE	O2P-P-O1P	2.23	119.39	110.68
3	E	402	PEE	O2P-P-O1P	2.21	119.34	110.68
3	D	401	PEE	O2P-P-O1P	2.21	119.32	110.68
3	B	401	PEE	O2P-P-O1P	2.21	119.32	110.68
3	E	404	PEE	O2P-P-O1P	2.17	119.18	110.68
3	B	401	PEE	C37-C38-C39	-2.16	113.86	131.07
3	C	404	PEE	C37-C38-C39	-2.15	113.99	131.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	404	PEE	C37-C38-C39	-2.14	114.07	131.07
3	D	401	PEE	C37-C38-C39	-2.11	114.33	131.07
3	B	404	PEE	C37-C38-C39	-2.10	114.40	131.07
3	E	403	PEE	O3P-P-O1P	2.01	112.12	106.47

There are no chirality outliers.

All (301) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PEE	O3P-C1-C2-O2
3	A	402	PEE	O2-C2-C3-O3
3	A	402	PEE	C1-O3P-P-O4P
3	A	403	PEE	C1-O3P-P-O2P
3	A	403	PEE	C1-O3P-P-O1P
3	A	403	PEE	C1-O3P-P-O4P
3	A	403	PEE	C4-O4P-P-O1P
3	A	405	PEE	C4-O4P-P-O3P
3	A	405	PEE	C4-O4P-P-O1P
3	A	406	PEE	C1-O3P-P-O4P
3	B	401	PEE	C1-O3P-P-O2P
3	B	401	PEE	C1-O3P-P-O4P
3	B	403	PEE	C11-C10-O2-C2
3	B	403	PEE	C1-O3P-P-O2P
3	B	403	PEE	C1-O3P-P-O4P
3	B	404	PEE	C1-O3P-P-O4P
3	B	406	PEE	C4-O4P-P-O1P
3	B	407	PEE	C1-O3P-P-O2P
3	B	407	PEE	C1-O3P-P-O1P
3	C	401	PEE	C17-C18-C19-C20
3	C	401	PEE	O4-C10-O2-C2
3	C	403	PEE	C1-O3P-P-O2P
3	C	403	PEE	C1-O3P-P-O4P
3	C	404	PEE	C11-C10-O2-C2
3	C	404	PEE	C1-O3P-P-O2P
3	C	404	PEE	C1-O3P-P-O4P
3	E	402	PEE	C11-C10-O2-C2
3	E	402	PEE	C1-O3P-P-O4P
3	E	403	PEE	O2-C2-C3-O3
3	E	404	PEE	C1-O3P-P-O2P
3	E	404	PEE	C1-O3P-P-O4P
3	E	404	PEE	C37-C38-C39-C40
3	E	407	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	E	407	PEE	C1-O3P-P-O1P
3	E	407	PEE	C1-O3P-P-O4P
3	D	401	PEE	O3P-C1-C2-O2
3	D	401	PEE	C1-O3P-P-O2P
3	D	401	PEE	C1-O3P-P-O1P
3	D	401	PEE	C1-O3P-P-O4P
3	D	403	PEE	C4-O4P-P-O1P
3	D	404	PEE	C1-O3P-P-O2P
3	D	404	PEE	C1-O3P-P-O4P
3	A	402	PEE	O5-C30-O3-C3
3	D	404	PEE	O5-C30-O3-C3
3	B	403	PEE	O4-C10-O2-C2
3	E	402	PEE	O4-C10-O2-C2
3	D	404	PEE	C31-C30-O3-C3
3	C	401	PEE	C11-C10-O2-C2
3	A	402	PEE	C31-C30-O3-C3
3	A	404	PEE	C17-C18-C19-C20
3	A	406	PEE	C17-C18-C19-C20
3	A	406	PEE	C37-C38-C39-C40
3	C	401	PEE	C37-C38-C39-C40
3	C	405	PEE	C17-C18-C19-C20
3	E	403	PEE	C17-C18-C19-C20
3	E	404	PEE	C17-C18-C19-C20
3	C	404	PEE	O4-C10-O2-C2
3	A	403	PEE	C31-C30-O3-C3
3	A	403	PEE	O5-C30-O3-C3
3	D	403	PEE	O2-C2-C3-O3
3	B	404	PEE	C10-C11-C12-C13
3	C	401	PEE	C30-C31-C32-C33
3	E	405	PEE	C20-C21-C22-C23
3	B	404	PEE	C11-C10-O2-C2
3	A	403	PEE	C37-C38-C39-C40
3	B	405	PEE	C17-C18-C19-C20
3	A	403	PEE	C4-O4P-P-O3P
3	A	405	PEE	C1-O3P-P-O4P
3	B	406	PEE	C1-O3P-P-O4P
3	B	407	PEE	C1-O3P-P-O4P
3	B	407	PEE	C4-O4P-P-O3P
3	D	403	PEE	C4-O4P-P-O3P
3	B	404	PEE	O4-C10-O2-C2
3	B	407	PEE	C30-C31-C32-C33
3	E	407	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
3	C	401	PEE	C11-C12-C13-C14
3	E	404	PEE	C13-C14-C15-C16
3	C	404	PEE	C3-C2-O2-C10
3	C	405	PEE	C14-C15-C16-C17
3	B	407	PEE	C37-C38-C39-C40
3	B	406	PEE	O2-C2-C3-O3
3	A	403	PEE	C31-C32-C33-C34
3	E	407	PEE	C31-C32-C33-C34
3	D	404	PEE	C31-C32-C33-C34
3	A	404	PEE	C22-C23-C24-C25
3	B	401	PEE	C12-C13-C14-C15
3	E	407	PEE	C34-C35-C36-C37
3	D	403	PEE	C34-C35-C36-C37
3	E	407	PEE	O4-C10-O2-C2
3	E	406	PEE	C11-C10-O2-C2
3	D	404	PEE	C11-C10-O2-C2
3	E	405	PEE	C19-C20-C21-C22
3	E	405	PEE	C15-C16-C17-C18
3	E	405	PEE	C12-C13-C14-C15
3	A	406	PEE	C31-C32-C33-C34
3	E	402	PEE	C31-C32-C33-C34
3	E	406	PEE	C31-C32-C33-C34
3	D	403	PEE	C31-C32-C33-C34
3	E	402	PEE	C1-C2-C3-O3
3	E	406	PEE	O4-C10-O2-C2
3	E	404	PEE	C11-C12-C13-C14
3	D	401	PEE	C11-C10-O2-C2
3	A	406	PEE	C33-C34-C35-C36
3	D	401	PEE	O4-C10-O2-C2
3	E	403	PEE	C12-C13-C14-C15
3	B	403	PEE	C13-C14-C15-C16
3	C	401	PEE	C14-C15-C16-C17
3	C	401	PEE	C15-C16-C17-C18
3	D	404	PEE	O4-C10-O2-C2
3	A	406	PEE	C10-C11-C12-C13
3	A	406	PEE	C12-C13-C14-C15
3	C	403	PEE	C11-C10-O2-C2
3	A	406	PEE	C14-C15-C16-C17
3	D	403	PEE	C13-C14-C15-C16
3	E	405	PEE	C18-C19-C20-C21
3	C	403	PEE	O4-C10-O2-C2
3	E	406	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	E	404	PEE	C32-C33-C34-C35
3	E	403	PEE	C10-C11-C12-C13
3	E	407	PEE	C37-C38-C39-C40
3	C	404	PEE	C34-C35-C36-C37
3	B	406	PEE	C4-O4P-P-O3P
3	E	407	PEE	O3P-C1-C2-C3
3	D	401	PEE	C13-C14-C15-C16
3	A	402	PEE	C1-C2-C3-O3
3	B	404	PEE	C1-C2-C3-O3
3	C	401	PEE	C1-C2-C3-O3
3	E	403	PEE	C1-C2-C3-O3
3	D	403	PEE	C1-C2-C3-O3
3	D	401	PEE	C10-C11-C12-C13
3	E	407	PEE	C11-C12-C13-C14
3	E	403	PEE	C18-C19-C20-C21
3	E	405	PEE	C16-C17-C18-C19
3	D	401	PEE	C18-C19-C20-C21
3	E	407	PEE	C35-C36-C37-C38
3	A	403	PEE	C32-C33-C34-C35
3	E	404	PEE	C31-C32-C33-C34
3	B	403	PEE	C31-C30-O3-C3
3	E	406	PEE	C3-C2-O2-C10
3	D	401	PEE	C30-C31-C32-C33
3	A	402	PEE	C1-O3P-P-O1P
3	A	406	PEE	C1-O3P-P-O1P
3	B	401	PEE	C1-O3P-P-O1P
3	B	403	PEE	C1-O3P-P-O1P
3	B	404	PEE	C1-O3P-P-O1P
3	E	402	PEE	C1-O3P-P-O1P
3	E	404	PEE	C1-O3P-P-O1P
3	E	407	PEE	C40-C41-C42-C43
3	C	404	PEE	O3P-C1-C2-O2
3	E	402	PEE	O3P-C1-C2-O2
3	E	403	PEE	C37-C38-C39-C40
3	E	407	PEE	C17-C18-C19-C20
3	A	405	PEE	C33-C34-C35-C36
3	B	407	PEE	C44-C45-C46-C47
3	B	406	PEE	C11-C10-O2-C2
3	A	406	PEE	C34-C35-C36-C37
3	E	407	PEE	C39-C40-C41-C42
3	A	402	PEE	O3P-C1-C2-C3
3	A	406	PEE	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	E	402	PEE	O3P-C1-C2-C3
3	D	401	PEE	O3P-C1-C2-C3
3	D	404	PEE	O3P-C1-C2-C3
3	B	401	PEE	C11-C12-C13-C14
3	D	403	PEE	C12-C13-C14-C15
3	A	405	PEE	C31-C30-O3-C3
3	D	404	PEE	C10-C11-C12-C13
3	B	403	PEE	O5-C30-O3-C3
3	D	404	PEE	C18-C19-C20-C21
3	A	406	PEE	C13-C14-C15-C16
3	A	403	PEE	C1-C2-C3-O3
3	C	404	PEE	C1-C2-C3-O3
3	D	401	PEE	C1-C2-C3-O3
3	D	404	PEE	C14-C15-C16-C17
3	B	406	PEE	C31-C32-C33-C34
3	E	407	PEE	C32-C33-C34-C35
3	C	401	PEE	C33-C34-C35-C36
3	B	401	PEE	C34-C35-C36-C37
3	A	406	PEE	O3P-C1-C2-O2
3	B	407	PEE	O3P-C1-C2-O2
3	E	404	PEE	C34-C35-C36-C37
3	C	403	PEE	C12-C13-C14-C15
3	E	402	PEE	C2-C1-O3P-P
3	D	404	PEE	C2-C1-O3P-P
3	C	405	PEE	C22-C23-C24-C25
3	E	405	PEE	C22-C23-C24-C25
3	B	401	PEE	C18-C19-C20-C21
3	E	403	PEE	C38-C39-C40-C41
3	E	407	PEE	C12-C13-C14-C15
3	A	405	PEE	O3P-C1-C2-C3
3	E	406	PEE	O3P-C1-C2-C3
3	B	401	PEE	C31-C32-C33-C34
3	C	403	PEE	C14-C15-C16-C17
3	A	402	PEE	C1-O3P-P-O2P
3	B	404	PEE	C34-C35-C36-C37
3	C	404	PEE	C33-C34-C35-C36
3	B	404	PEE	C3-C2-O2-C10
3	E	407	PEE	C3-C2-O2-C10
3	B	401	PEE	C1-C2-C3-O3
3	B	406	PEE	C1-C2-C3-O3
3	A	405	PEE	O5-C30-O3-C3
3	E	407	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	404	PEE	O3P-C1-C2-O2
3	B	406	PEE	O4-C10-O2-C2
3	A	403	PEE	O2-C2-C3-O3
3	B	401	PEE	O2-C2-C3-O3
3	C	404	PEE	O2-C2-C3-O3
3	E	402	PEE	O2-C2-C3-O3
3	D	404	PEE	O2-C2-C3-O3
3	A	402	PEE	C13-C14-C15-C16
3	D	404	PEE	C19-C20-C21-C22
3	A	403	PEE	C2-C1-O3P-P
3	E	406	PEE	C2-C1-O3P-P
3	A	403	PEE	C4-O4P-P-O2P
3	A	405	PEE	C1-O3P-P-O1P
3	B	406	PEE	C1-O3P-P-O1P
3	B	406	PEE	C4-O4P-P-O2P
3	B	407	PEE	C4-O4P-P-O1P
3	D	403	PEE	C4-O4P-P-O2P
3	B	407	PEE	O3P-C1-C2-C3
3	C	404	PEE	O3P-C1-C2-C3
3	E	403	PEE	O3P-C1-C2-C3
3	B	404	PEE	C16-C17-C18-C19
3	D	404	PEE	C30-C31-C32-C33
3	E	406	PEE	O3P-C1-C2-O2
3	B	403	PEE	C31-C32-C33-C34
3	D	404	PEE	C1-C2-C3-O3
3	D	401	PEE	O2-C2-C3-O3
3	A	406	PEE	C11-C12-C13-C14
3	B	406	PEE	C2-C1-O3P-P
3	C	405	PEE	C20-C21-C22-C23
3	E	403	PEE	C14-C15-C16-C17
3	B	401	PEE	C16-C17-C18-C19
3	B	407	PEE	C38-C39-C40-C41
3	D	403	PEE	C38-C39-C40-C41
3	E	402	PEE	C1-C2-O2-C10
3	E	402	PEE	C3-C2-O2-C10
3	A	403	PEE	C30-C31-C32-C33
3	D	403	PEE	C2-C1-O3P-P
3	A	405	PEE	O3P-C1-C2-O2
3	A	403	PEE	C36-C37-C38-C39
3	C	404	PEE	C36-C37-C38-C39
3	D	401	PEE	C16-C17-C18-C19
3	B	404	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
3	B	404	PEE	O5-C30-O3-C3
3	A	402	PEE	C2-C1-O3P-P
3	B	403	PEE	C2-C1-O3P-P
3	A	404	PEE	C16-C17-C18-C19
3	D	403	PEE	C18-C19-C20-C21
3	B	404	PEE	C33-C34-C35-C36
3	C	404	PEE	C32-C33-C34-C35
3	C	401	PEE	C16-C17-C18-C19
3	B	401	PEE	C36-C37-C38-C39
3	B	407	PEE	O2-C2-C3-O3
3	B	406	PEE	C33-C34-C35-C36
3	C	401	PEE	C12-C13-C14-C15
3	A	406	PEE	C16-C17-C18-C19
3	A	403	PEE	C12-C13-C14-C15
3	E	405	PEE	C13-C14-C15-C16
3	E	403	PEE	C31-C30-O3-C3
3	E	403	PEE	O5-C30-O3-C3
3	E	407	PEE	C18-C19-C20-C21
3	D	401	PEE	C36-C37-C38-C39
3	B	406	PEE	O3P-C1-C2-O2
3	C	401	PEE	C38-C39-C40-C41
3	B	401	PEE	O2-C10-C11-C12
3	A	403	PEE	C16-C17-C18-C19
3	A	406	PEE	C1-O3P-P-O2P
3	E	402	PEE	C1-O3P-P-O2P
3	E	404	PEE	C24-C25-C26-C27
3	A	404	PEE	C13-C14-C15-C16
3	A	406	PEE	C18-C19-C20-C21
3	D	403	PEE	C16-C17-C18-C19
3	D	403	PEE	C36-C37-C38-C39
3	A	403	PEE	O3-C30-C31-C32
3	E	407	PEE	C14-C15-C16-C17
3	C	401	PEE	C18-C19-C20-C21
3	B	407	PEE	C1-C2-C3-O3
3	B	403	PEE	C11-C12-C13-C14
3	C	403	PEE	O3P-C1-C2-O2
3	D	403	PEE	C14-C15-C16-C17
3	B	405	PEE	C18-C19-C20-C21
3	E	404	PEE	C16-C17-C18-C19
3	A	406	PEE	O2-C2-C3-O3
3	E	403	PEE	C35-C36-C37-C38
3	A	406	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	C	405	PEE	C16-C17-C18-C19
3	B	401	PEE	O4-C10-C11-C12
3	E	404	PEE	C18-C19-C20-C21
3	B	407	PEE	C31-C30-O3-C3
3	A	403	PEE	O5-C30-C31-C32
3	A	403	PEE	C11-C12-C13-C14
3	A	406	PEE	C1-C2-C3-O3
3	C	404	PEE	C2-C1-O3P-P
3	B	407	PEE	O5-C30-O3-C3
3	A	405	PEE	C5-C4-O4P-P
3	A	403	PEE	C13-C14-C15-C16
3	C	404	PEE	C37-C38-C39-C40
3	A	405	PEE	O5-C30-C31-C32
3	A	405	PEE	O3-C30-C31-C32
3	E	403	PEE	O3-C30-C31-C32
3	E	406	PEE	C35-C36-C37-C38

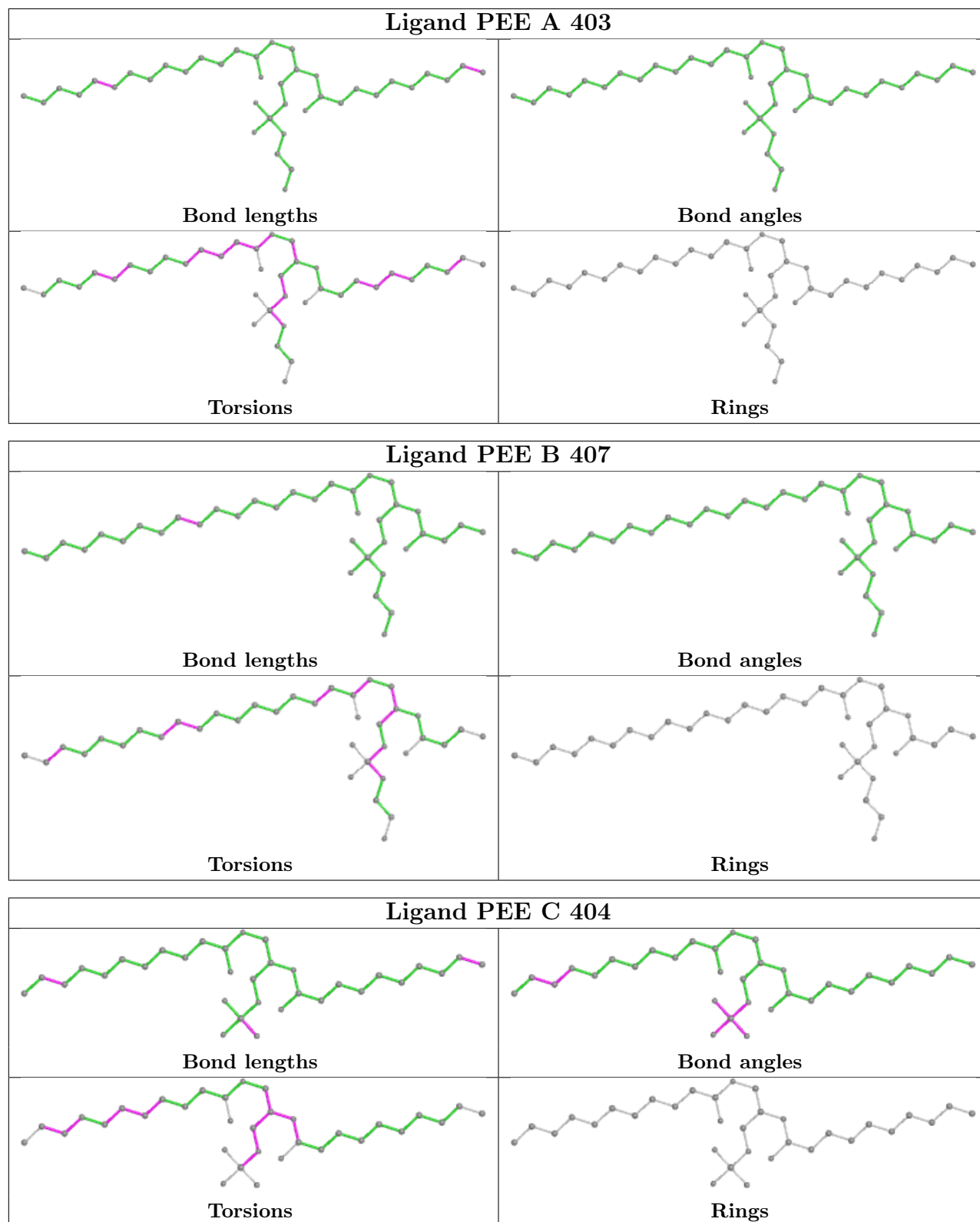
There are no ring outliers.

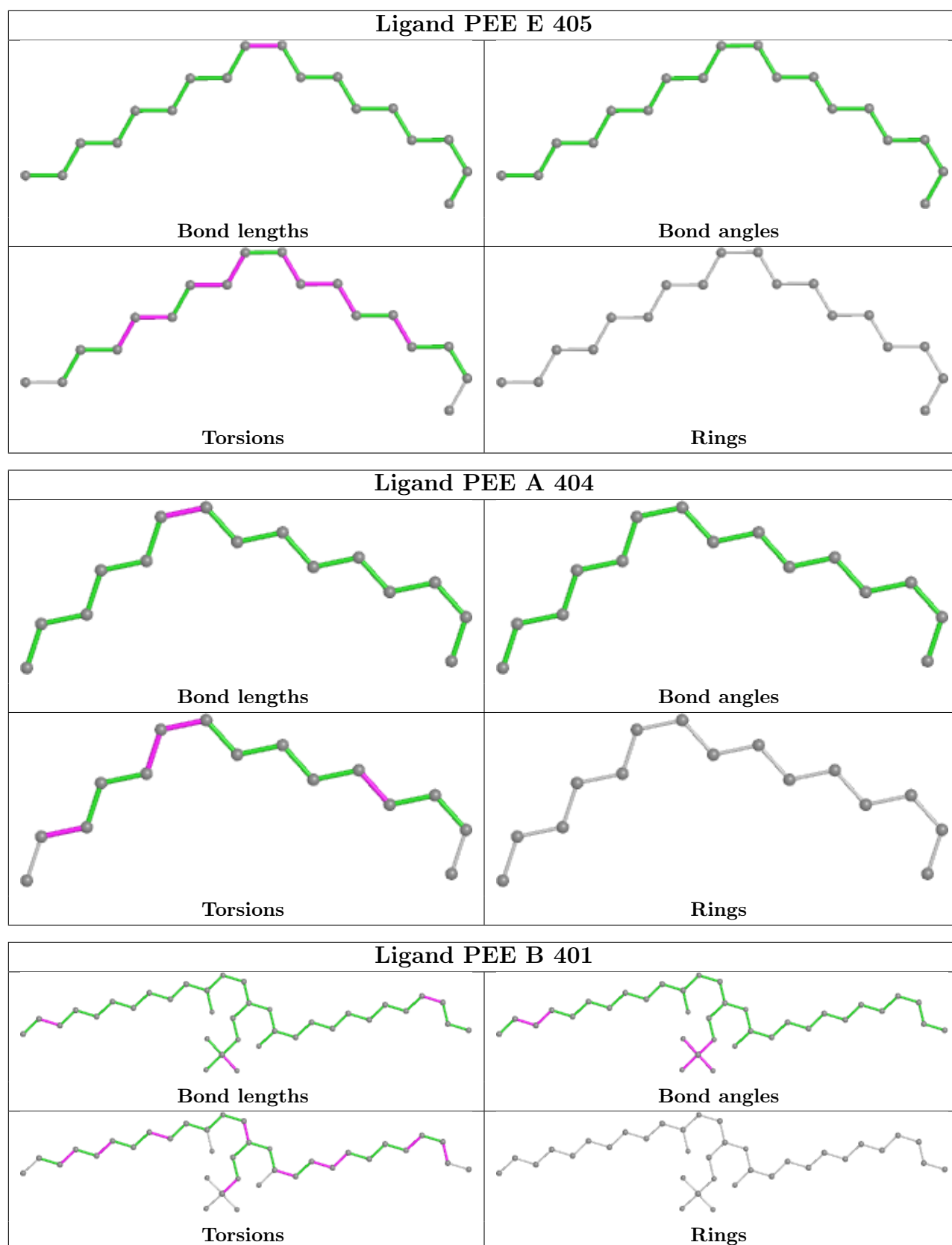
11 monomers are involved in 17 short contacts:

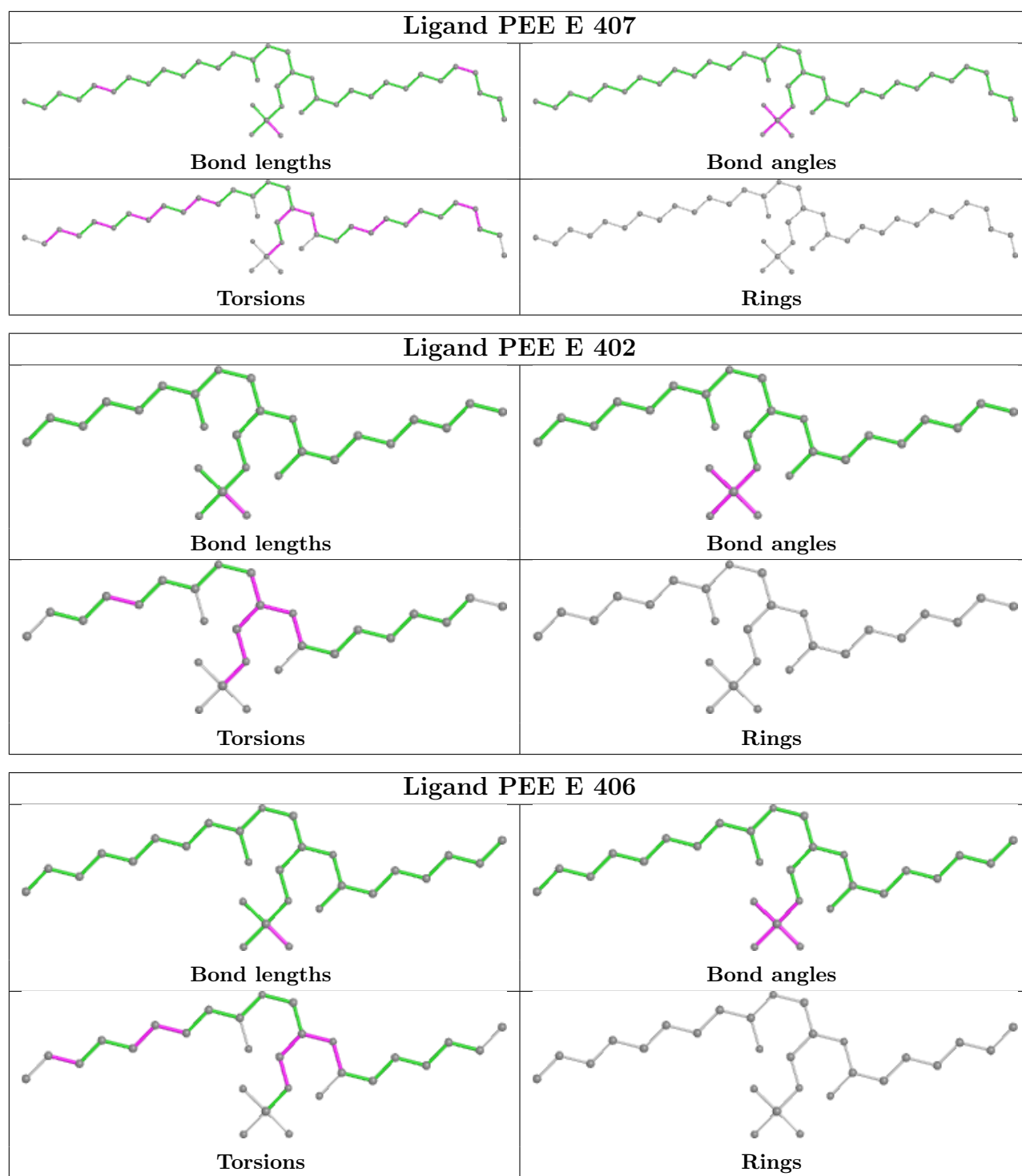
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	PEE	1	0
3	B	407	PEE	1	0
3	C	404	PEE	2	0
3	E	405	PEE	2	0
3	A	404	PEE	1	0
3	B	401	PEE	1	0
3	E	404	PEE	2	0
3	B	404	PEE	1	0
3	D	403	PEE	3	0
3	E	403	PEE	2	0
3	B	406	PEE	1	0

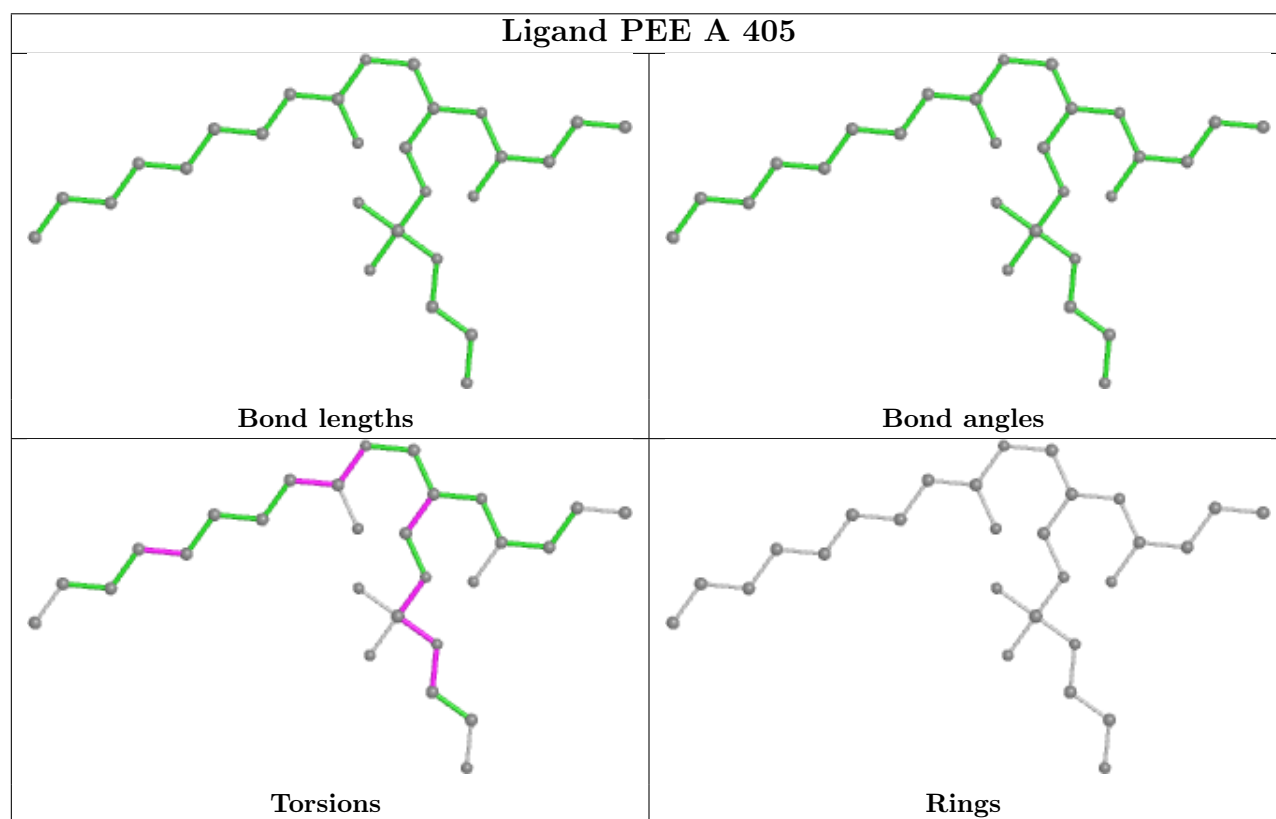
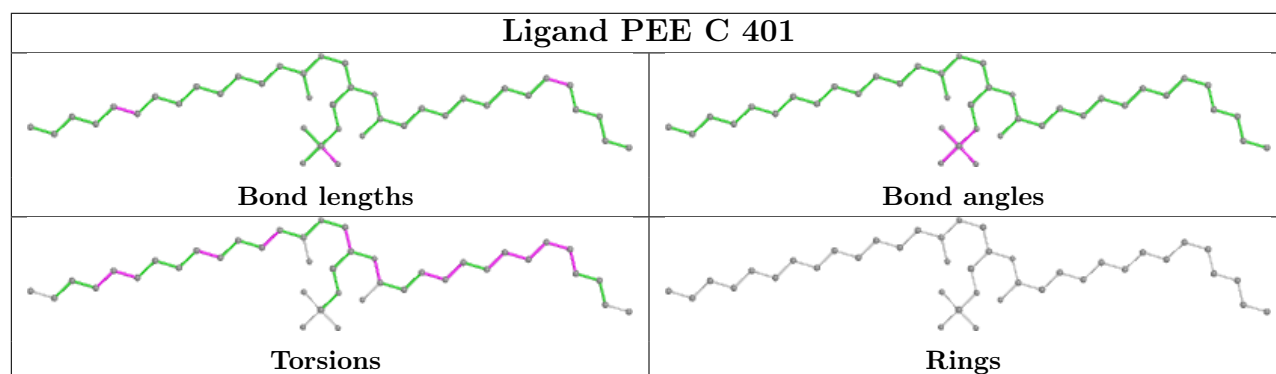
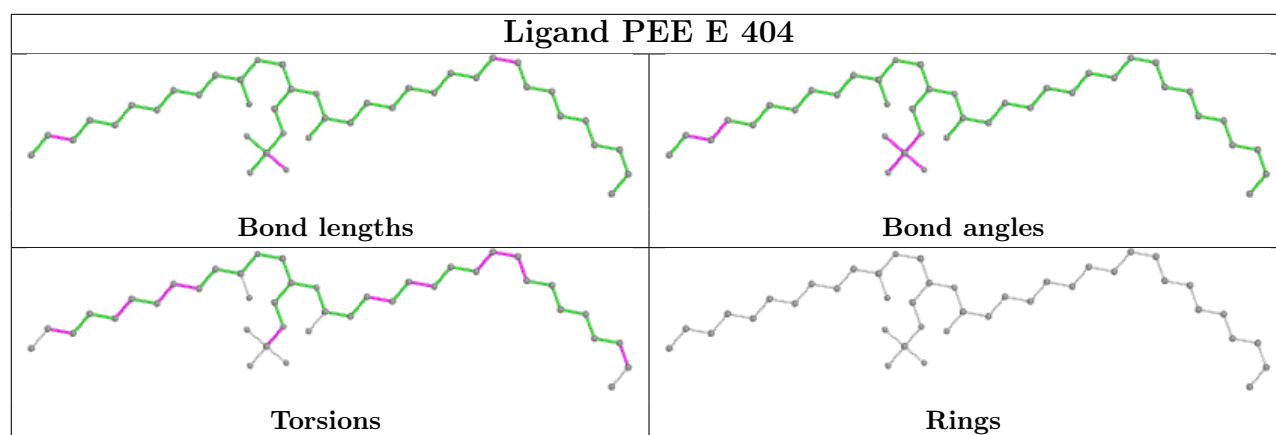
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

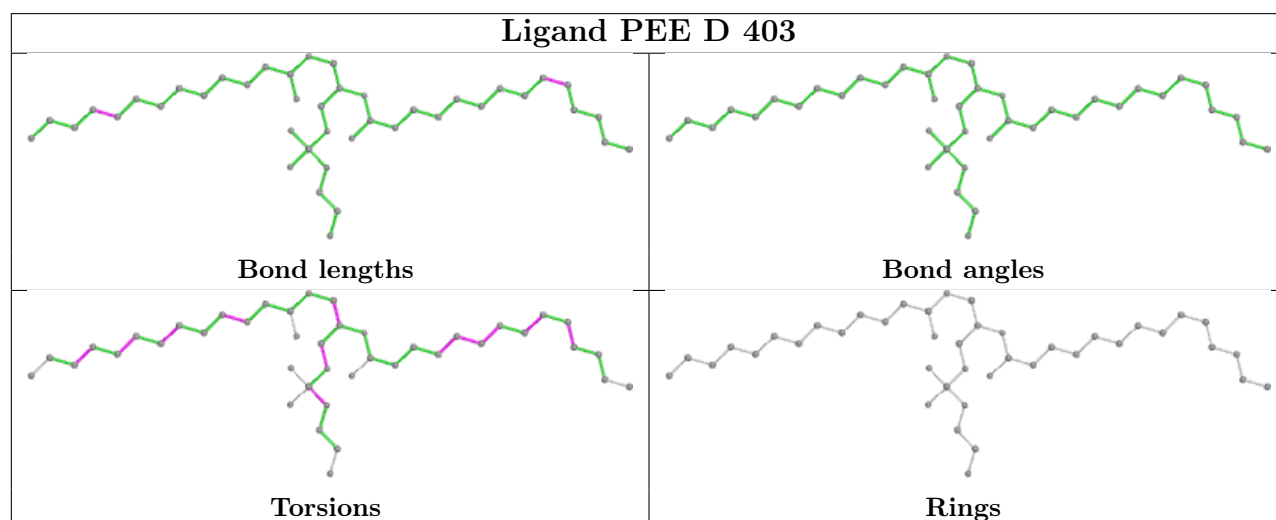
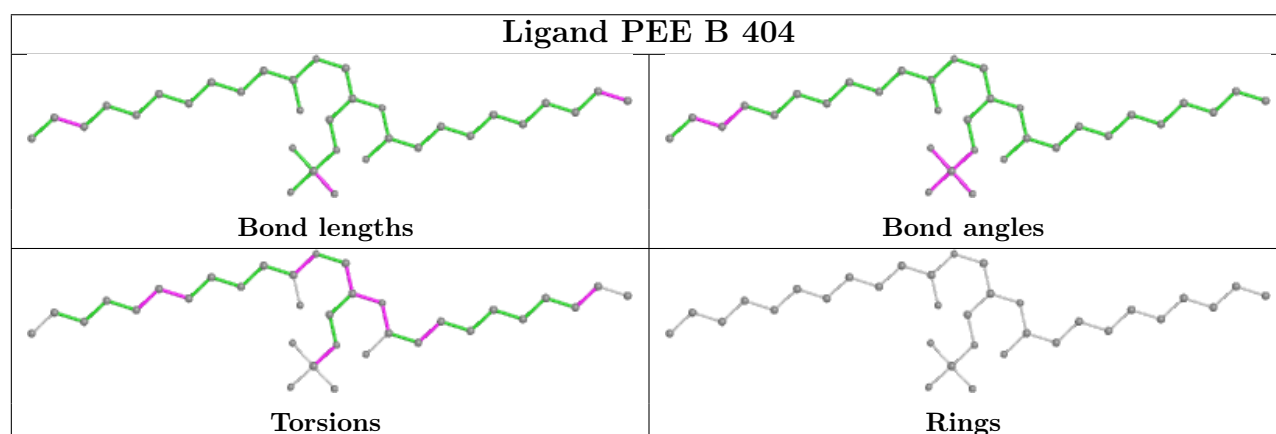
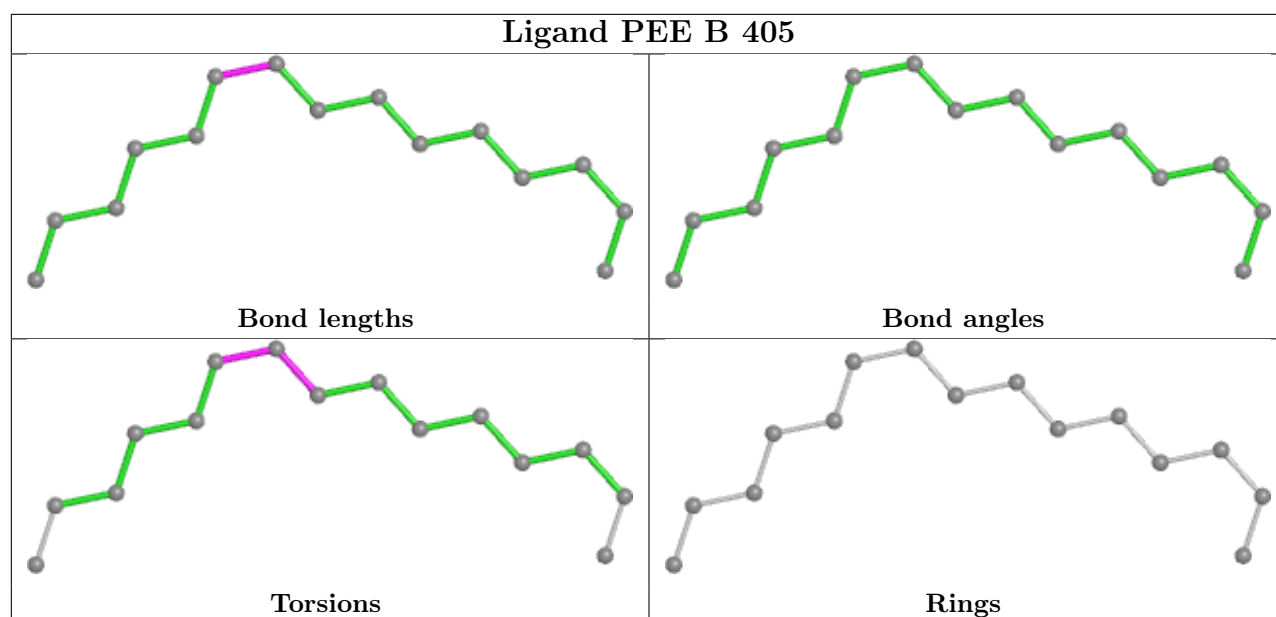
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



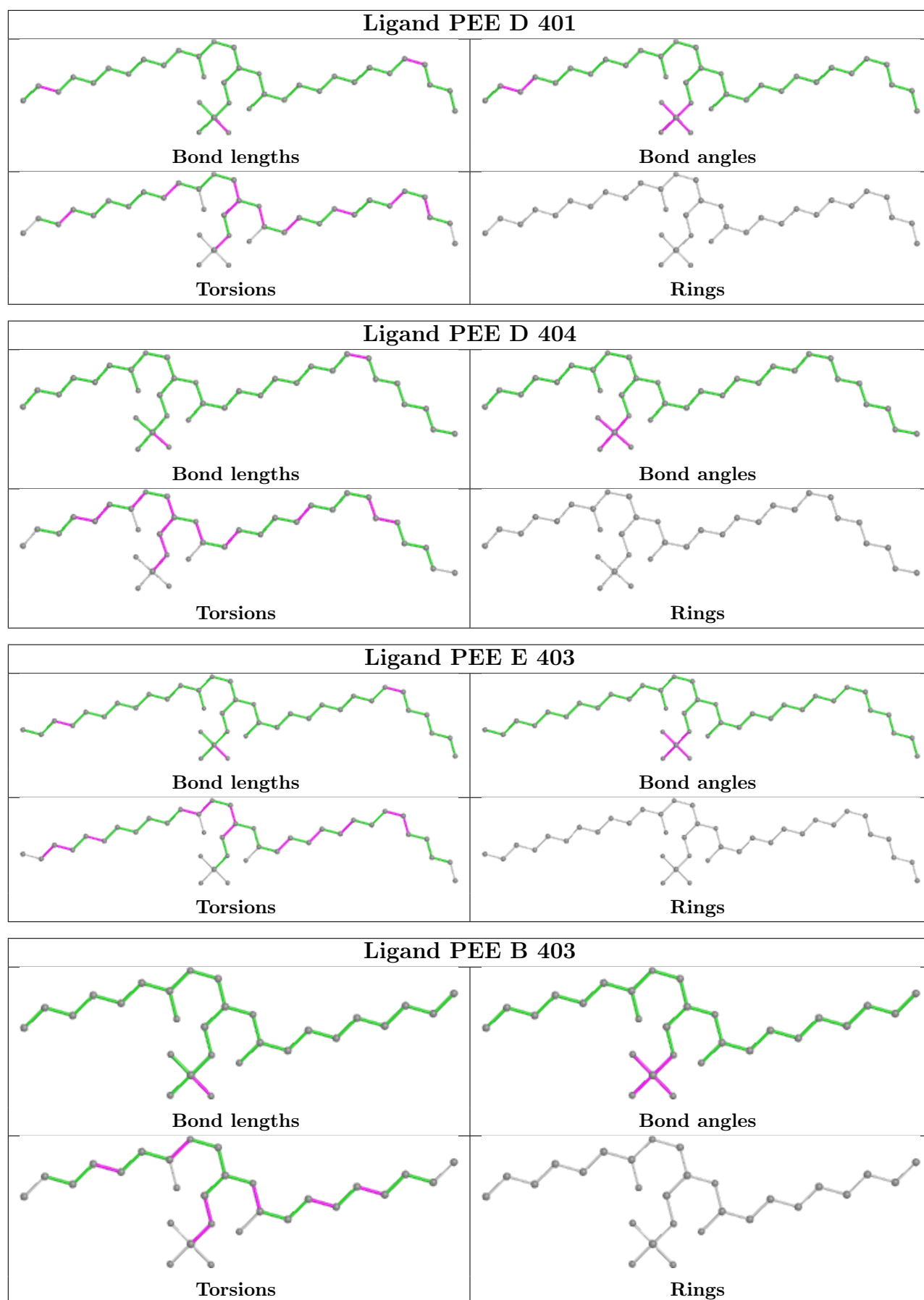


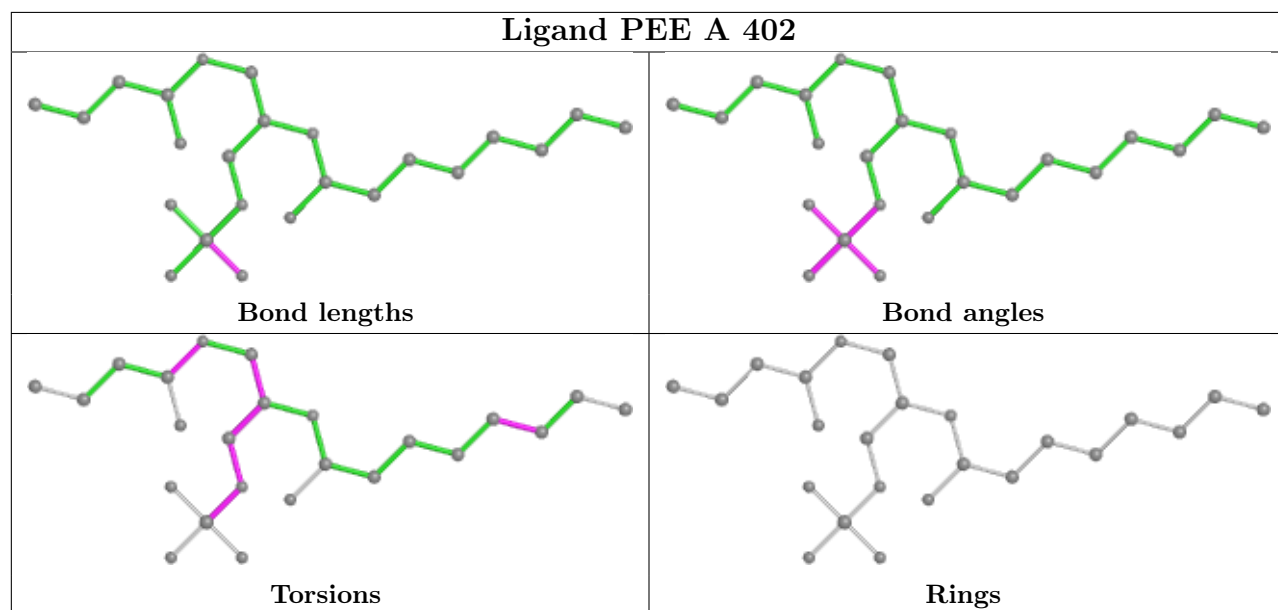
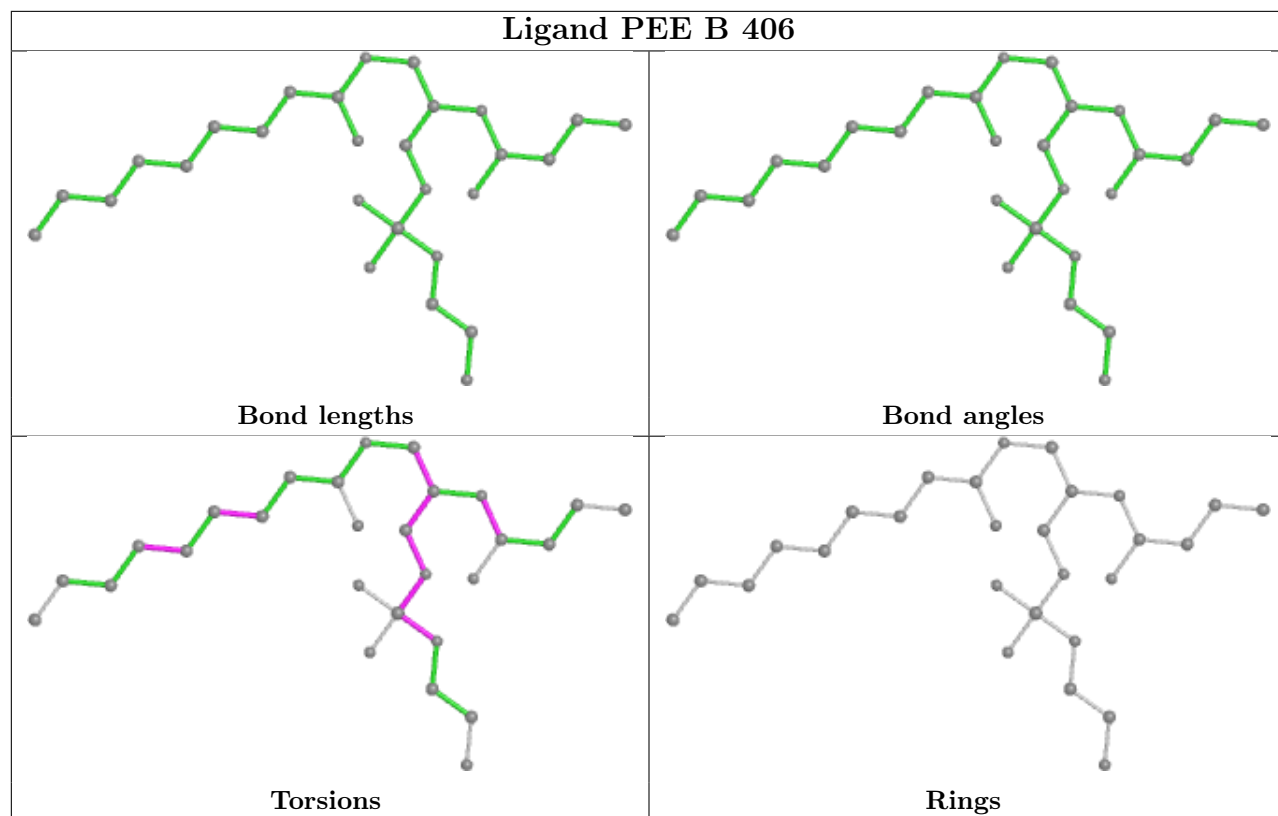


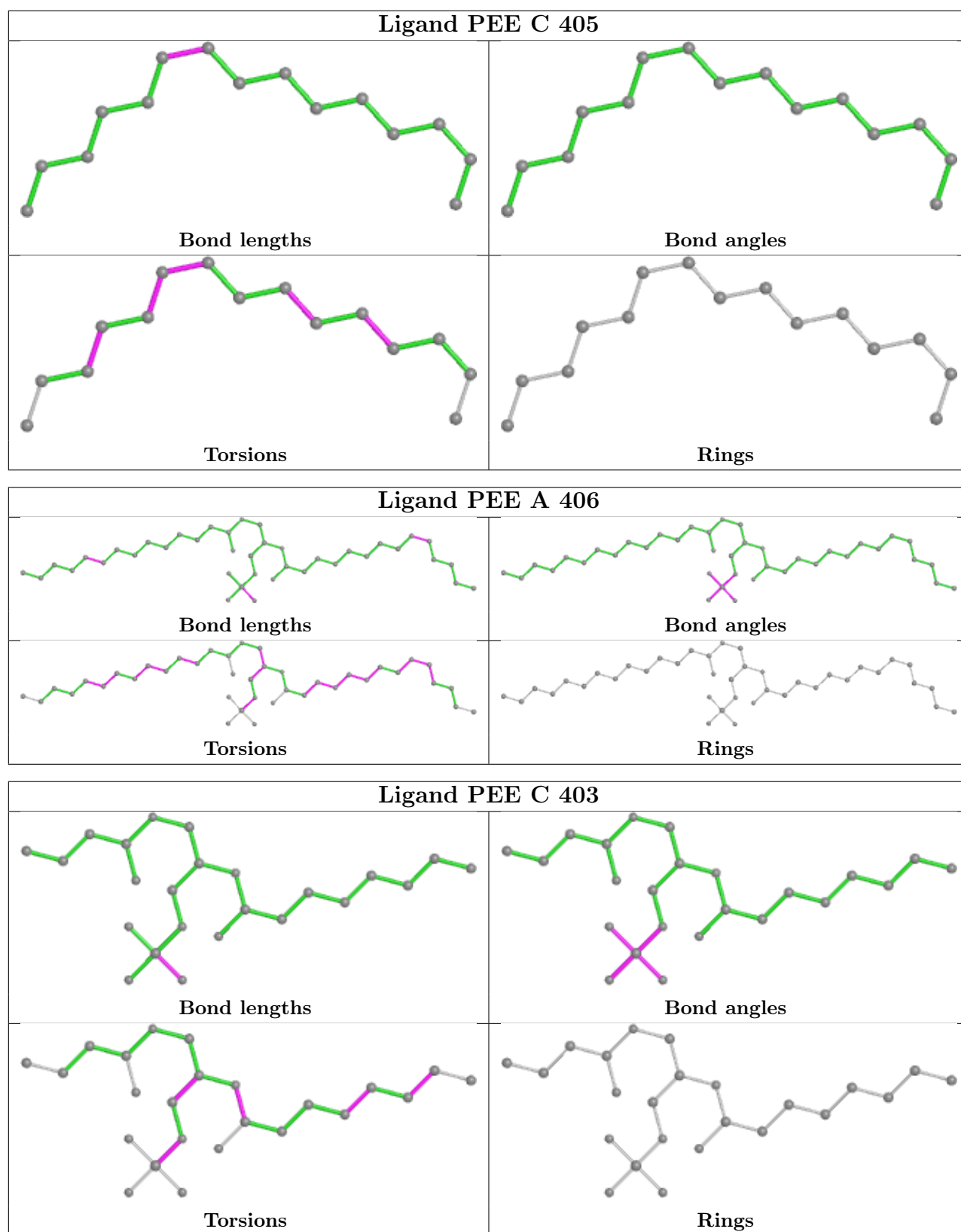












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

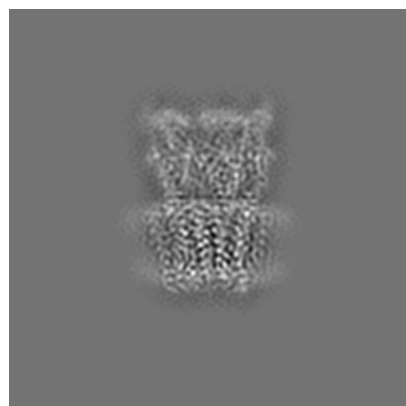
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62929. These allow visual inspection of the internal detail of the map and identification of artifacts.

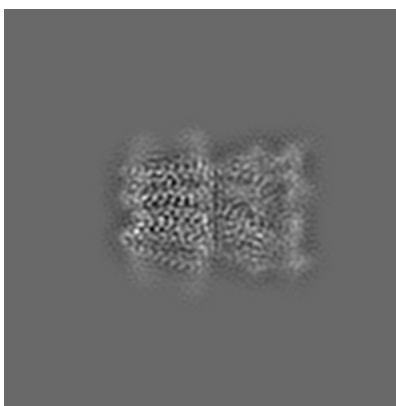
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

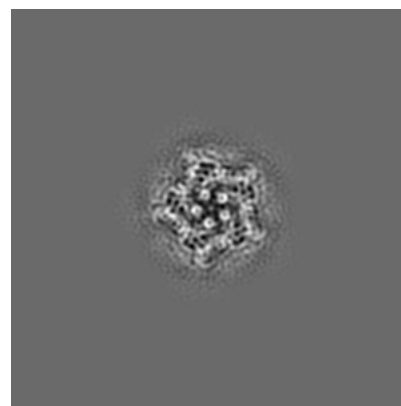
#### 6.1.1 Primary map



X

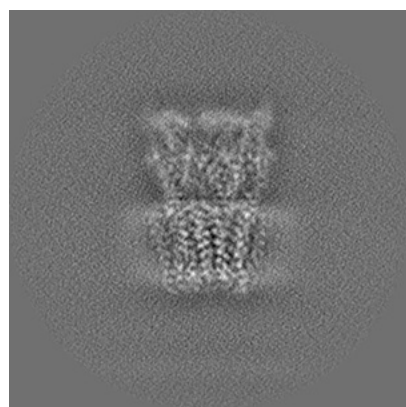


Y

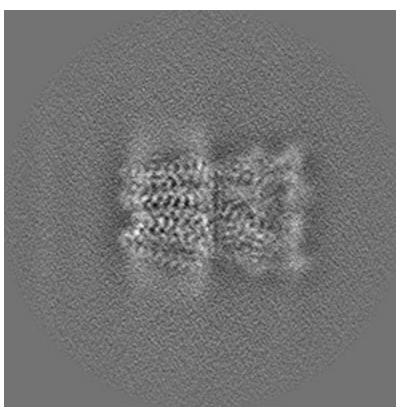


Z

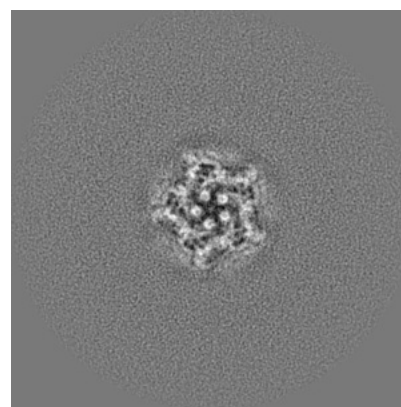
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

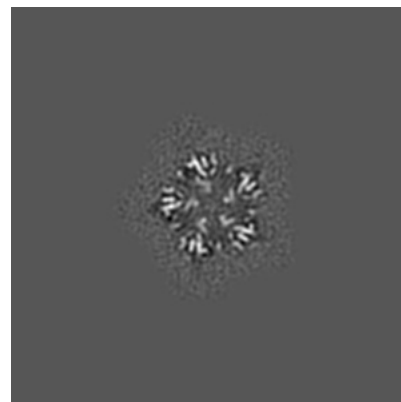
### 6.2.1 Primary map



X Index: 150

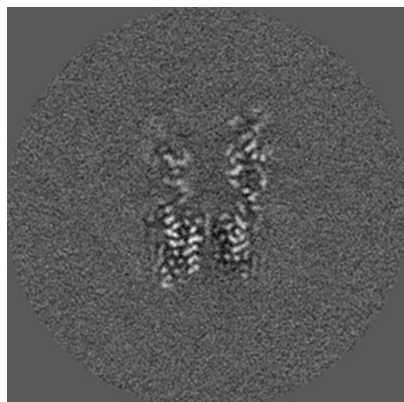


Y Index: 150

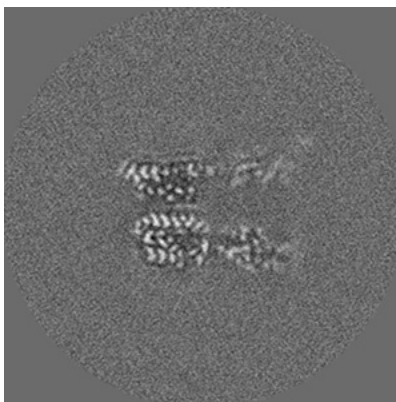


Z Index: 150

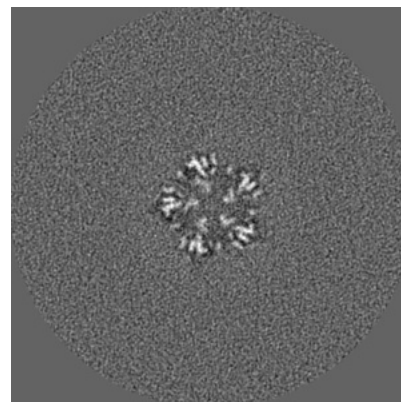
### 6.2.2 Raw map



X Index: 150



Y Index: 150

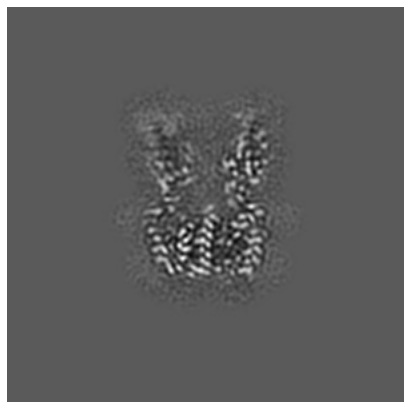


Z Index: 150

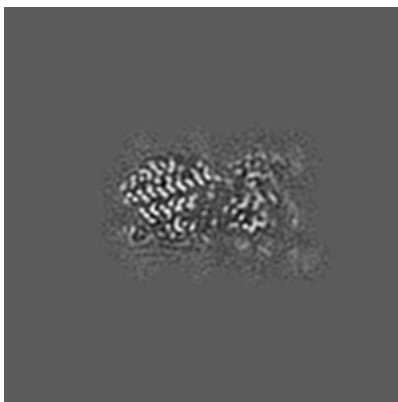
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 138

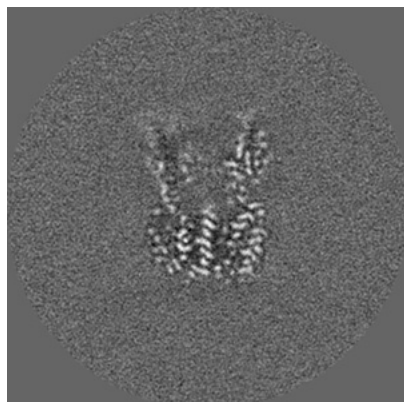


Y Index: 173

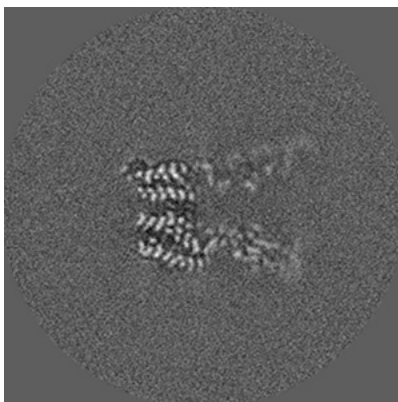


Z Index: 125

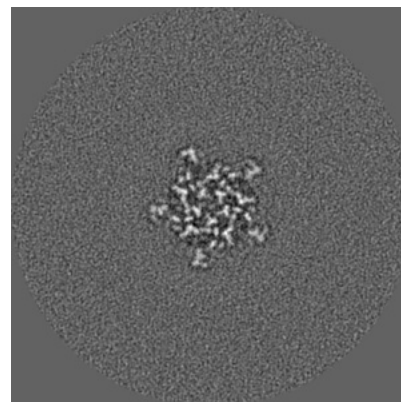
### 6.3.2 Raw map



X Index: 137



Y Index: 146

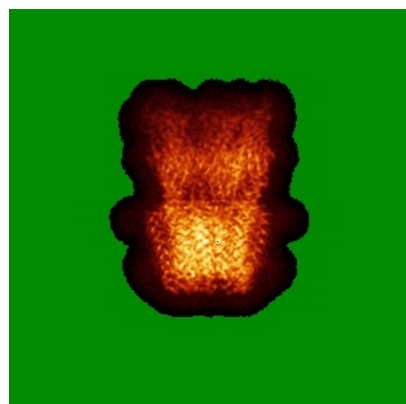


Z Index: 132

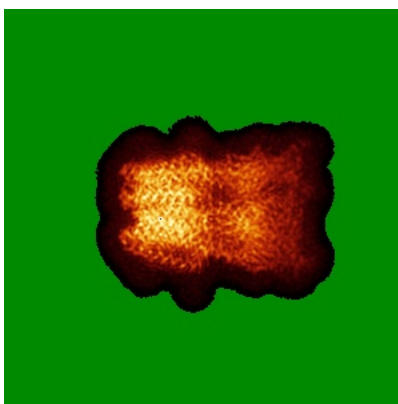
The images above show the largest variance slices of the map in three orthogonal directions.

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

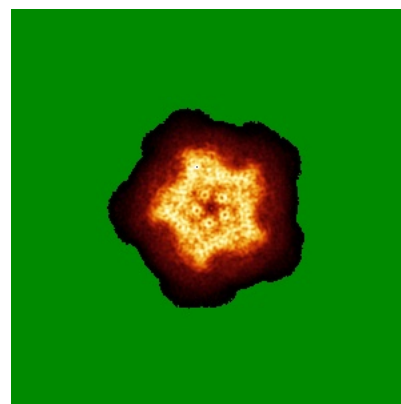
### 6.4.1 Primary map



X

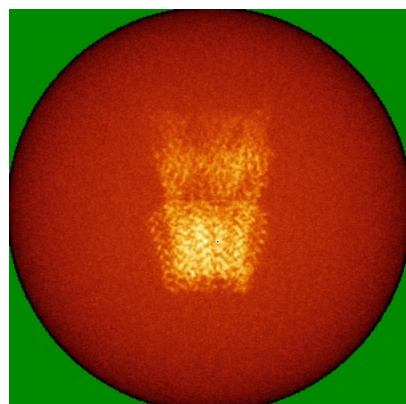


Y

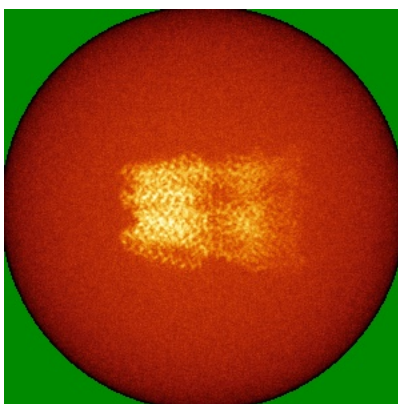


Z

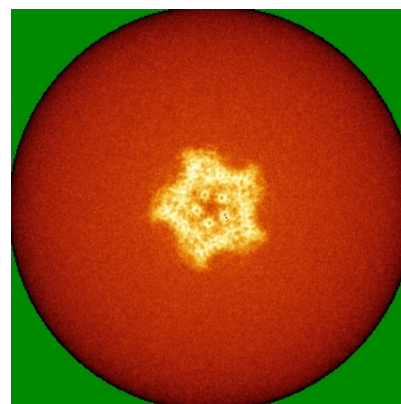
### 6.4.2 Raw map



X



Y



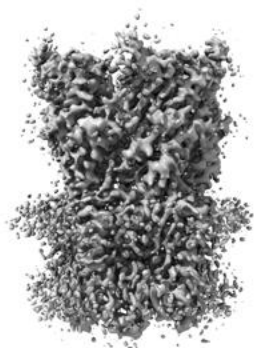
Z

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



## 6.5 Orthogonal surface views [i](#)

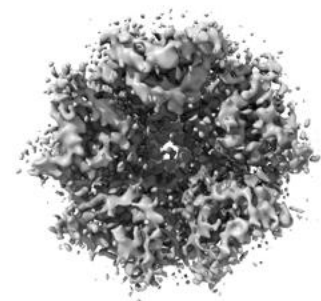
### 6.5.1 Primary map



X



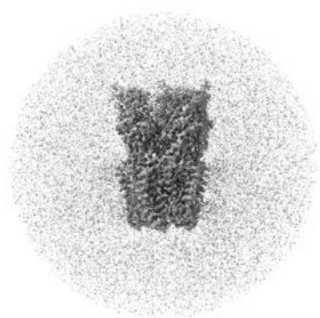
Y



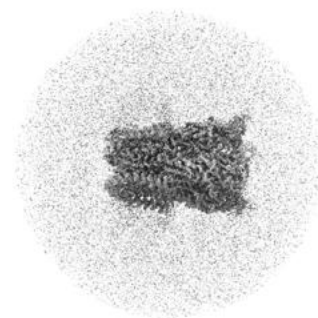
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

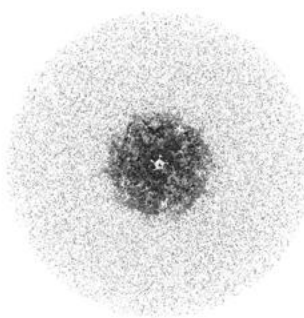
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

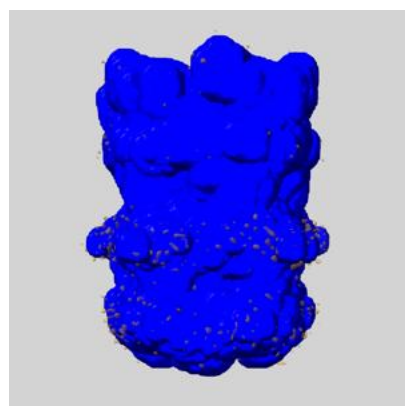
## 6.6 Mask visualisation [i](#)

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

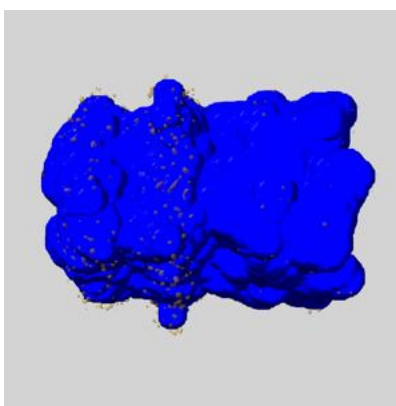
A mask typically either:

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

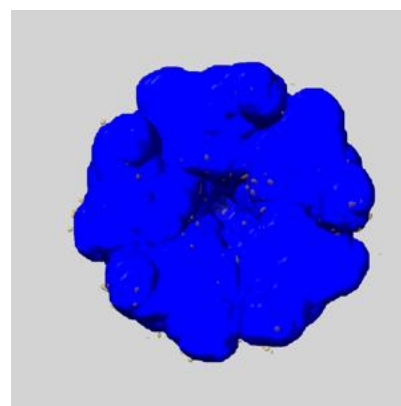
### 6.6.1 emd\_62929\_msk\_1.map [i](#)



X



Y

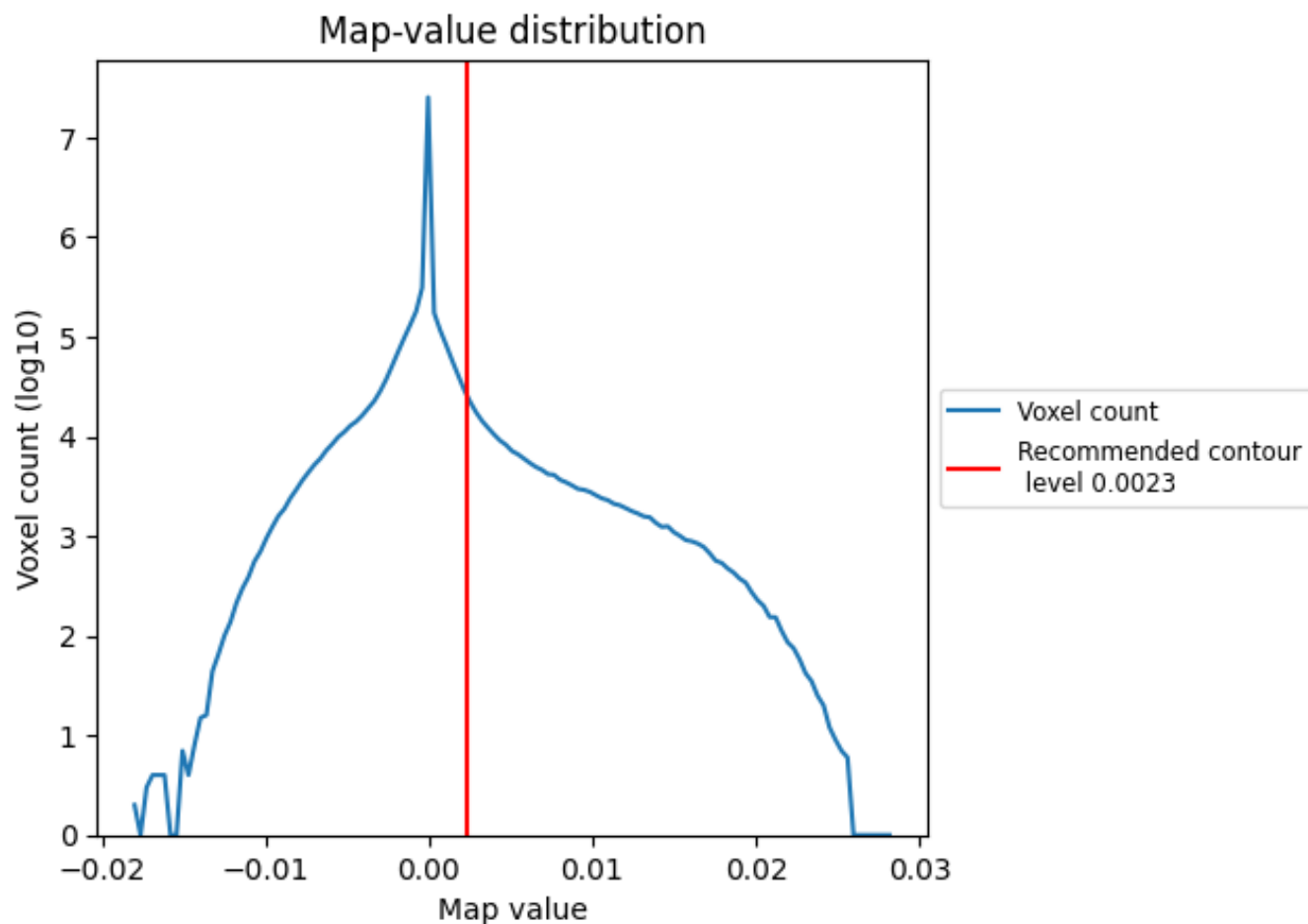


Z

## 7 Map analysis [i](#)

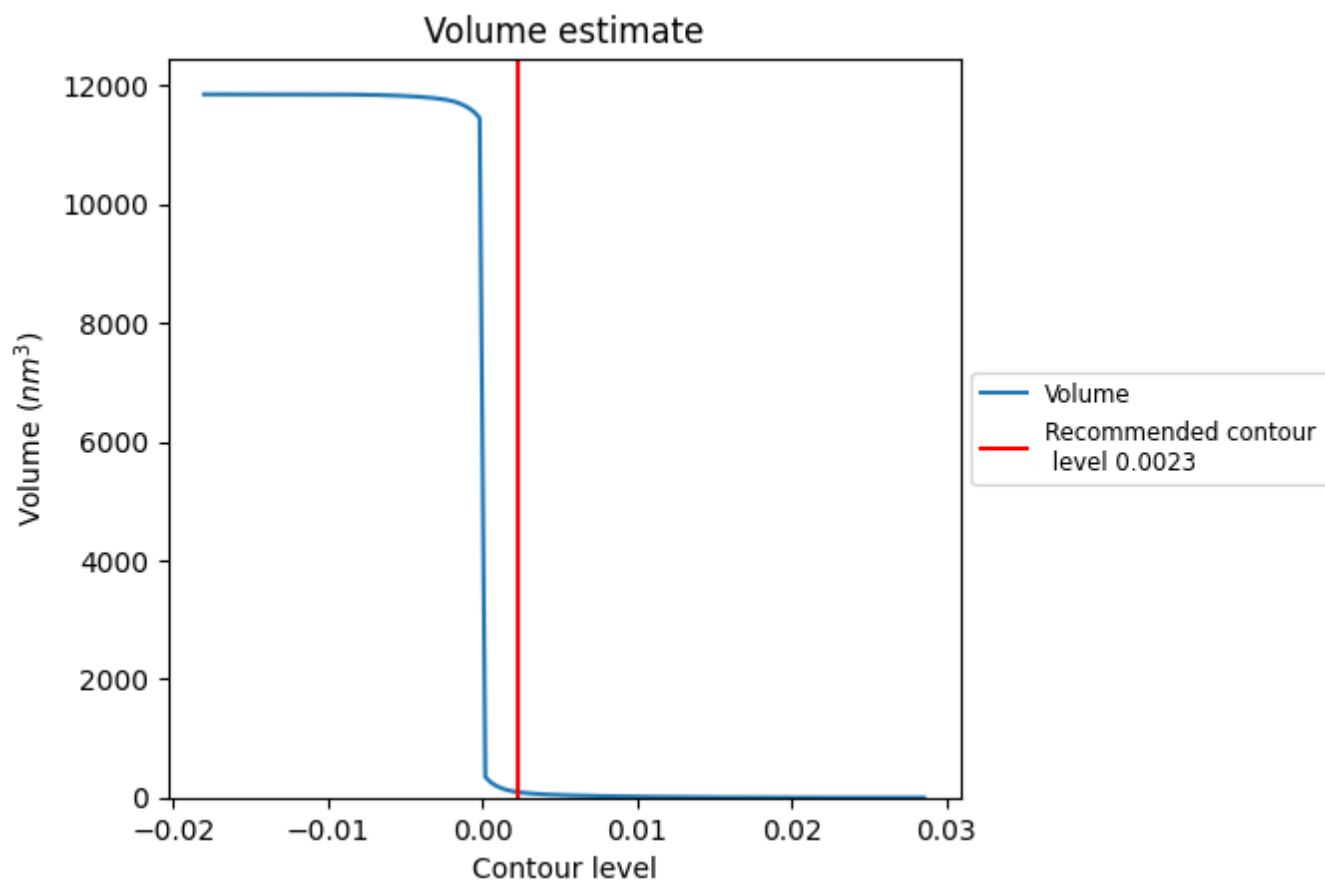
This section contains the results of statistical analysis of the map.

### 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.

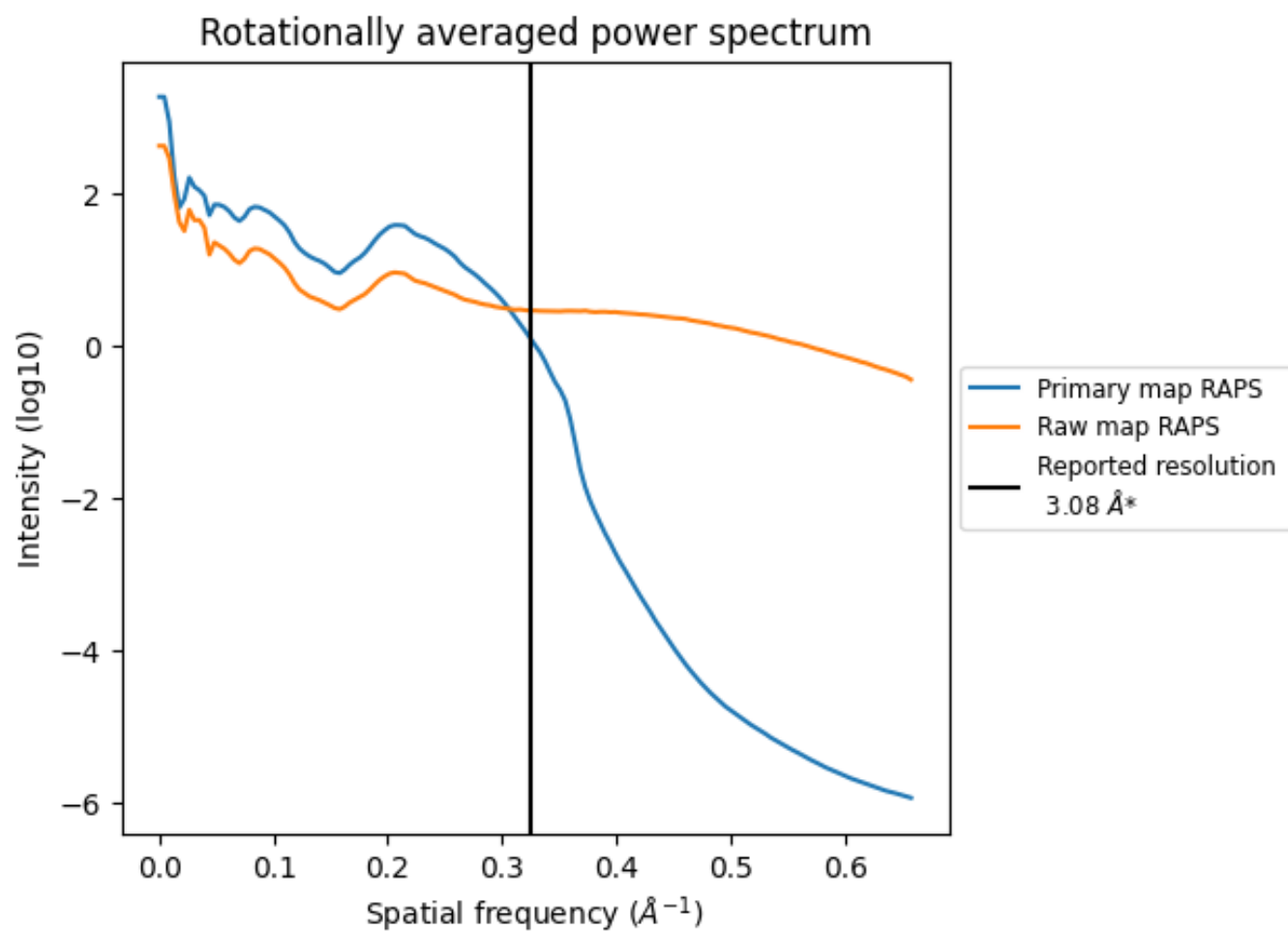
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm<sup>3</sup>; this corresponds to an approximate mass of 82 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

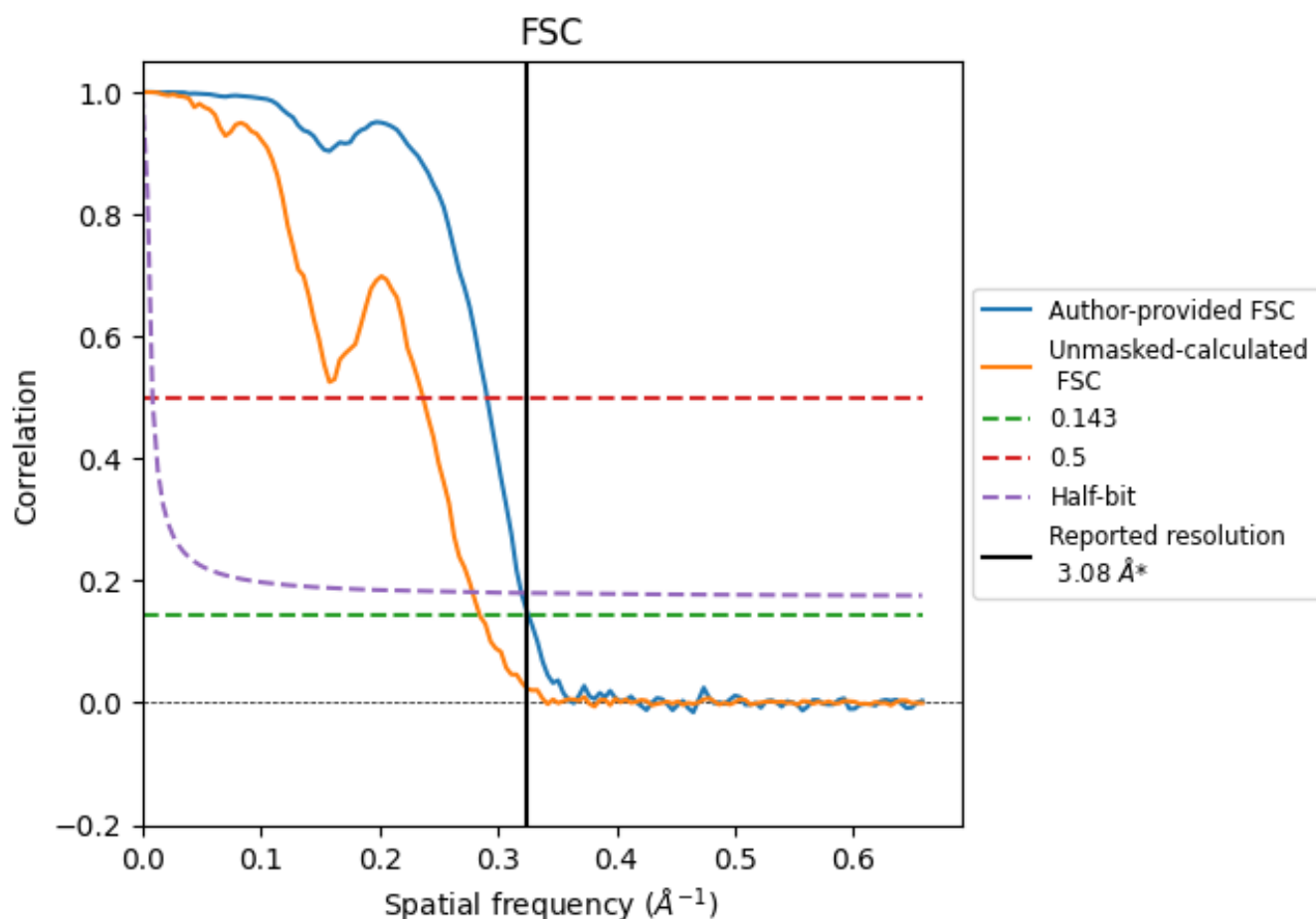


\*Reported resolution corresponds to spatial frequency of 0.325  $\text{\AA}^{-1}$

## 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  $0.325 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

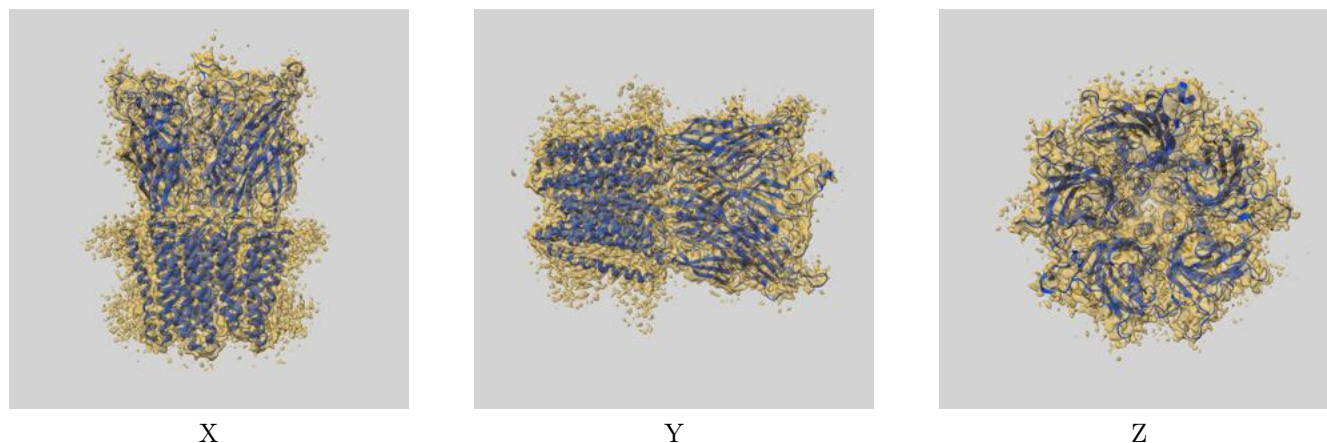
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.07	3.44	3.13
Unmasked-calculated*	3.51	4.22	3.59

\*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 3.51 differs from the reported value 3.08 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62929 and PDB model 9LAI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

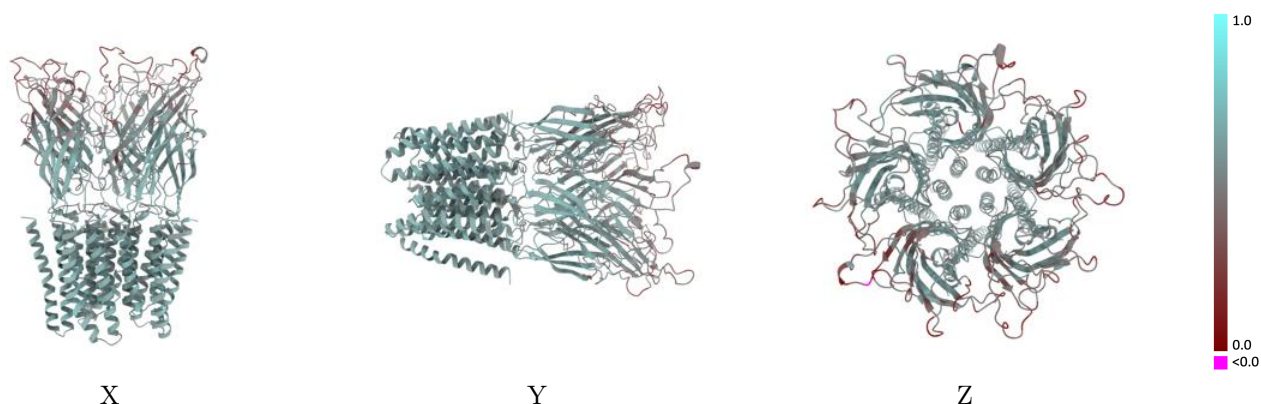
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0023 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.

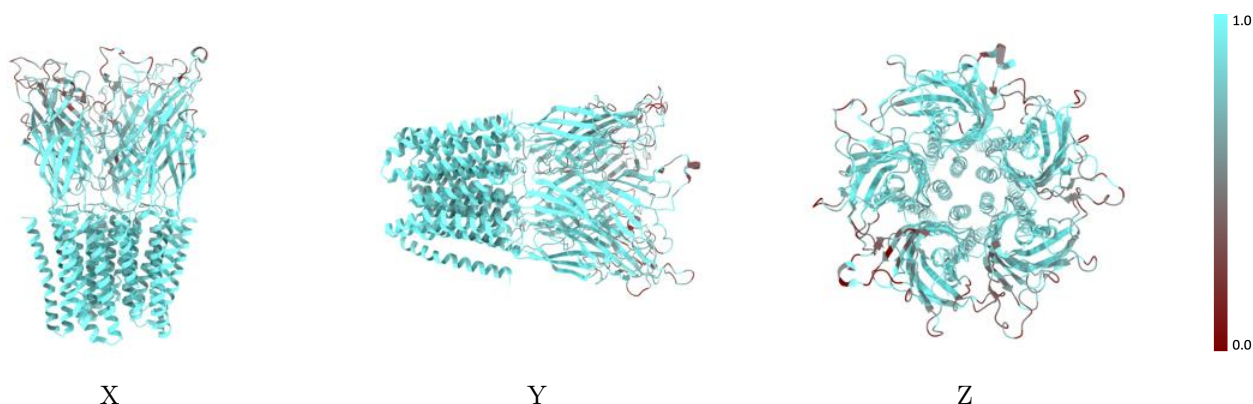


## 9.2 Q-score mapped to coordinate model [i](#)



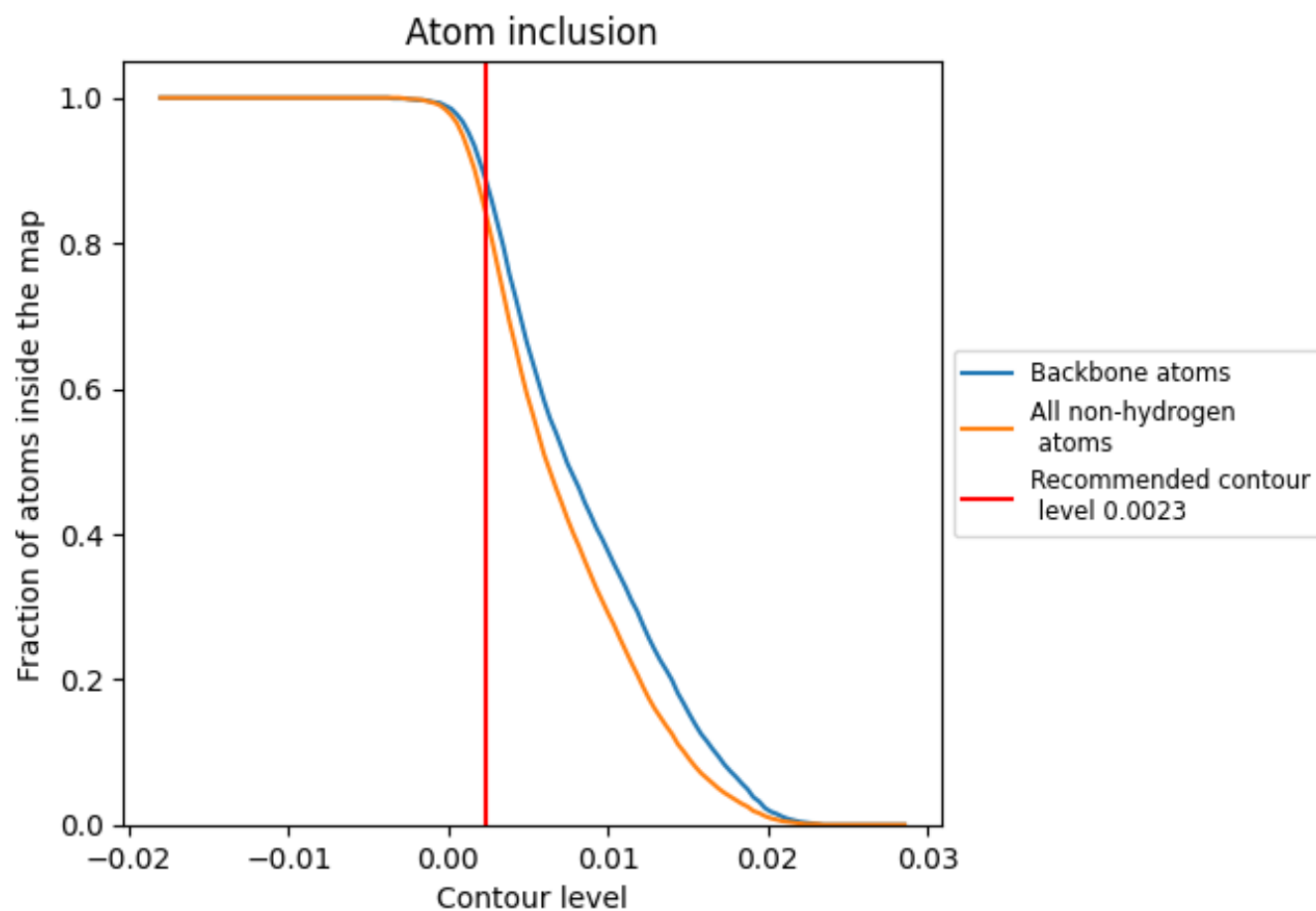
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0023).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.0023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8450	<div><div></div></div> 0.5400
A	<div><div></div></div> 0.8350	<div><div></div></div> 0.5310
B	<div><div></div></div> 0.8250	<div><div></div></div> 0.5320
C	<div><div></div></div> 0.8180	<div><div></div></div> 0.5260
D	<div><div></div></div> 0.8540	<div><div></div></div> 0.5490
E	<div><div></div></div> 0.8890	<div><div></div></div> 0.5600

