



# Full wwPDB EM Validation Report ⓘ

Aug 3, 2024 – 02:22 PM EDT

PDB ID : 9AVV  
EMDB ID : EMD-43924  
Title : Bovine adult muscle nAChR resting state  
Authors : Li, H.; Hibbs, R.E.  
Deposited on : 2024-03-05  
Resolution : 2.09 Å(reported)  
Based on initial model : .

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>.

---

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

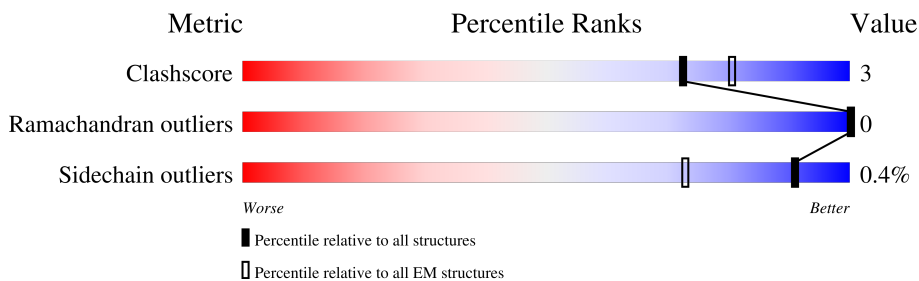
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.09 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	437	85% 5% 8%
1	C	437	86% 6% 8%
2	E	481	81% 15%
3	D	495	83% 13%
4	B	471	80% 6% 13%
5	F	62	97% ..
5	G	62	97% ..
6	J	10	50% 50%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
7	K	4	<p>50% 75% 25%</p>
7	N	4	<p>25% 100%</p>
8	L	11	<p>73% 27%</p>
9	M	6	<p>17% 67% 33%</p>

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 36425 atoms, of which 18249 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 Acetylcholine receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	400	Total	C	H	N	O	S	0	0
			6487	2118	3257	513	580	19		
1	C	401	Total	C	H	N	O	S	0	0
			6501	2123	3264	514	581	19		

- Molecule 2 is a protein called Acetylcholine receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	E	410	Total	C	H	N	O	S	0	0
			6670	2174	3333	543	609	11		

- Molecule 3 is a protein called Acetylcholine receptor subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	D	429	Total	C	H	N	O	S	0	0
			6949	2259	3483	562	629	16		

- Molecule 4 is a protein called Acetylcholine receptor subunit epsilon.

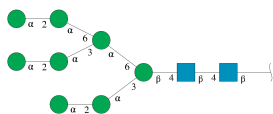
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	B	408	Total	C	H	N	O	S	0	0
			6440	2091	3216	517	601	15		

- Molecule 5 is a protein called Toxin.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	F	61	Total	C	H	N	O	S	0	0
			942	287	466	91	89	9		
5	G	62	Total	C	H	N	O	S	0	0
			951	289	471	92	90	9		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyra

nose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



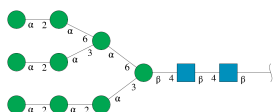
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
6	J	10	220	64	104	2	50	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



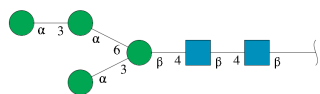
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
7	K	4	96	28	46	2	20	0	0
7	N	4	96	28	46	2	20	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



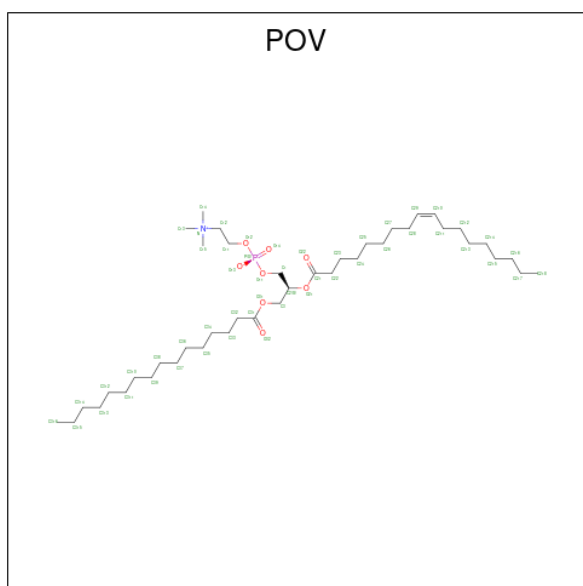
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
8	L	11	241	70	114	2	55	0	0

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



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
9	M	6	137	40	65	2	30	0	0

- Molecule 10 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						AltConf	
			Total	C	H	N	O	P		
10	A	1	Total	79	25	44	1	8	1	0
10	A	1	Total	85	27	48	1	8	1	0
10	E	1	Total	79	25	44	1	8	1	0
10	E	1	Total	79	25	44	1	8	1	0
10	E	1	Total	79	25	44	1	8	1	0
10	C	1	Total	85	27	48	1	8	1	0
10	C	1	Total	70	22	38	1	8	1	0
10	B	1	Total	85	27	48	1	8	1	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



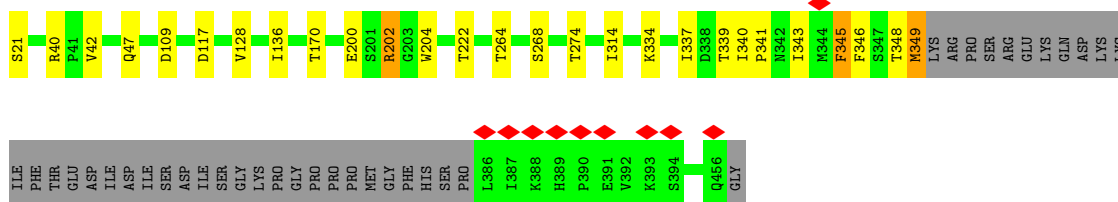
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
11	D	1	Total	C	H	N	O	0
			27	8	13	1	5	
11	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

### 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.

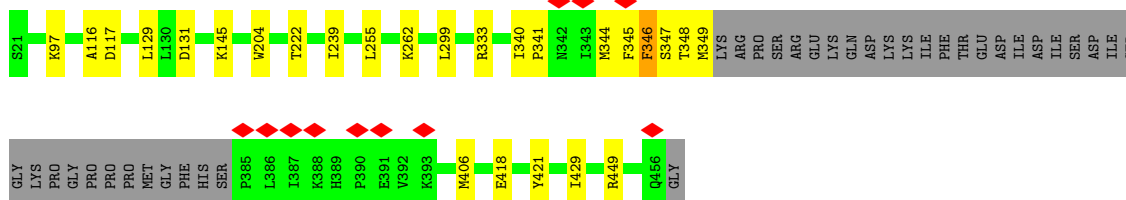
- Molecule 1: Acetylcholine receptor subunit alpha

Chain A: 85% 5% 8%



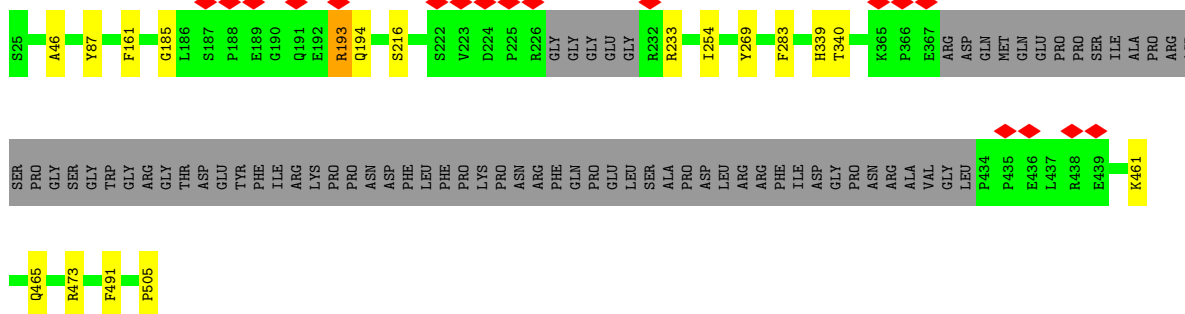
- Molecule 1: Acetylcholine receptor subunit alpha

Chain C: 86% 6% 8%



- Molecule 2: Acetylcholine receptor subunit beta

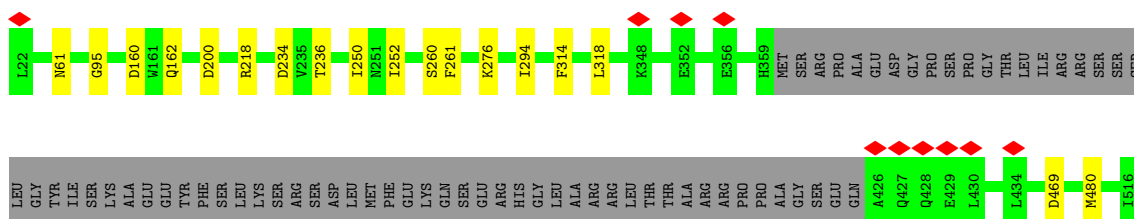
Chain E: 81% 15% 8%



- Molecule 3: Acetylcholine receptor subunit delta

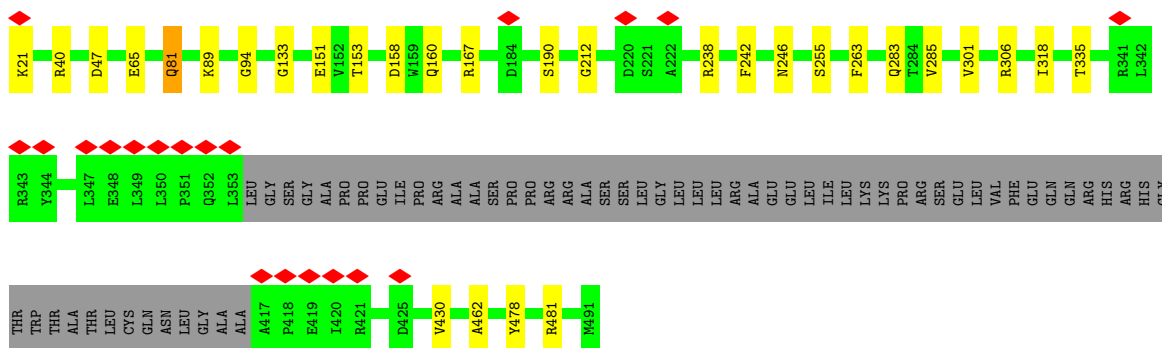


Chain D: 83% 13%



- Molecule 4: Acetylcholine receptor subunit epsilon

Chain B: 80% 6% 13%



- Molecule 5: Toxin

Chain F: 97%



- Molecule 5: Toxin

Chain G: 97%

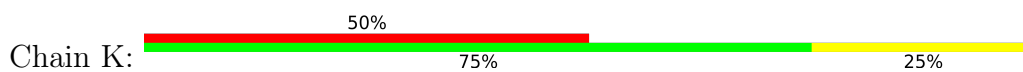


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 50%



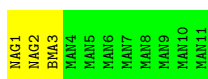
- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209258	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)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.786	Depositor
Minimum map value	-1.804	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	478.72, 478.72, 478.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	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: BMA, NAG, MAN, POV

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	0.32	0/3316	0.58	0/4524
1	C	0.32	0/3324	0.60	0/4535
2	E	0.31	0/3427	0.60	0/4674
3	D	0.31	0/3558	0.62	1/4854 (0.0%)
4	B	0.32	0/3301	0.61	0/4512
5	F	0.37	0/485	0.68	0/651
5	G	0.32	0/489	0.76	1/656 (0.2%)
All	All	0.32	0/17900	0.61	2/24406 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	E	0	2
4	B	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	200	ASP	CB-CG-OD1	5.22	123.00	118.30
5	G	29	ASP	CB-CG-OD1	5.12	122.90	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	ARG	Sidechain
4	B	167	ARG	Sidechain
1	C	449	ARG	Sidechain
2	E	233	ARG	Sidechain
2	E	473	ARG	Sidechain

## 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	3230	3257	3249	36	0
1	C	3237	3264	3257	23	0
2	E	3337	3333	3328	16	0
3	D	3466	3483	3476	14	0
4	B	3224	3216	3209	28	0
5	F	476	466	468	1	0
5	G	480	471	471	1	0
6	J	116	104	97	6	0
7	K	50	46	43	2	0
7	N	50	46	43	0	0
8	L	127	114	106	3	0
9	M	72	65	61	3	0
10	A	72	92	92	16	0
10	B	37	48	48	3	0
10	C	69	86	86	5	0
10	E	105	132	132	11	0
11	B	14	13	13	3	0
11	D	14	13	13	1	0
All	All	18176	18249	18192	123	0

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

All (123) 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)
4:B:81:GLN:OE1	11:B:502:NAG:C8	2.18	0.91

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD23	10:C:502:POV:H33	1.55	0.86
2:E:161:PHE:CZ	10:E:601:POV:H23A	2.12	0.83
1:C:340:ILE:HG21	1:C:429:ILE:HD11	1.59	0.82
10:E:603:POV:O13	10:E:603:POV:C33	2.27	0.82
1:C:239:ILE:HG21	10:C:501:POV:H27A	1.62	0.81
1:A:343:ILE:HG13	10:A:502:POV:H14A	1.61	0.81
1:A:343:ILE:HG13	10:A:502:POV:C14	2.13	0.79
10:E:603:POV:O13	10:E:603:POV:H33	1.83	0.79
4:B:81:GLN:OE1	11:B:502:NAG:H83	1.81	0.78
1:A:345:PHE:HB3	10:A:502:POV:O14	1.84	0.77
10:A:501:POV:H3	4:B:263:PHE:CD1	2.20	0.76
1:A:339:THR:C	1:A:341:PRO:HD3	2.08	0.73
3:D:314:PHE:O	3:D:318:LEU:HD13	1.89	0.72
10:A:501:POV:H1A	4:B:263:PHE:HD1	1.55	0.71
2:E:491:PHE:CD1	10:E:601:POV:H24A	2.26	0.70
2:E:491:PHE:CE1	10:E:601:POV:H24A	2.27	0.70
10:A:501:POV:H1A	4:B:263:PHE:CD1	2.27	0.69
3:D:261:PHE:HA	3:D:480:MET:HE1	1.74	0.68
1:C:204:TRP:HB2	8:L:2:NAG:H82	1.74	0.68
1:A:348:THR:O	1:A:348:THR:HG22	1.94	0.68
4:B:89:LYS:CG	4:B:94:GLY:HA2	2.25	0.67
1:C:347:SER:HB2	4:B:335:THR:HA	1.76	0.67
1:A:340:ILE:N	1:A:341:PRO:HD3	2.11	0.66
1:A:343:ILE:HG21	10:A:502:POV:H14A	1.76	0.65
1:A:128:VAL:HG13	1:A:136:ILE:HG23	1.79	0.65
3:D:314:PHE:CE1	3:D:318:LEU:HD11	2.32	0.65
1:A:21:SER:N	2:E:87:TYR:HH	1.95	0.65
1:A:343:ILE:HB	10:A:502:POV:H13B	1.80	0.64
1:A:343:ILE:CG2	10:A:502:POV:H11	2.28	0.64
1:A:340:ILE:HG22	1:A:340:ILE:O	1.98	0.63
2:E:505:PRO:O	7:K:2:NAG:C6	2.47	0.63
1:A:264:THR:O	1:A:268:SER:OG	2.12	0.62
1:A:42:VAL:O	4:B:21:LYS:N	2.33	0.61
1:A:40:ARG:NH2	1:A:47:GLN:O	2.33	0.61
2:E:505:PRO:O	7:K:2:NAG:H62	2.00	0.61
8:L:1:NAG:H62	8:L:2:NAG:C7	2.31	0.61
1:A:343:ILE:HG21	10:A:502:POV:H11	1.84	0.60
1:C:255:LEU:O	1:C:262:LYS:NZ	2.35	0.59
4:B:89:LYS:HG2	4:B:94:GLY:HA2	1.83	0.59
4:B:40:ARG:NH2	4:B:47:ASP:O	2.35	0.59
1:A:337:ILE:O	1:A:349:MET:HG2	2.04	0.58

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:95:GLY:HA2	11:D:601:NAG:H83	1.86	0.58
4:B:301:VAL:O	4:B:306:ARG:NH1	2.36	0.58
5:G:59:ASN:OD1	5:G:59:ASN:N	2.37	0.57
1:C:340:ILE:HB	1:C:341:PRO:HD3	1.86	0.57
1:C:344:MET:HB3	10:B:501:POV:C13	2.35	0.56
1:A:348:THR:O	1:A:349:MET:C	2.44	0.56
1:C:116:ALA:HA	3:D:61:ASN:HD21	1.72	0.55
10:E:603:POV:O13	10:E:603:POV:H33A	2.03	0.55
2:E:185:GLY:O	2:E:193:ARG:NE	2.40	0.55
1:A:346:PHE:HA	2:E:340:THR:O	2.05	0.54
3:D:160:ASP:OD2	3:D:162:GLN:NE2	2.40	0.54
4:B:81:GLN:OE1	11:B:502:NAG:H82	2.03	0.54
3:D:260:SER:O	3:D:480:MET:HE3	2.08	0.53
4:B:89:LYS:HG3	4:B:94:GLY:HA2	1.89	0.53
2:E:461:LYS:HE3	2:E:465:GLN:OE1	2.09	0.53
10:A:501:POV:C1	4:B:263:PHE:CD1	2.92	0.52
10:C:502:POV:H3	10:C:502:POV:H14B	1.91	0.52
1:C:222:THR:HB	8:L:2:NAG:H81	1.92	0.52
1:A:109:ASP:OD2	1:A:170:THR:OG1	2.23	0.51
3:D:252:ILE:HG21	3:D:294:ILE:HD11	1.92	0.51
4:B:478:TYR:CZ	4:B:481:ARG:NH2	2.68	0.50
1:C:333:ARG:NH1	1:C:418:GLU:OE1	2.41	0.50
4:B:478:TYR:CE1	4:B:481:ARG:NH2	2.79	0.50
3:D:260:SER:O	3:D:480:MET:CE	2.60	0.50
4:B:158:ASP:OD2	4:B:160:GLN:NE2	2.40	0.50
1:C:345:PHE:C	1:C:346:PHE:CG	2.86	0.49
4:B:151:GLU:OE2	4:B:153:THR:CB	2.60	0.49
1:A:21:SER:N	2:E:46:ALA:O	2.46	0.49
1:A:340:ILE:N	1:A:341:PRO:CD	2.74	0.48
4:B:151:GLU:OE2	4:B:153:THR:OG1	2.25	0.48
6:J:1:NAG:H62	6:J:2:NAG:C7	2.43	0.48
2:E:269:TYR:CE1	10:E:602:POV:H1	2.49	0.48
1:C:344:MET:HB3	10:B:501:POV:H13B	1.94	0.48
3:D:218:ARG:HH11	9:M:2:NAG:H83	1.77	0.48
1:C:346:PHE:CD1	1:C:346:PHE:N	2.82	0.48
1:A:343:ILE:HG13	10:A:502:POV:H14	1.94	0.47
1:C:117:ASP:OD1	1:C:145:LYS:HD3	2.14	0.47
2:E:194:GLN:O	2:E:216:SER:N	2.47	0.47
1:A:117:ASP:OD1	1:A:117:ASP:N	2.46	0.47
1:A:222:THR:HB	6:J:2:NAG:H81	1.95	0.47
1:C:344:MET:HB3	10:B:501:POV:H13	1.97	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ILE:CG1	10:A:502:POV:H14A	2.38	0.47
1:C:406:MET:SD	4:B:430:VAL:HG12	2.55	0.46
1:A:128:VAL:CG1	1:A:136:ILE:HG23	2.45	0.46
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.81	0.46
10:A:501:POV:H3	4:B:263:PHE:CE1	2.50	0.46
1:A:345:PHE:C	1:A:345:PHE:CD1	2.90	0.45
10:E:603:POV:H3A	10:E:603:POV:H32A	1.65	0.45
1:A:204:TRP:HB2	6:J:2:NAG:H82	1.99	0.45
2:E:193:ARG:O	2:E:194:GLN:NE2	2.44	0.45
1:A:200:GLU:OE2	6:J:1:NAG:C8	2.65	0.45
4:B:190:SER:O	4:B:212:GLY:N	2.48	0.45
2:E:254:ILE:HD12	10:E:601:POV:H24	1.98	0.44
1:C:97:LYS:HG2	1:C:131:ASP:OD1	2.18	0.44
1:C:344:MET:HB2	1:C:346:PHE:CZ	2.52	0.44
4:B:242:PHE:O	4:B:246:ASN:ND2	2.46	0.44
1:A:314:ILE:CG1	10:A:501:POV:O32	2.66	0.43
2:E:339:HIS:CD2	2:E:340:THR:HG23	2.53	0.43
1:C:97:LYS:HD3	1:C:129:LEU:HD11	2.00	0.43
10:C:501:POV:H39	10:C:501:POV:H36	1.76	0.43
1:A:348:THR:O	1:A:348:THR:CG2	2.64	0.43
3:D:234:ASP:OD1	3:D:236:THR:OG1	2.36	0.43
10:E:603:POV:H24	10:E:603:POV:H27	1.75	0.42
4:B:65:GLU:OE2	4:B:238:ARG:NH1	2.44	0.42
2:E:161:PHE:CE2	10:E:601:POV:H25A	2.55	0.42
4:B:81:GLN:OE1	4:B:133:GLY:O	2.38	0.42
1:C:349:MET:HG2	1:C:418:GLU:HA	2.01	0.42
5:F:36:GLU:OE1	6:J:5:MAN:H4	2.20	0.42
9:M:2:NAG:H83	9:M:2:NAG:H2	1.93	0.41
1:A:334:LYS:O	1:A:339:THR:HG23	2.21	0.41
1:C:348:THR:HA	1:C:421:TYR:CZ	2.55	0.41
10:C:502:POV:H22A	3:D:250:ILE:HD11	2.02	0.41
4:B:255:SER:OG	4:B:283:GLN:NE2	2.46	0.41
1:A:200:GLU:OE2	6:J:1:NAG:H82	2.21	0.41
1:A:274:THR:HG22	4:B:285:VAL:HG11	2.03	0.41
10:A:502:POV:H22A	10:A:502:POV:H2	1.88	0.41
9:M:1:NAG:H82	9:M:1:NAG:H2	1.97	0.41
3:D:261:PHE:CA	3:D:480:MET:HE1	2.46	0.40
3:D:276:LYS:NZ	3:D:469:ASP:OD2	2.51	0.40
1:C:345:PHE:O	1:C:346:PHE:CG	2.75	0.40
4:B:318:ILE:HD11	4:B:462:ALA:HB1	2.03	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	396/437 (91%)	385 (97%)	11 (3%)	0	100	100
1	C	397/437 (91%)	387 (98%)	10 (2%)	0	100	100
2	E	404/481 (84%)	397 (98%)	7 (2%)	0	100	100
3	D	425/495 (86%)	420 (99%)	5 (1%)	0	100	100
4	B	404/471 (86%)	399 (99%)	5 (1%)	0	100	100
5	F	59/62 (95%)	59 (100%)	0	0	100	100
5	G	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	2145/2445 (88%)	2104 (98%)	41 (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	369/402 (92%)	367 (100%)	2 (0%)	88	92
1	C	370/402 (92%)	369 (100%)	1 (0%)	92	95
2	E	380/438 (87%)	378 (100%)	2 (0%)	88	92
3	D	395/451 (88%)	395 (100%)	0	100	100
4	B	360/410 (88%)	359 (100%)	1 (0%)	92	95
5	F	57/57 (100%)	57 (100%)	0	100	100
5	G	57/57 (100%)	56 (98%)	1 (2%)	59	65

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1988/2217 (90%)	1981 (100%)	7 (0%)	91 94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	PHE
1	A	349	MET
2	E	193	ARG
2	E	283	PHE
1	C	346	PHE
4	B	81	GLN
5	G	59	ASN

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

35 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	$\# Z  > 2$
6	NAG	J	1	6	14,14,15	0.40	0	17,19,21	0.63	0
6	MAN	J	10	6	11,11,12	0.29	0	15,15,17	0.52	0
6	NAG	J	2	6	14,14,15	0.39	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	J	3	6	11,11,12	0.32	0	15,15,17	0.68	1 (6%)
6	MAN	J	4	6	11,11,12	0.26	0	15,15,17	0.62	0
6	MAN	J	5	6	11,11,12	0.39	0	15,15,17	0.53	0
6	MAN	J	6	6	11,11,12	0.43	0	15,15,17	0.88	1 (6%)
6	MAN	J	7	6	11,11,12	0.43	0	15,15,17	0.57	0
6	MAN	J	8	6	11,11,12	0.31	0	15,15,17	0.53	0
6	MAN	J	9	6	11,11,12	0.45	0	15,15,17	0.63	0
7	NAG	K	1	2,7	14,14,15	0.38	0	17,19,21	0.54	0
7	NAG	K	2	7	14,14,15	0.39	0	17,19,21	0.52	0
7	BMA	K	3	7	11,11,12	0.32	0	15,15,17	0.46	0
7	MAN	K	4	7	11,11,12	0.30	0	15,15,17	0.51	0
8	NAG	L	1	1,8	14,14,15	0.43	0	17,19,21	0.75	0
8	MAN	L	10	8	11,11,12	0.47	0	15,15,17	0.59	0
8	MAN	L	11	8	11,11,12	0.34	0	15,15,17	0.55	0
8	NAG	L	2	8	14,14,15	0.40	0	17,19,21	0.66	0
8	BMA	L	3	8	11,11,12	0.32	0	15,15,17	0.72	1 (6%)
8	MAN	L	4	8	11,11,12	0.44	0	15,15,17	0.50	0
8	MAN	L	5	8	11,11,12	0.43	0	15,15,17	0.59	0
8	MAN	L	6	8	11,11,12	0.33	0	15,15,17	0.53	0
8	MAN	L	7	8	11,11,12	0.38	0	15,15,17	0.60	0
8	MAN	L	8	8	11,11,12	0.51	0	15,15,17	0.53	0
8	MAN	L	9	8	11,11,12	0.35	0	15,15,17	0.58	0
9	NAG	M	1	3,9	14,14,15	0.40	0	17,19,21	0.60	0
9	NAG	M	2	9	14,14,15	0.36	0	17,19,21	0.50	0
9	BMA	M	3	9	11,11,12	0.65	0	15,15,17	0.54	0
9	MAN	M	4	9	11,11,12	0.33	0	15,15,17	0.50	0
9	MAN	M	5	9	11,11,12	0.31	0	15,15,17	0.52	0
9	MAN	M	6	9	11,11,12	0.27	0	15,15,17	0.48	0
7	NAG	N	1	4,7	14,14,15	0.42	0	17,19,21	0.65	0
7	NAG	N	2	7	14,14,15	0.39	0	17,19,21	0.43	0
7	BMA	N	3	7	11,11,12	0.30	0	15,15,17	0.48	0
7	MAN	N	4	7	11,11,12	0.25	0	15,15,17	0.51	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	1	6	-	0/6/23/26	0/1/1/1
6	MAN	J	10	6	-	0/2/19/22	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
6	MAN	J	7	6	-	1/2/19/22	0/1/1/1
6	MAN	J	8	6	-	0/2/19/22	0/1/1/1
6	MAN	J	9	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	1/2/19/22	0/1/1/1
8	NAG	L	1	1,8	-	2/6/23/26	0/1/1/1
8	MAN	L	10	8	-	0/2/19/22	0/1/1/1
8	MAN	L	11	8	-	0/2/19/22	0/1/1/1
8	NAG	L	2	8	-	2/6/23/26	0/1/1/1
8	BMA	L	3	8	-	0/2/19/22	0/1/1/1
8	MAN	L	4	8	-	0/2/19/22	0/1/1/1
8	MAN	L	5	8	-	0/2/19/22	0/1/1/1
8	MAN	L	6	8	-	0/2/19/22	0/1/1/1
8	MAN	L	7	8	-	0/2/19/22	0/1/1/1
8	MAN	L	8	8	-	0/2/19/22	0/1/1/1
8	MAN	L	9	8	-	0/2/19/22	0/1/1/1
9	NAG	M	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	0/2/19/22	0/1/1/1
9	MAN	M	6	9	-	0/2/19/22	0/1/1/1
7	NAG	N	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	6	MAN	C1-O5-C5	2.34	115.37	112.19
8	L	3	BMA	C1-O5-C5	2.06	114.98	112.19
6	J	3	BMA	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

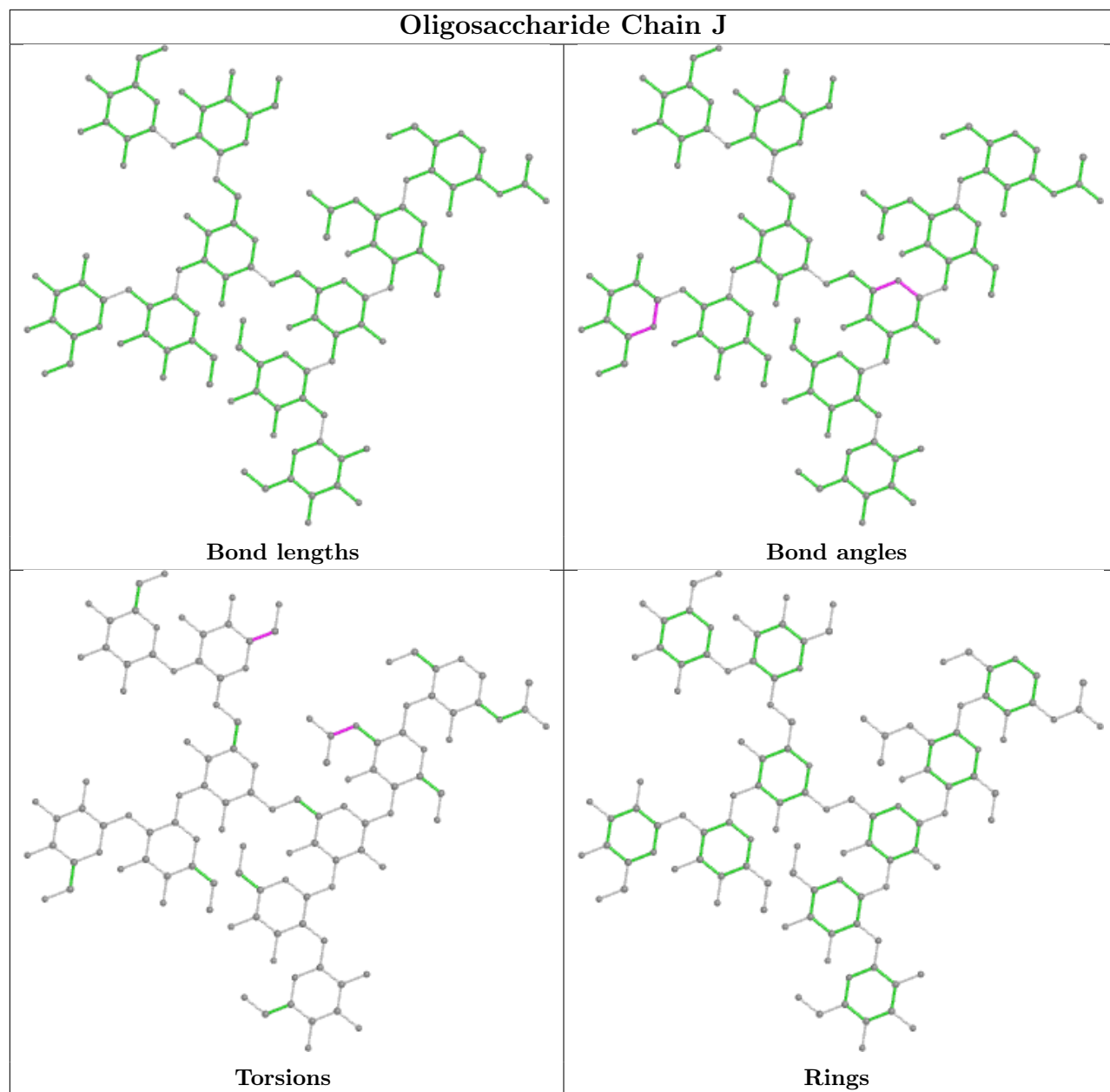
Mol	Chain	Res	Type	Atoms
7	N	1	NAG	C8-C7-N2-C2
9	M	2	NAG	C8-C7-N2-C2
9	M	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
8	L	1	NAG	C8-C7-N2-C2
9	M	1	NAG	C8-C7-N2-C2
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
7	N	2	NAG	O7-C7-N2-C2
8	L	1	NAG	O7-C7-N2-C2
8	L	2	NAG	C8-C7-N2-C2
8	L	2	NAG	O7-C7-N2-C2
9	M	1	NAG	O7-C7-N2-C2
7	K	4	MAN	O5-C5-C6-O6
6	J	7	MAN	O5-C5-C6-O6

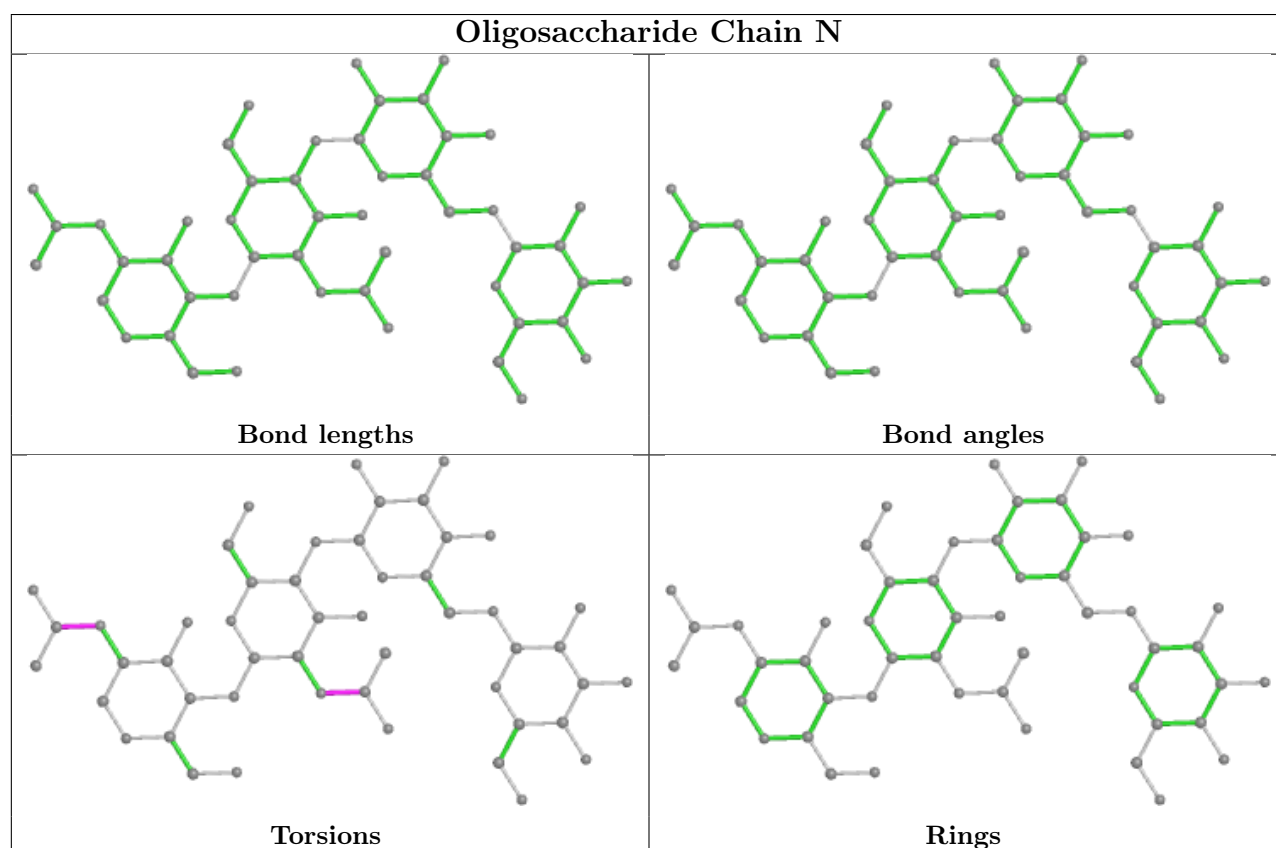
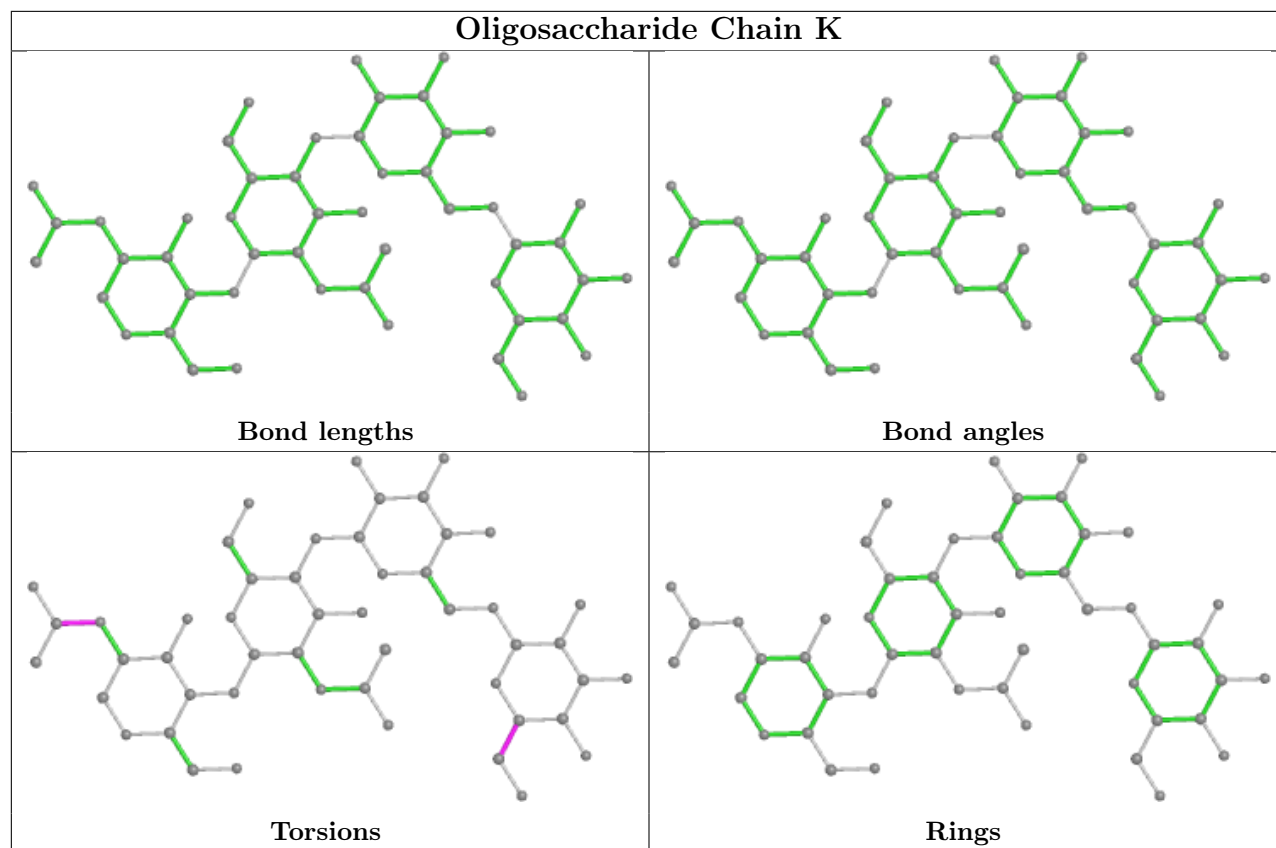
There are no ring outliers.

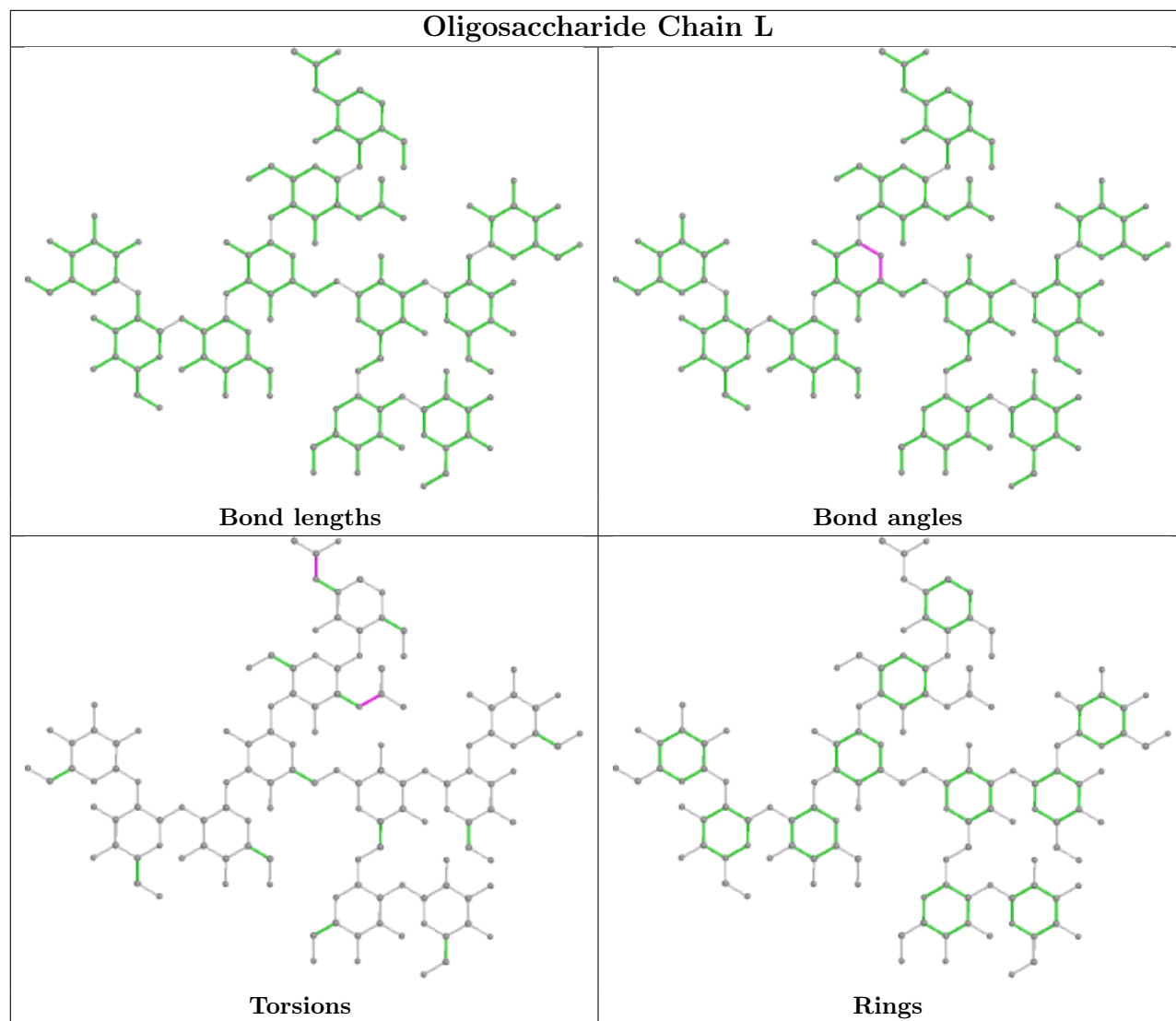
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	3	0
9	M	2	NAG	2	0
6	J	2	NAG	3	0
8	L	1	NAG	1	0
8	L	2	NAG	3	0
9	M	1	NAG	1	0
7	K	2	NAG	2	0
6	J	5	MAN	1	0

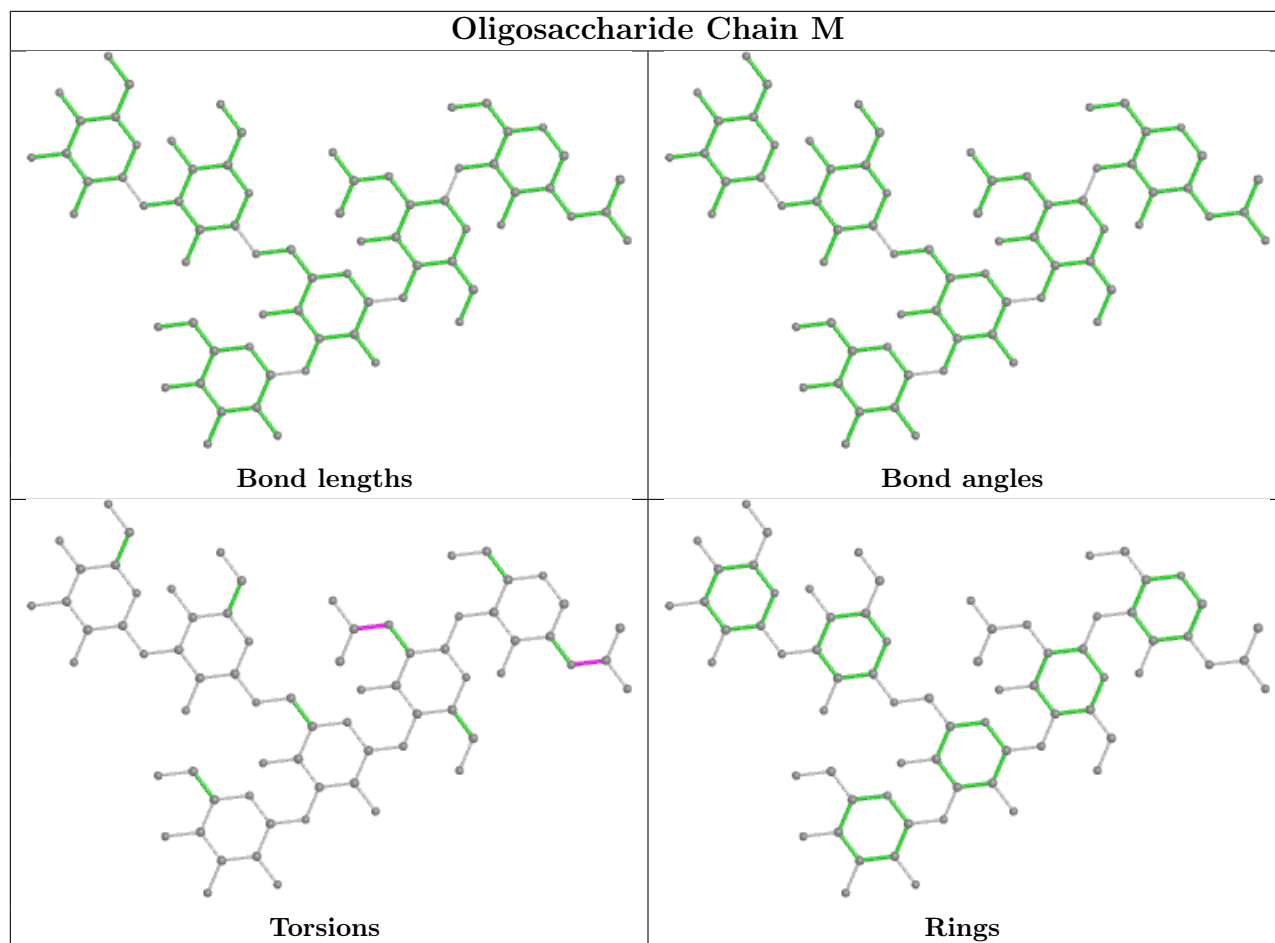
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	POV	A	502	-	36,36,51	0.32	0	42,44,59	0.41	0
10	POV	E	603	-	34,34,51	0.34	0	40,42,59	0.37	0
11	NAG	B	502	4	14,14,15	0.39	0	17,19,21	0.42	0
10	POV	C	501	-	36,36,51	0.31	0	42,44,59	0.34	0
11	NAG	D	601	3	14,14,15	0.39	0	17,19,21	0.90	1 (5%)
10	POV	E	601	-	34,34,51	0.34	0	40,42,59	0.35	0
10	POV	E	602	-	34,34,51	0.33	0	40,42,59	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	POV	C	502	-	31,31,51	0.34	0	37,39,59	0.40	0
10	POV	B	501	-	36,36,51	0.31	0	42,44,59	0.34	0
10	POV	A	501	-	34,34,51	0.32	0	40,42,59	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	POV	A	502	-	-	8/40/40/55	-
10	POV	E	603	-	-	30/38/38/55	-
11	NAG	B	502	4	-	0/6/23/26	0/1/1/1
10	POV	C	501	-	-	17/40/40/55	-
11	NAG	D	601	3	-	2/6/23/26	0/1/1/1
10	POV	E	601	-	-	15/38/38/55	-
10	POV	E	602	-	-	11/38/38/55	-
10	POV	C	502	-	-	8/35/35/55	-
10	POV	B	501	-	-	8/40/40/55	-
10	POV	A	501	-	-	12/38/38/55	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	601	NAG	C2-N2-C7	3.20	127.45	122.90

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	501	POV	C1-O11-P-O12
10	A	501	POV	C1-O11-P-O14
10	A	501	POV	C11-O12-P-O11
10	A	501	POV	C11-O12-P-O14
10	A	501	POV	C32-C31-O31-C3
10	A	501	POV	O32-C31-O31-C3
10	A	502	POV	C1-O11-P-O14
10	A	502	POV	C22-C21-O21-C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	A	502	POV	O22-C21-O21-C2
10	E	601	POV	C22-C21-O21-C2
10	E	602	POV	C11-O12-P-O13
10	E	603	POV	C1-O11-P-O12
10	E	603	POV	C1-O11-P-O13
10	E	603	POV	C1-O11-P-O14
10	E	603	POV	C11-O12-P-O14
10	C	501	POV	O12-C11-C12-N
10	C	502	POV	C22-C21-O21-C2
10	C	502	POV	O22-C21-O21-C2
10	E	601	POV	O32-C31-O31-C3
10	E	601	POV	C32-C31-O31-C3
10	E	603	POV	O32-C31-O31-C3
10	C	501	POV	O32-C31-O31-C3
10	E	601	POV	O22-C21-O21-C2
10	C	502	POV	O32-C31-O31-C3
10	A	502	POV	C32-C31-O31-C3
10	C	501	POV	C32-C31-O31-C3
10	E	603	POV	C32-C31-O31-C3
10	C	502	POV	C32-C31-O31-C3
10	A	502	POV	O32-C31-O31-C3
10	E	603	POV	C22-C21-O21-C2
10	E	603	POV	C34-C35-C36-C37
10	E	601	POV	C11-C12-N-C13
10	E	601	POV	C11-C12-N-C15
10	B	501	POV	C32-C31-O31-C3
10	C	501	POV	C36-C37-C38-C39
10	E	603	POV	O22-C21-O21-C2
10	E	603	POV	C11-C12-N-C14
10	B	501	POV	O32-C31-O31-C3
10	E	602	POV	C11-O12-P-O11
10	E	603	POV	C11-O12-P-O11
10	C	501	POV	C11-O12-P-O11
10	A	502	POV	C34-C35-C36-C37
10	E	601	POV	C21-C22-C23-C24
10	C	501	POV	C21-C22-C23-C24
10	B	501	POV	C22-C21-O21-C2
10	B	501	POV	O22-C21-O21-C2
10	E	603	POV	C31-C32-C33-C34
10	E	601	POV	C36-C37-C38-C39
10	E	603	POV	C22-C23-C24-C25
10	E	601	POV	C11-C12-N-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	E	603	POV	C25-C26-C27-C28
10	A	501	POV	O22-C21-O21-C2
10	E	603	POV	C11-C12-N-C13
10	C	501	POV	C23-C24-C25-C26
10	A	501	POV	C22-C21-O21-C2
10	C	501	POV	C25-C26-C27-C28
10	C	501	POV	C35-C36-C37-C38
10	E	601	POV	C34-C35-C36-C37
10	E	601	POV	C31-C32-C33-C34
10	E	601	POV	C33-C34-C35-C36
10	E	602	POV	C22-C21-O21-C2
10	C	501	POV	C22-C21-O21-C2
10	E	603	POV	O21-C2-C3-O31
10	E	603	POV	C11-C12-N-C15
10	C	501	POV	O22-C21-O21-C2
10	A	502	POV	C1-O11-P-O12
10	E	601	POV	C37-C38-C39-C310
10	E	602	POV	O22-C21-O21-C2
10	E	603	POV	C26-C27-C28-C29
10	B	501	POV	C32-C33-C34-C35
10	E	603	POV	C23-C24-C25-C26
10	E	601	POV	C311-C310-C39-C38
11	D	601	NAG	O5-C5-C6-O6
10	E	603	POV	C24-C25-C26-C27
10	C	501	POV	C311-C310-C39-C38
10	E	603	POV	C21-C22-C23-C24
10	C	501	POV	O11-C1-C2-C3
10	E	603	POV	C1-C2-C3-O31
10	A	501	POV	O11-C1-C2-O21
10	C	501	POV	O11-C1-C2-O21
10	E	602	POV	O21-C2-C3-O31
10	E	603	POV	C32-C33-C34-C35
10	C	502	POV	O11-C1-C2-O21
10	E	603	POV	C11-O12-P-O13
10	C	501	POV	C11-O12-P-O14
10	E	602	POV	C12-C11-O12-P
10	B	501	POV	C12-C11-O12-P
10	C	501	POV	C33-C34-C35-C36
10	A	502	POV	O12-C11-C12-N
10	E	602	POV	O12-C11-C12-N
10	B	501	POV	O12-C11-C12-N
10	E	602	POV	C33-C34-C35-C36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	A	501	POV	C3-C2-O21-C21
10	C	502	POV	C11-O12-P-O11
10	B	501	POV	C1-O11-P-O12
11	D	601	NAG	C3-C2-N2-C7
10	E	603	POV	C2-C1-O11-P
10	E	601	POV	C23-C24-C25-C26
10	C	502	POV	O11-C1-C2-C3
10	A	501	POV	C32-C33-C34-C35
10	A	501	POV	C33-C34-C35-C36
10	E	603	POV	O31-C31-C32-C33
10	E	602	POV	C1-C2-C3-O31
10	E	603	POV	O11-C1-C2-O21
10	E	603	POV	O21-C21-C22-C23
10	E	603	POV	O32-C31-C32-C33
10	E	603	POV	O22-C21-C22-C23
10	C	501	POV	C1-O11-P-O14
10	C	502	POV	O31-C31-C32-C33
10	E	602	POV	O21-C21-C22-C23
10	E	602	POV	O22-C21-C22-C23

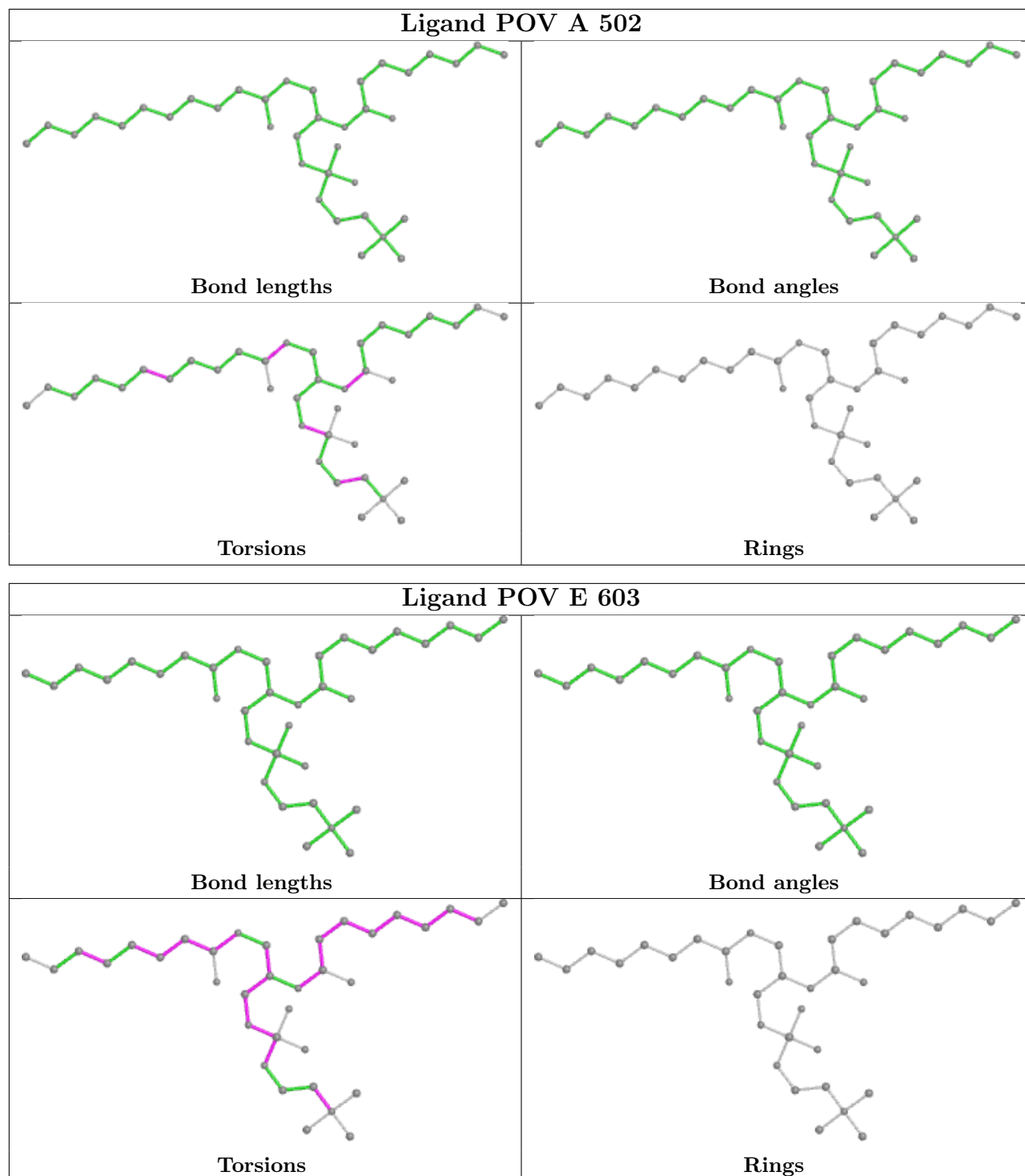
There are no ring outliers.

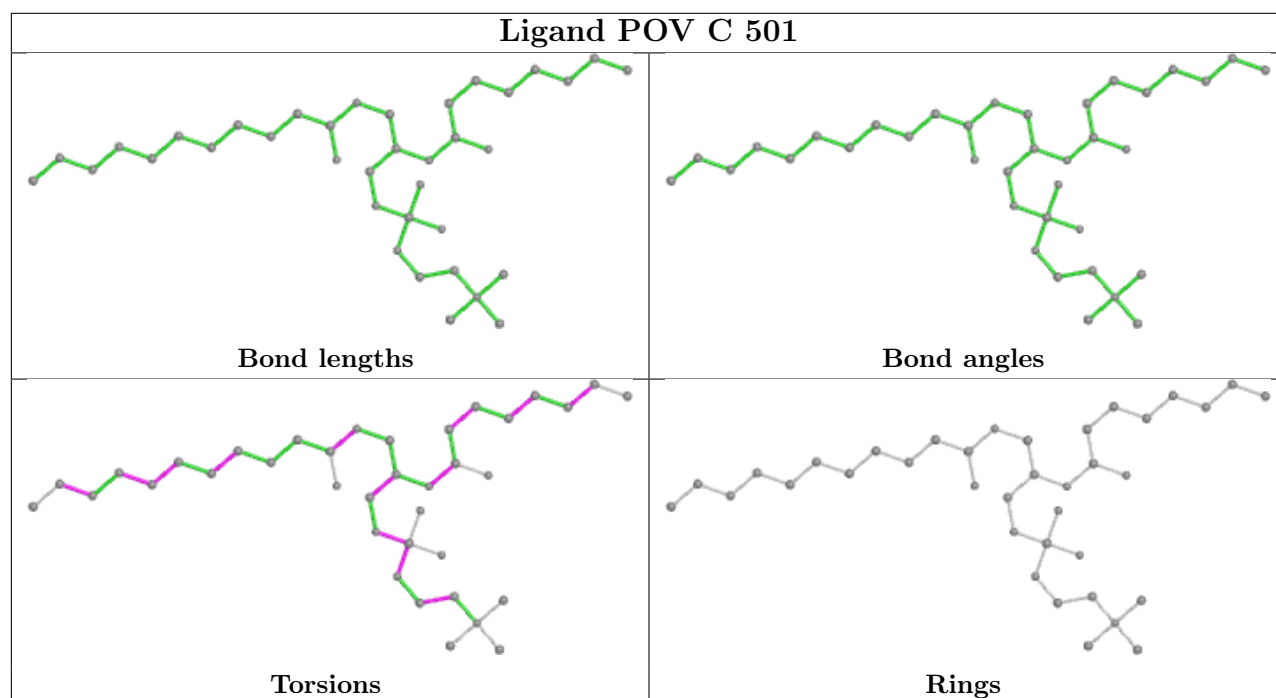
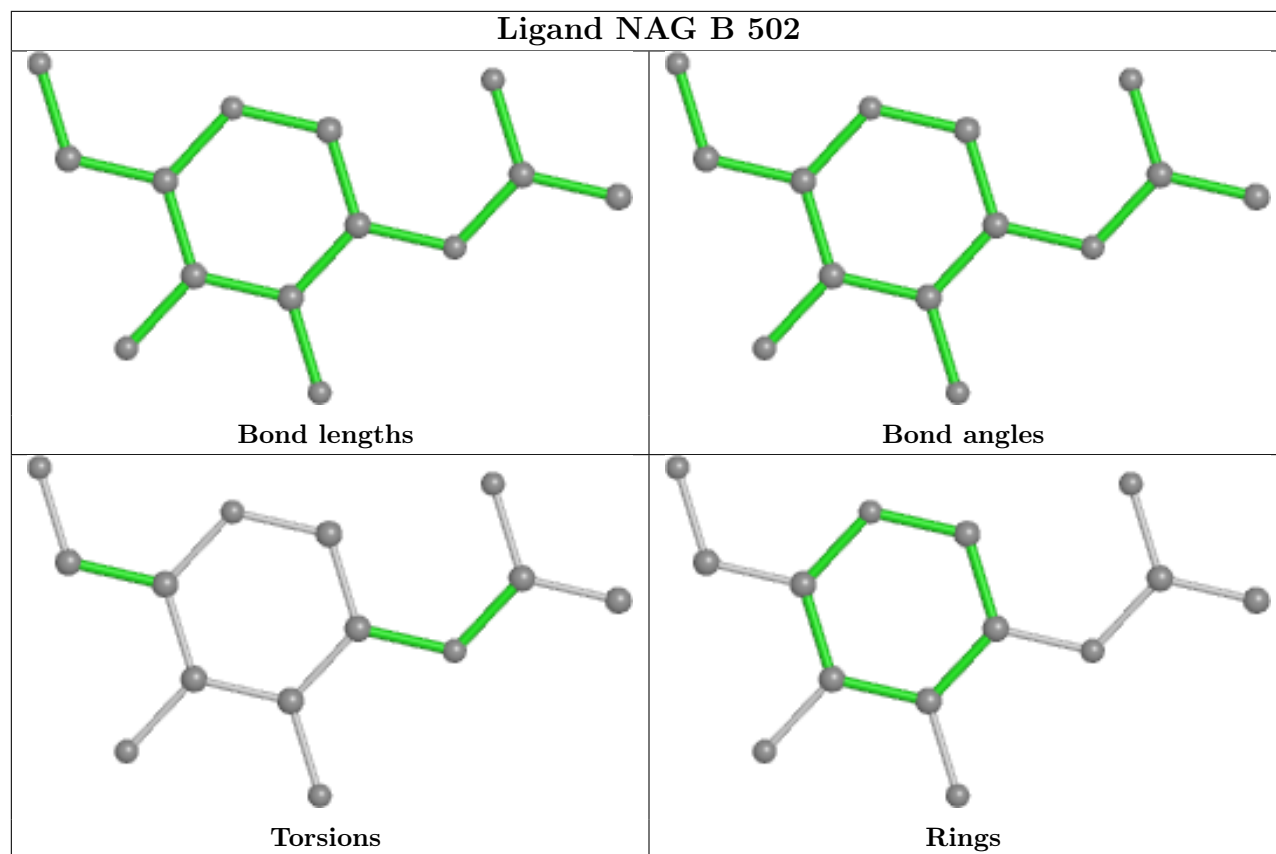
10 monomers are involved in 39 short contacts:

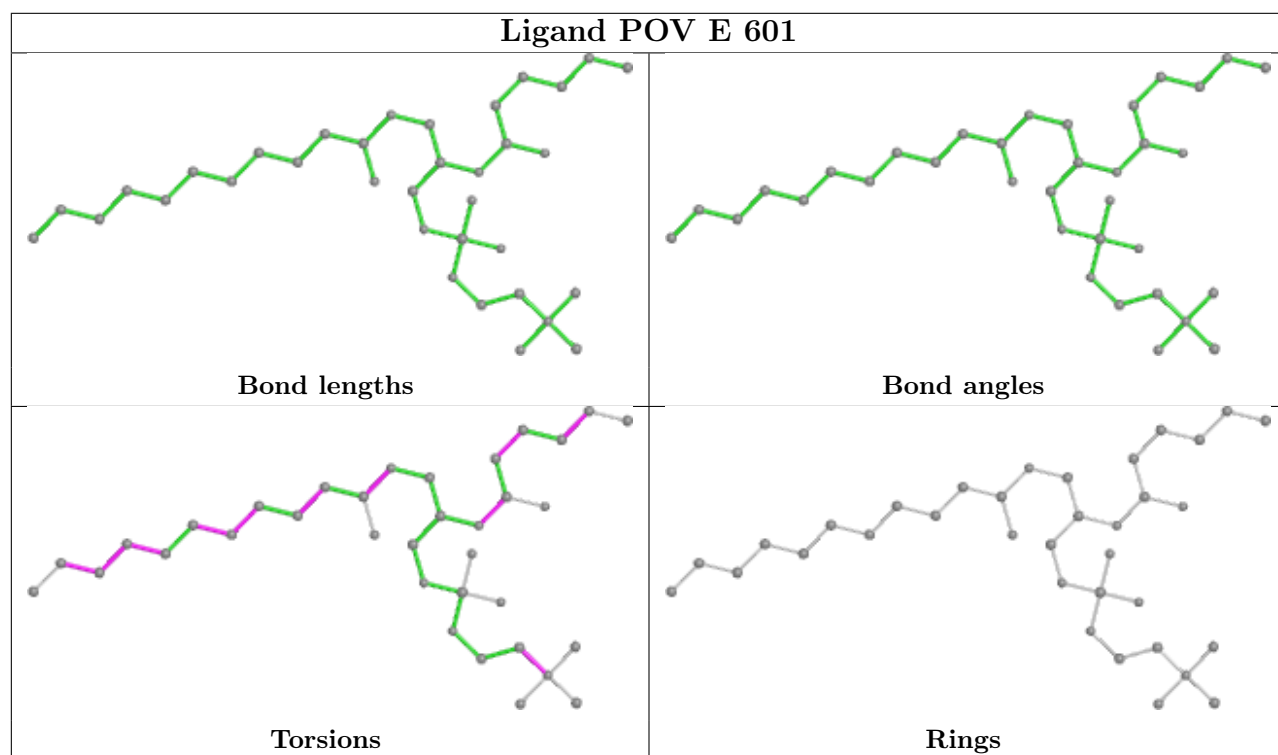
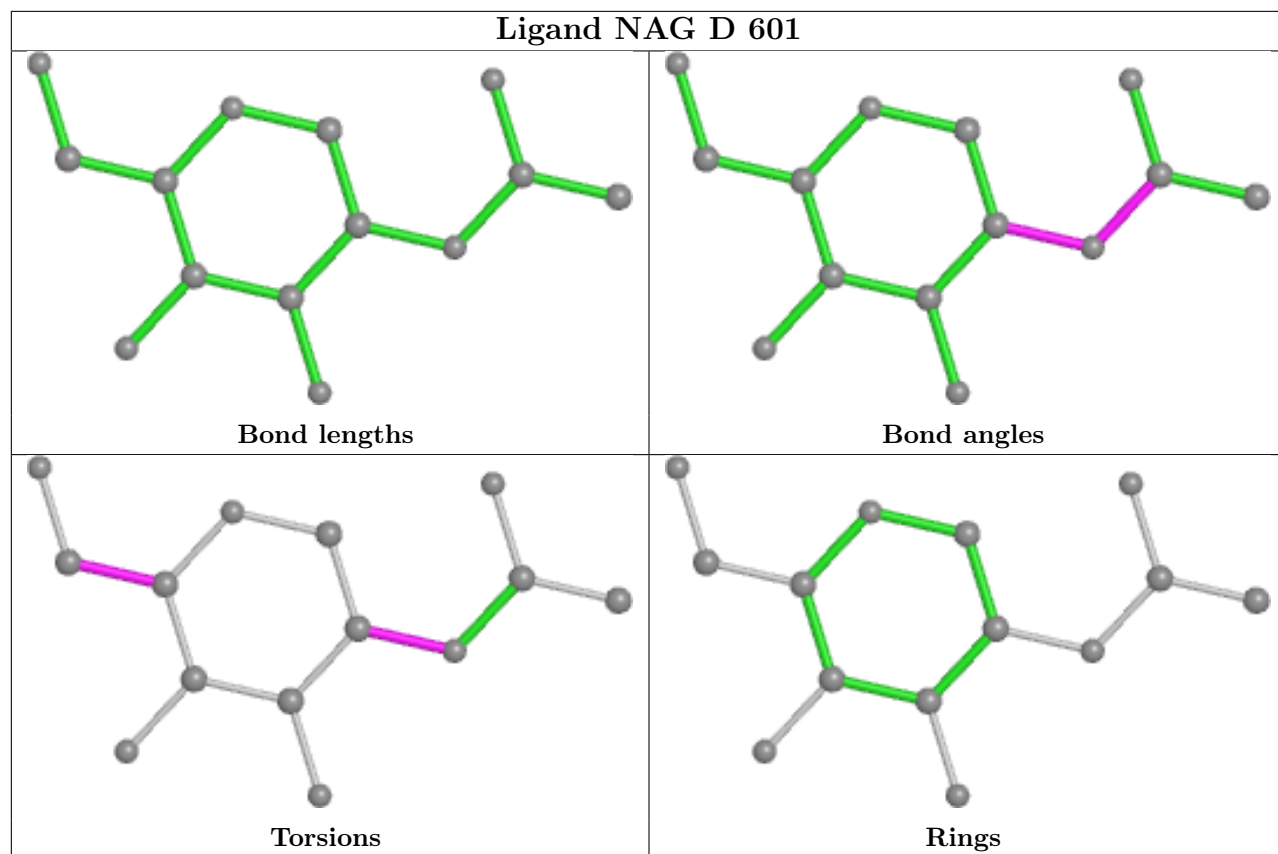
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	502	POV	10	0
10	E	603	POV	5	0
11	B	502	NAG	3	0
10	C	501	POV	2	0
11	D	601	NAG	1	0
10	E	601	POV	5	0
10	E	602	POV	1	0
10	C	502	POV	3	0
10	B	501	POV	3	0
10	A	501	POV	6	0

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

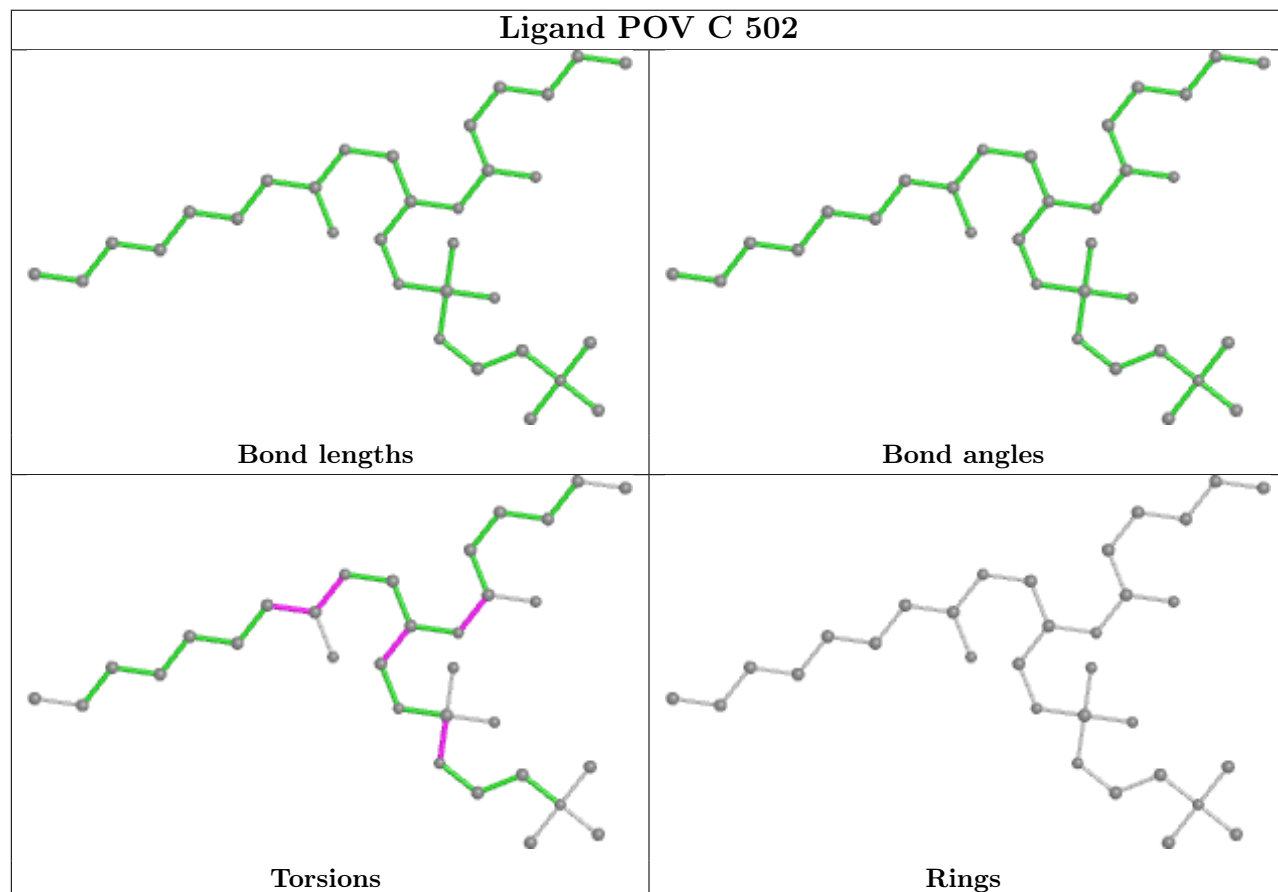
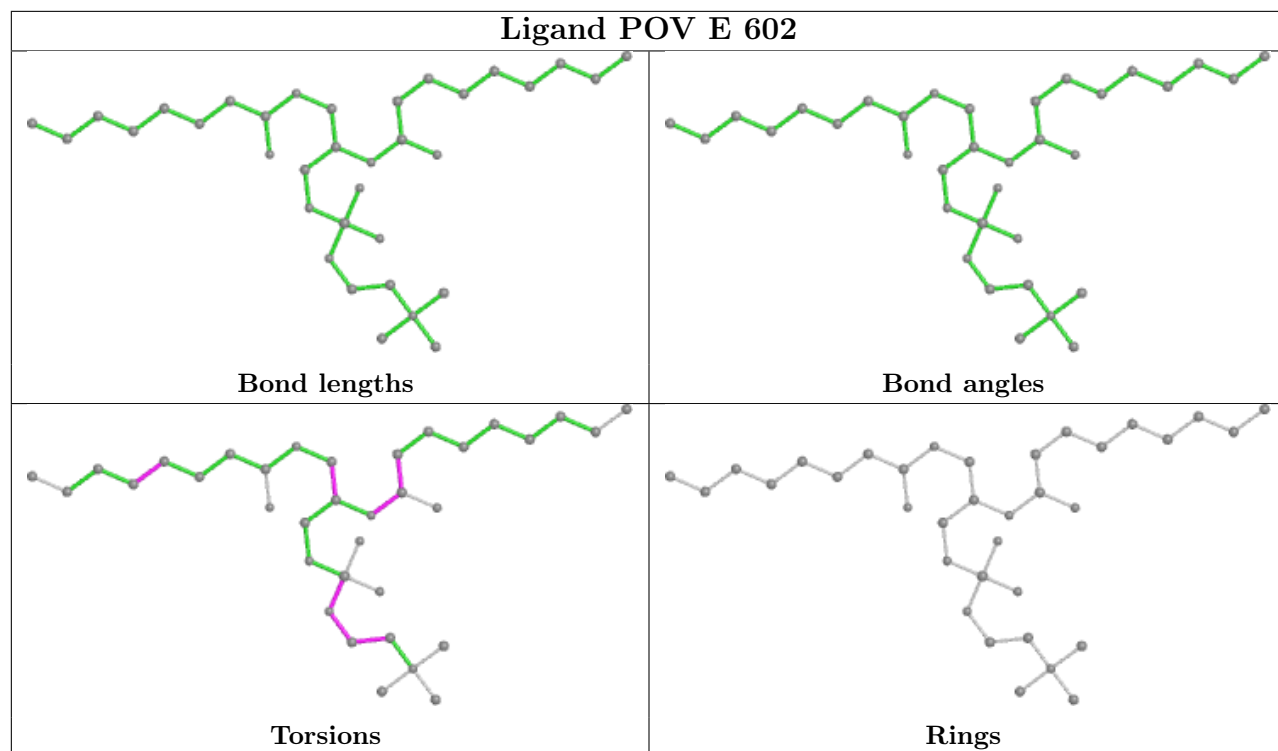
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

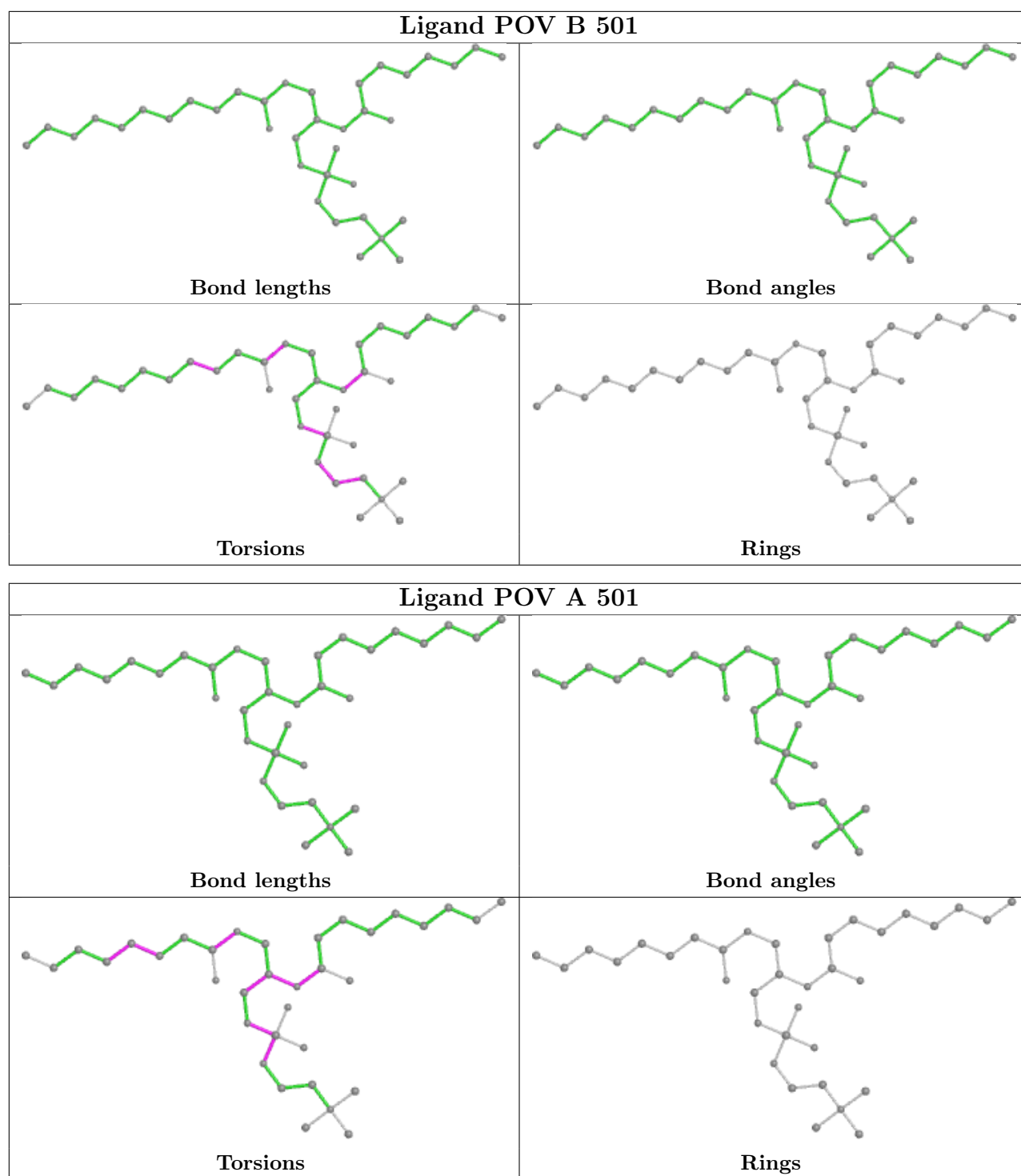












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

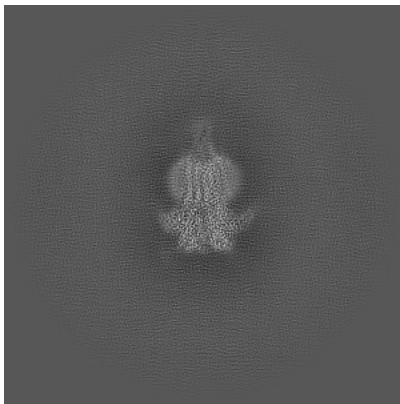
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43924. These allow visual inspection of the internal detail of the map and identification of artifacts.

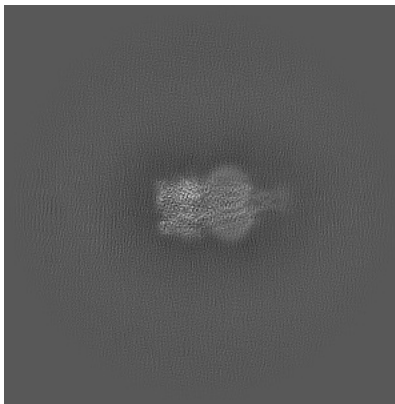
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

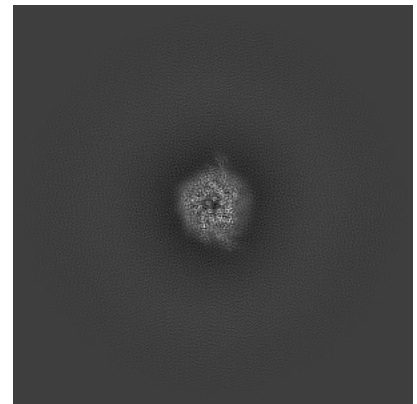
#### 6.1.1 Primary map



X

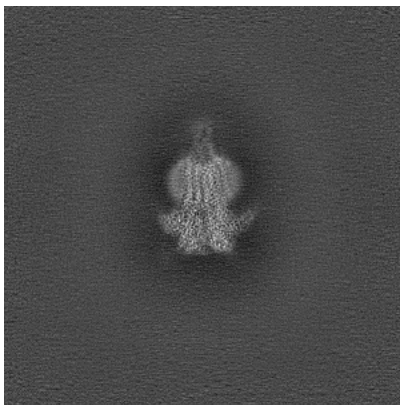


Y

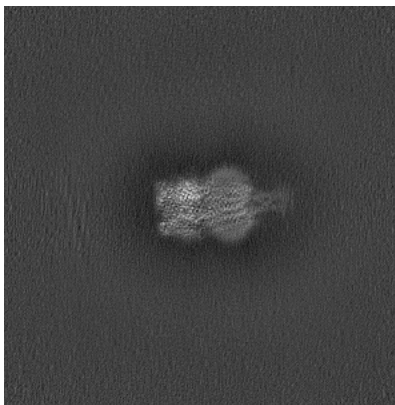


Z

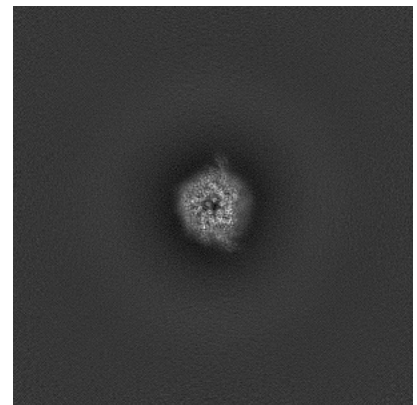
#### 6.1.2 Raw map



X



Y

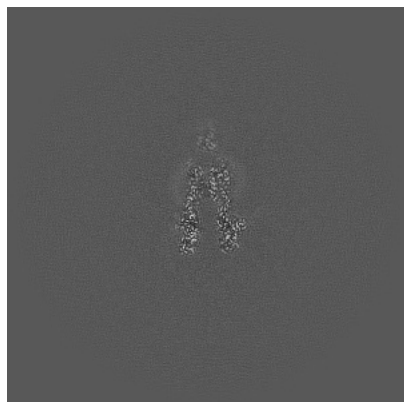


Z

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

## 6.2 Central slices [i](#)

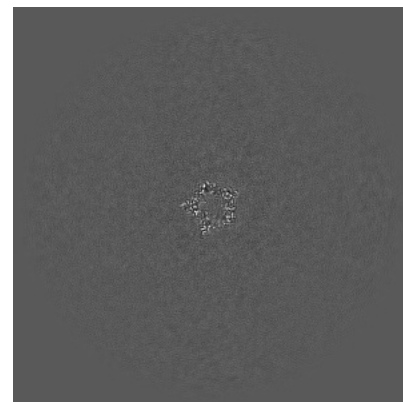
### 6.2.1 Primary map



X Index: 256



Y Index: 256

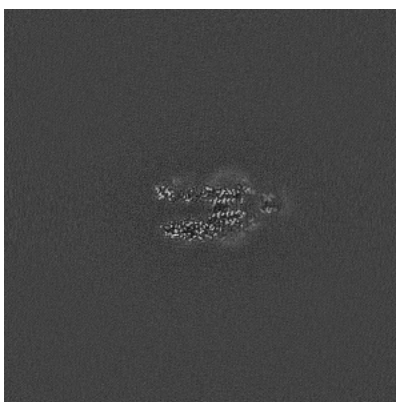


Z Index: 256

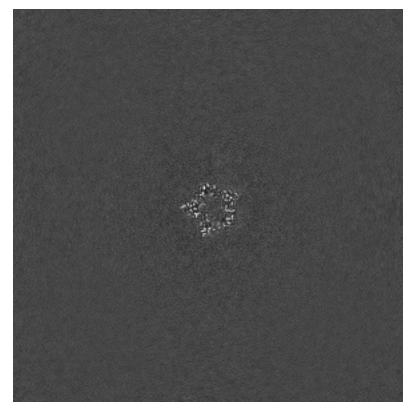
### 6.2.2 Raw map



X Index: 256



Y Index: 256

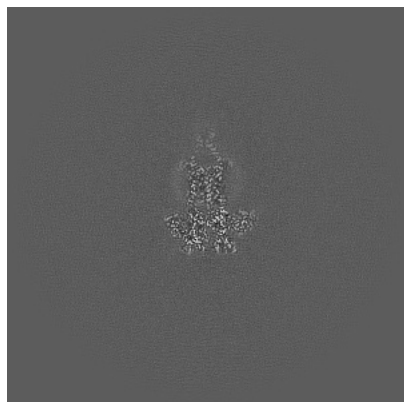


Z Index: 256

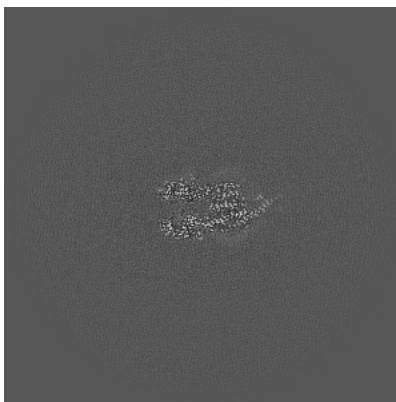
The images above show central slices of the map in three orthogonal directions.

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

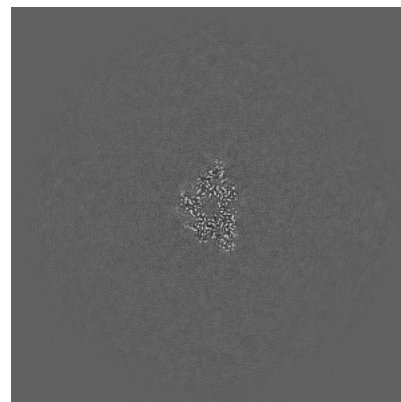
### 6.3.1 Primary map



X Index: 267

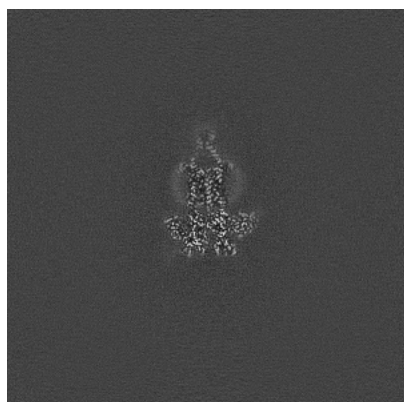


Y Index: 265



Z Index: 233

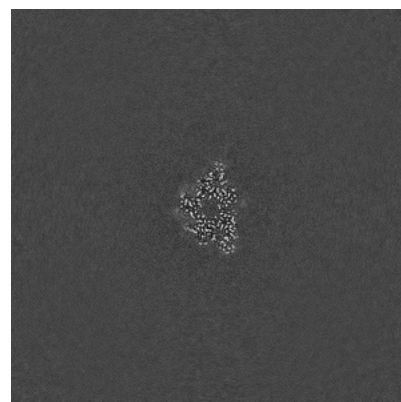
### 6.3.2 Raw map



X Index: 267



Y Index: 265

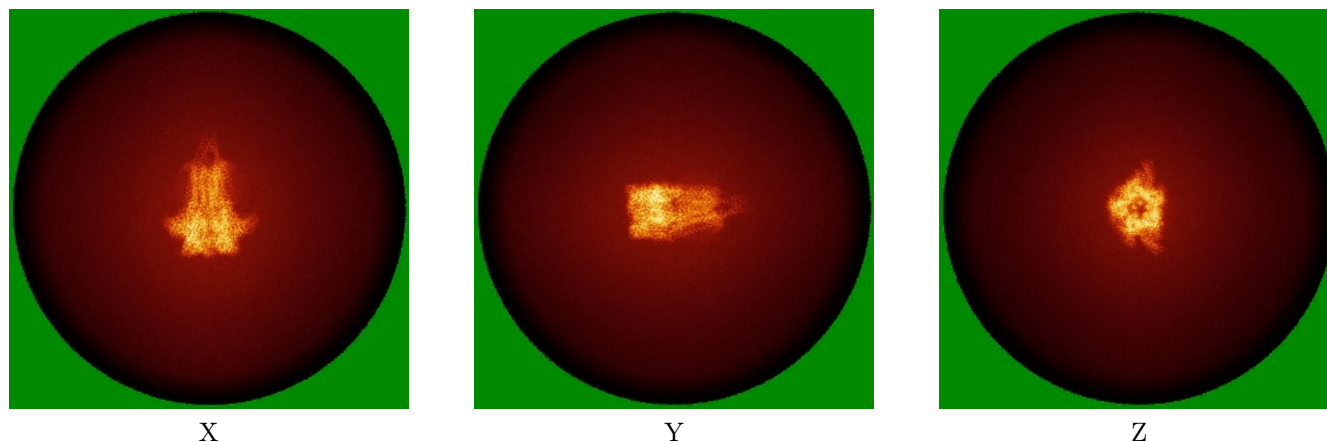


Z Index: 233

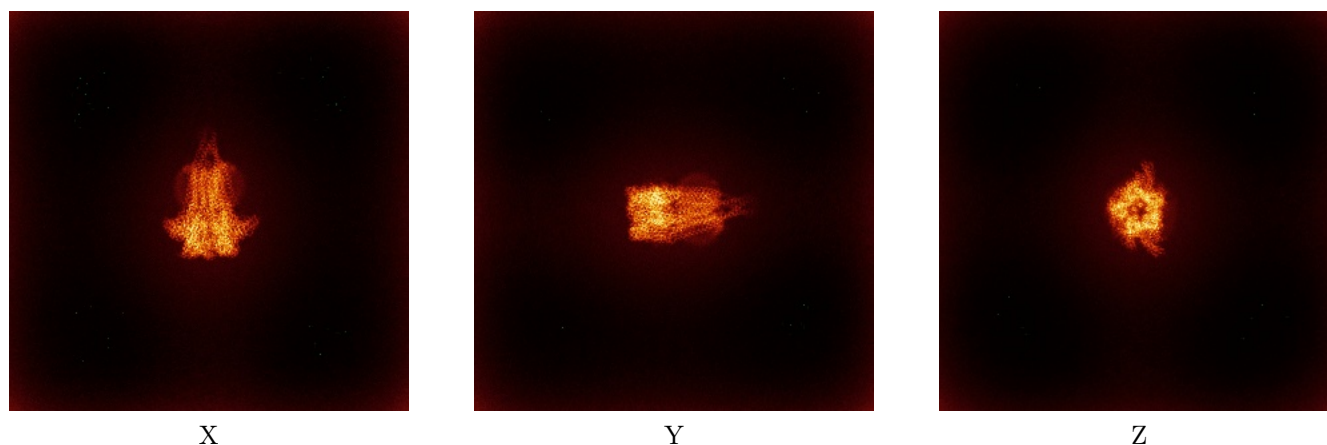
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



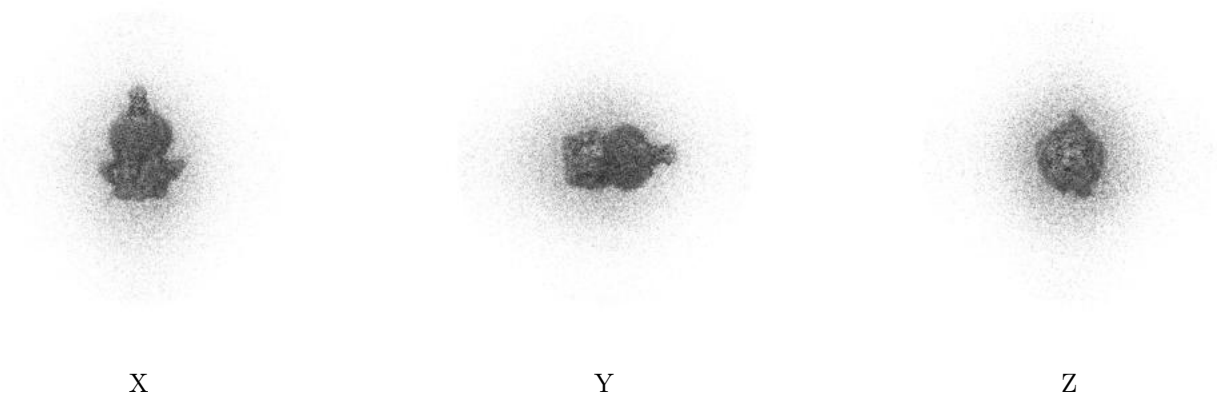
### 6.4.2 Raw map



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.

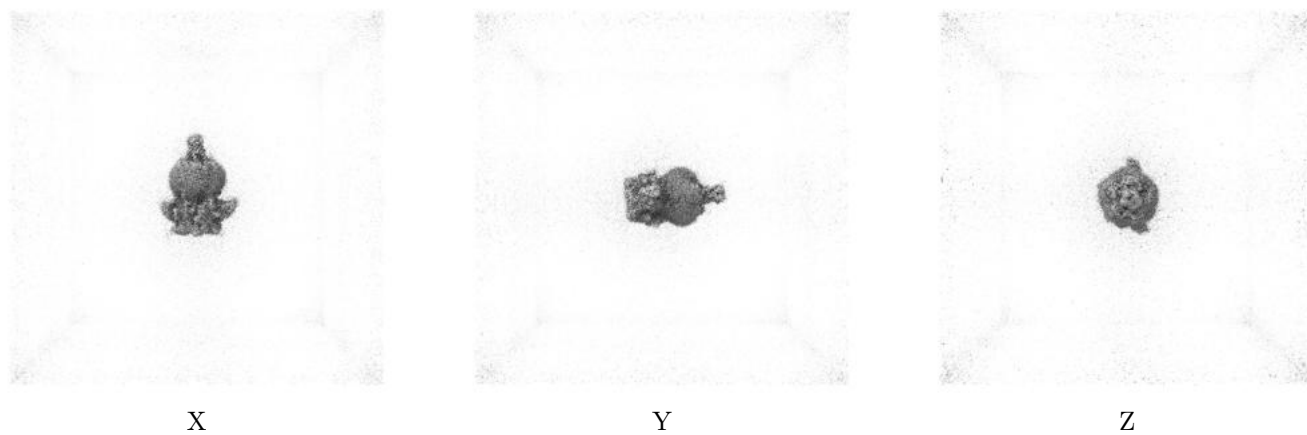
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

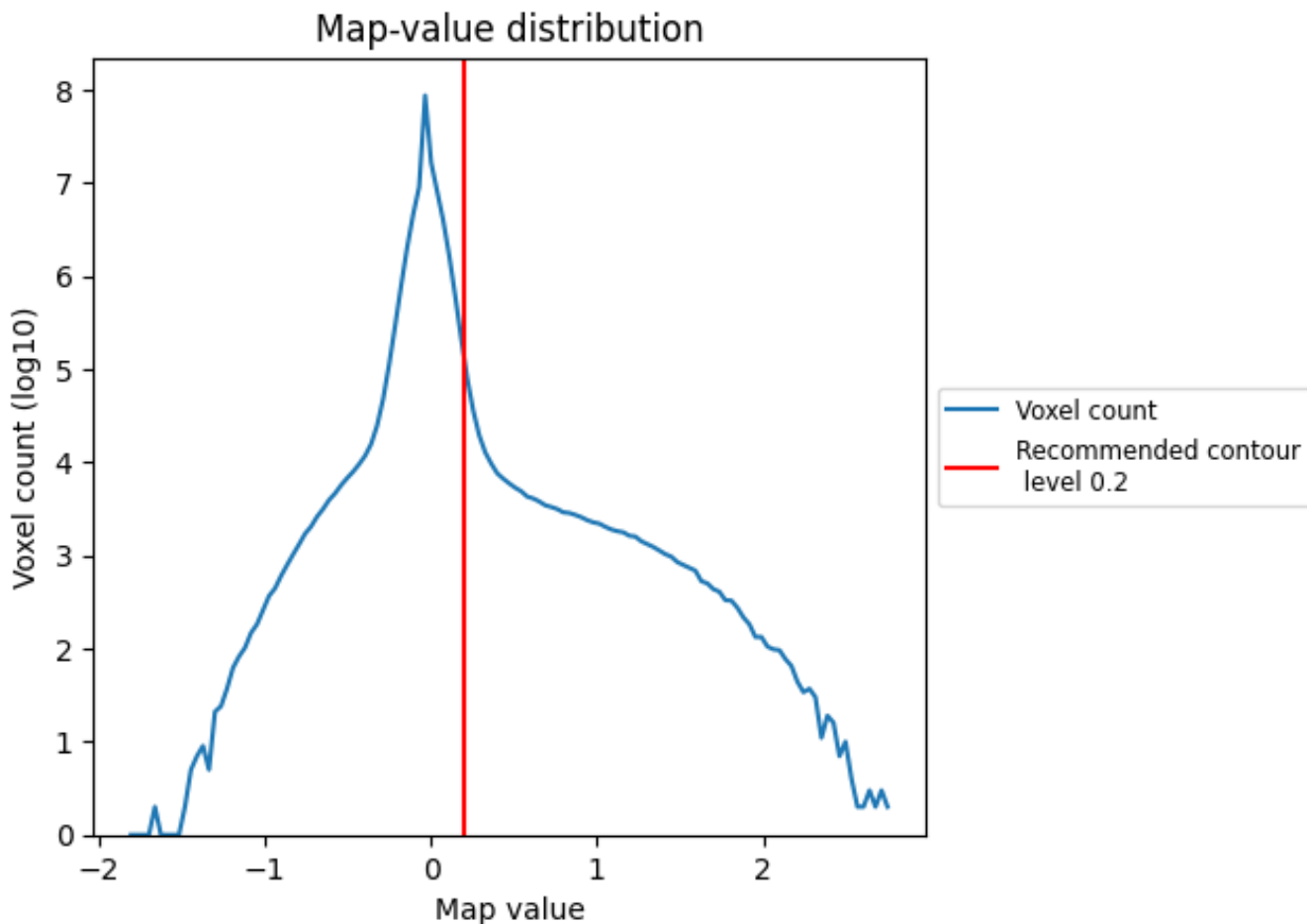
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

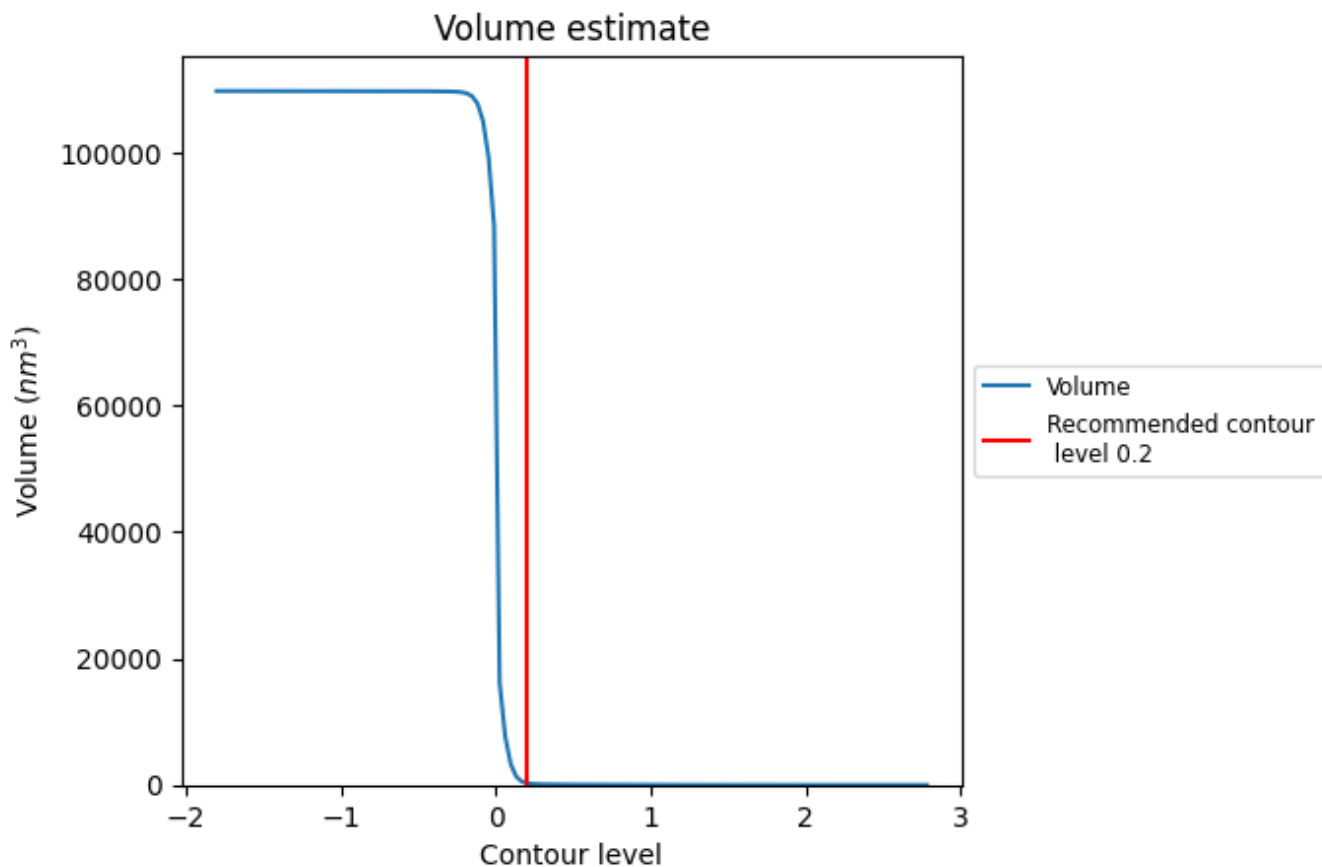
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

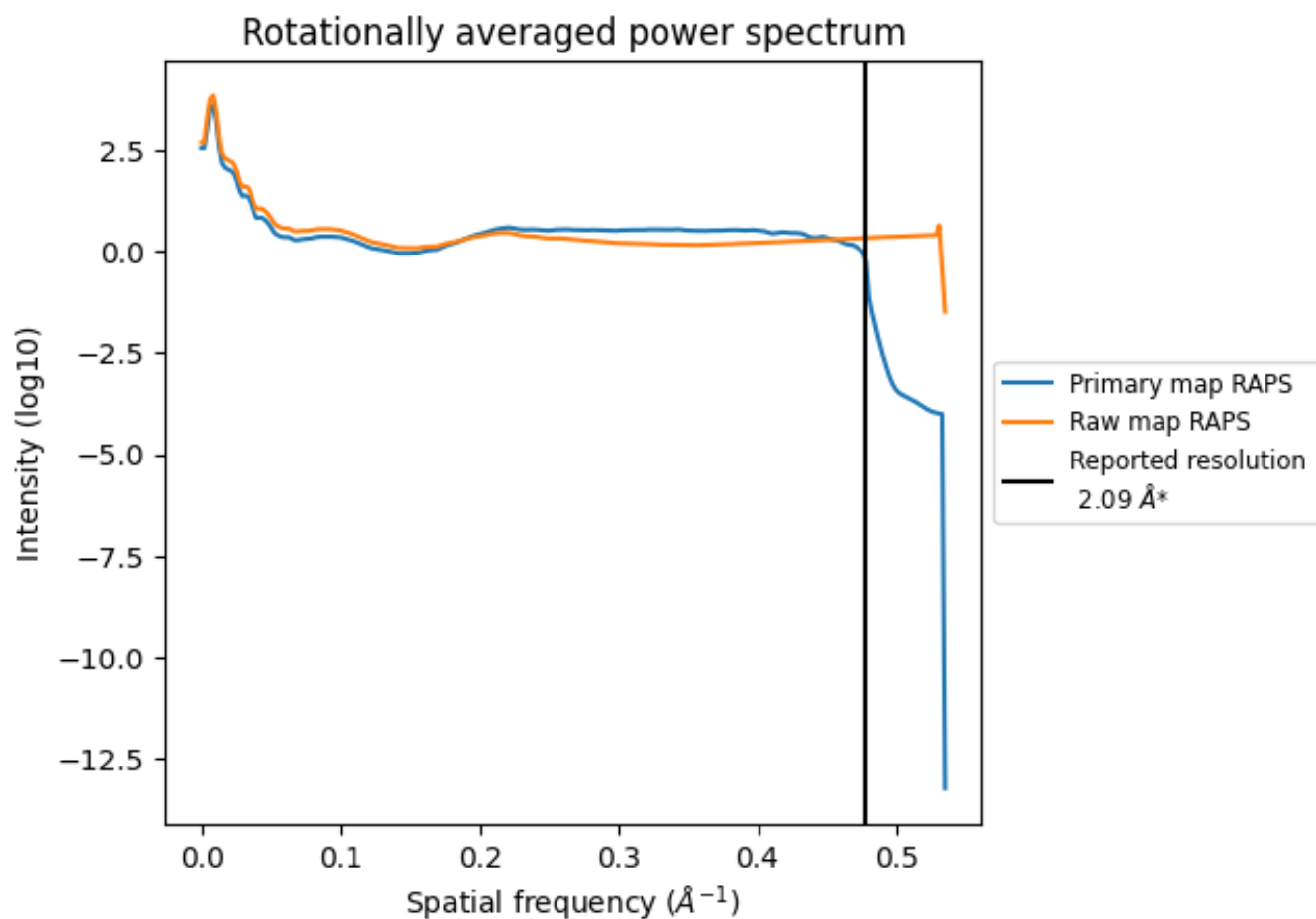
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 293  $\text{nm}^3$ ; this corresponds to an approximate mass of 264 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](#)

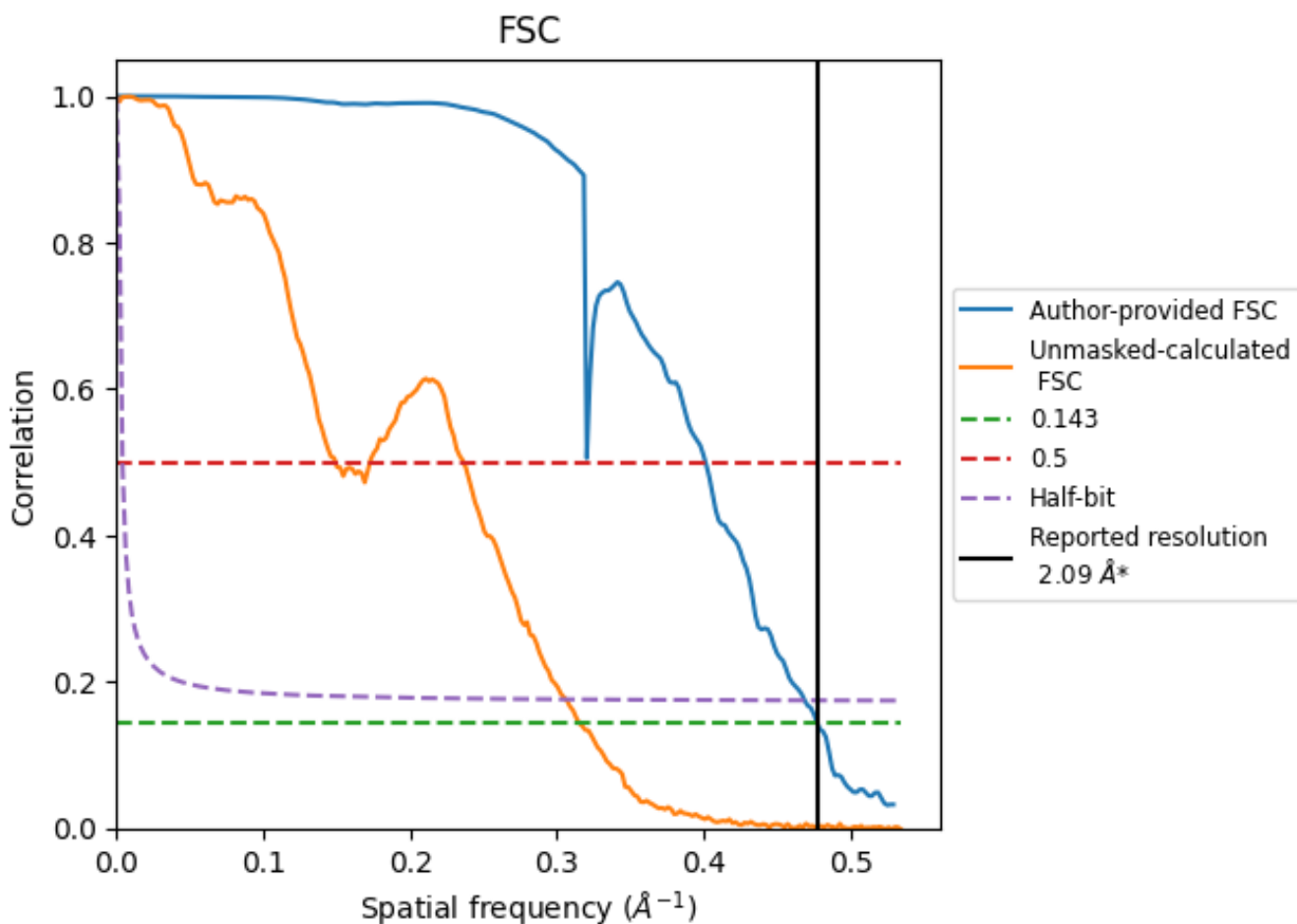


\*Reported resolution corresponds to spatial frequency of 0.478 Å<sup>-1</sup>

## 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 0.478 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

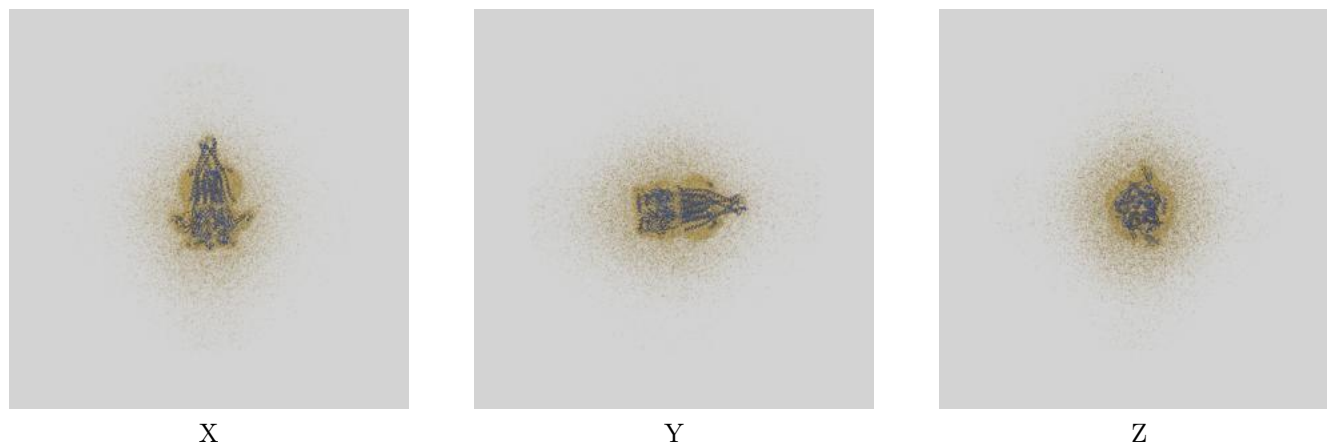
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.09	-	-
Author-provided FSC curve	2.09	2.49	2.13
Unmasked-calculated*	3.17	6.70	3.27

\*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 3.17 differs from the reported value 2.09 by more than 10 %

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

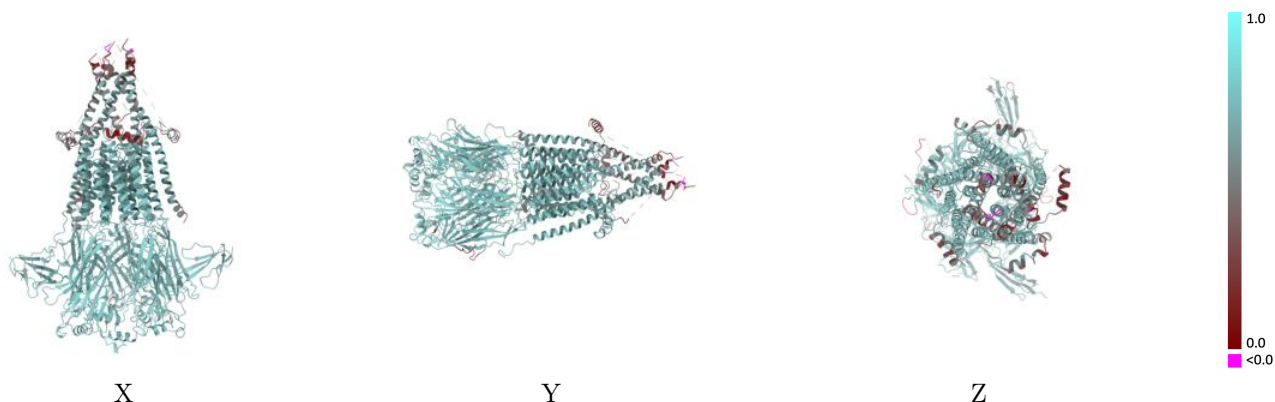
This section contains information regarding the fit between EMDB map EMD-43924 and PDB model 9AVV. Per-residue inclusion information can be found in section 3 on page 8.

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



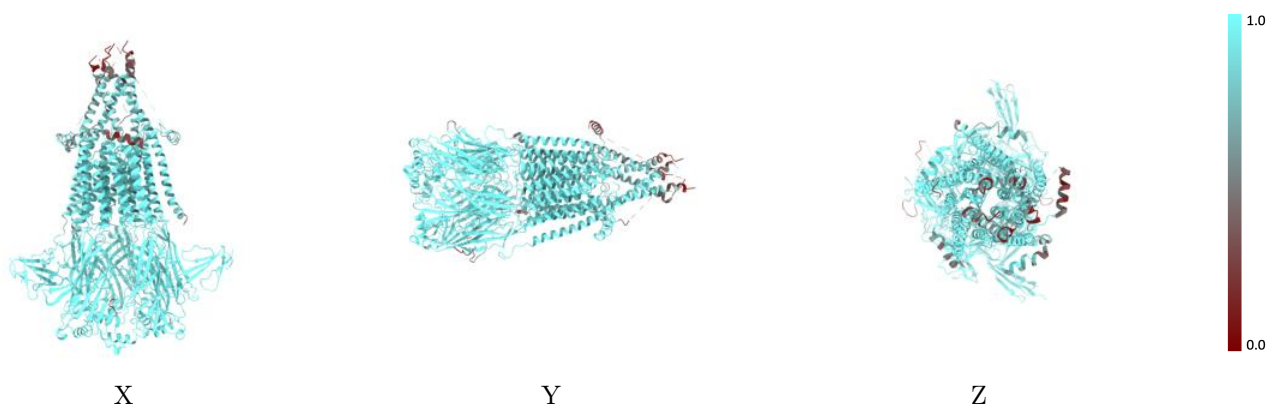
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



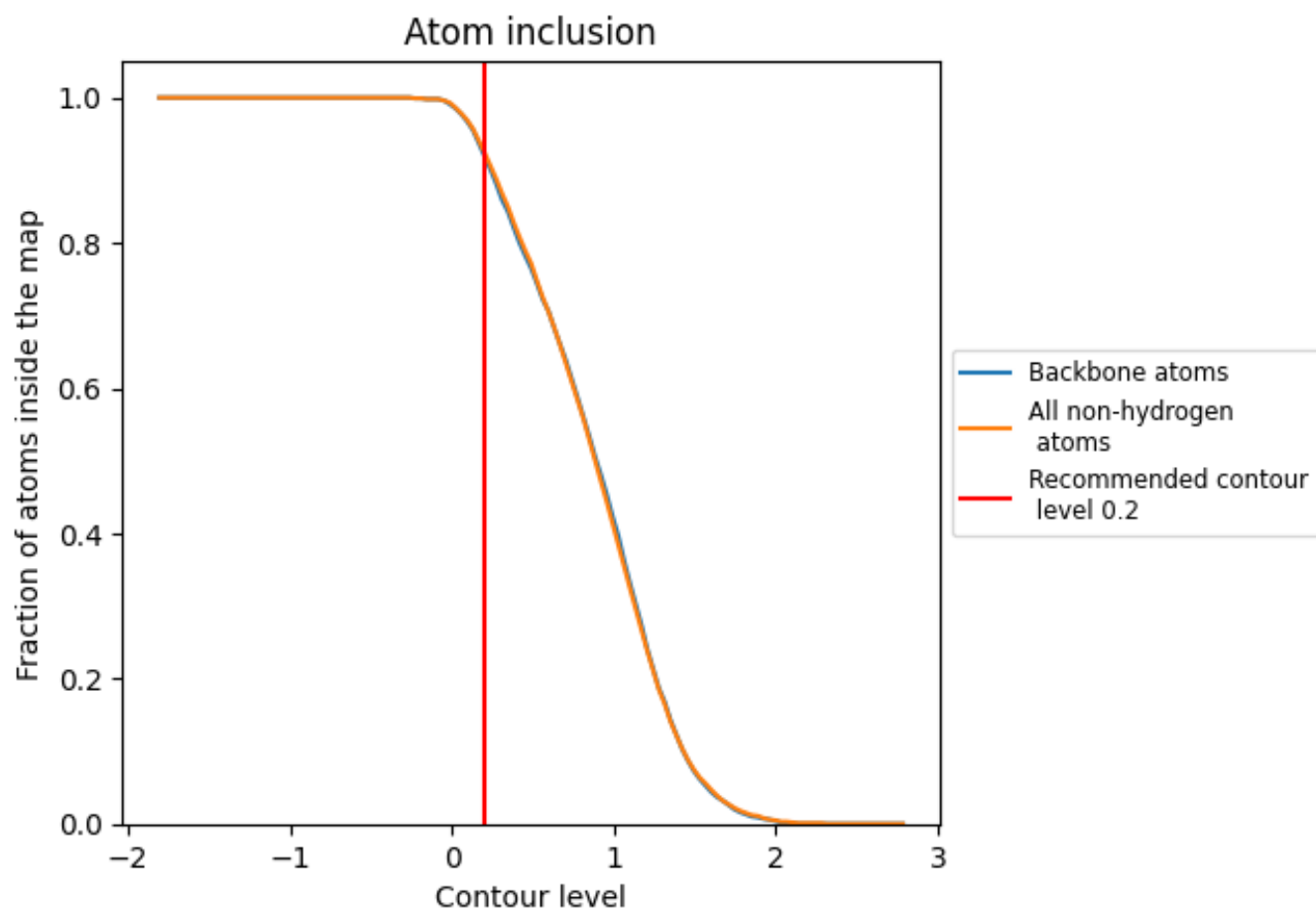
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)





























At the recommended contour level, 92% of all backbone atoms, 93% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.6580
A	 0.9300	 0.6640
B	 0.9170	 0.6530
C	 0.9250	 0.6580
D	 0.9400	 0.6670
E	 0.9300	 0.6640
F	 0.9530	 0.6380
G	 0.9770	 0.6690
J	 0.9740	 0.6460
K	 0.6000	 0.2980
L	 0.9450	 0.6250
M	 0.7360	 0.4940
N	 0.6000	 0.3590

