



Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 08:18 PM EST

PDB ID : 9AWK
EMDB ID : EMD-43926
Title : Bovine fetal muscle nAChR resting state
Authors : Li, H.; Hibbs, R.E.
Deposited on : 2024-03-05
Resolution : 2.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

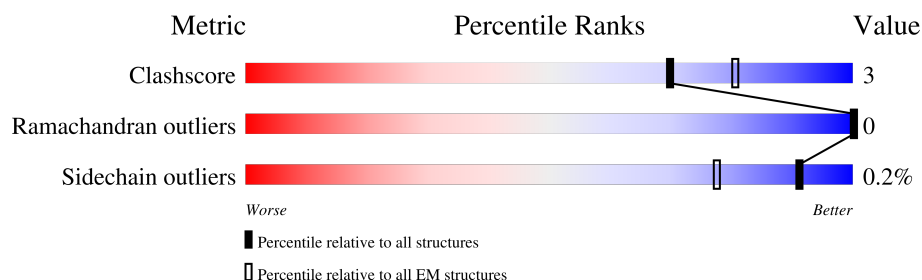
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.14 Å.

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




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

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

Mol	Chain	Length	Quality of chain
1	A	437	
1	C	437	
2	E	481	
3	D	495	
4	F	62	
4	G	62	
5	B	497	
6	I	10	

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Mol	Chain	Length	Quality of chain
7	J	4	 100%
7	M	4	 100%
8	K	11	 73%18%9%
9	L	6	 67%33%
10	N	2	 100%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 36310 atoms, of which 18199 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
1	A	402	Total	C	H	N	O	S	0	0
			6508	2125	3267	515	582	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
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
3	D	429	Total	C	H	N	O	S	0	0
			6949	2259	3483	562	629	16		

- Molecule 4 is a protein called Toxin.

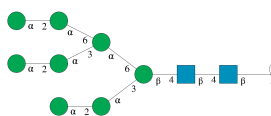
Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	61	Total	C	H	N	O	S	0	0
			942	287	466	91	89	9		
4	G	62	Total	C	H	N	O	S	0	0
			951	289	471	92	90	9		

- Molecule 5 is a protein called Acetylcholine receptor subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	396	Total	C	H	N	O	S	0	0
			6325	2051	3166	531	560	17		

- 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.



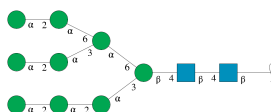
Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	10	Total	C	H	N	O	0	0
			220	64	104	2	50		

- 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.



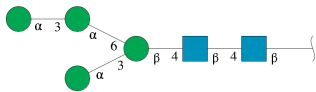
Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	4	Total	C	H	N	O	0	0
			96	28	46	2	20		
7	M	4	Total	C	H	N	O	0	0
			96	28	46	2	20		

- 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
8	K	11	Total	C	H	N	O	0	0
			241	70	114	2	55		

- 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.



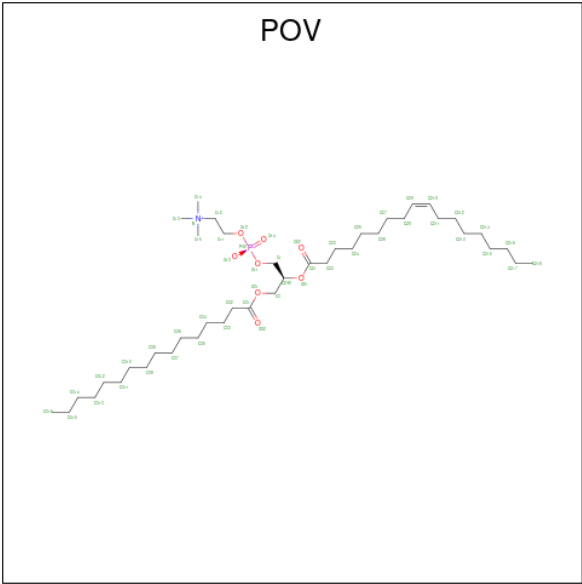
Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	6	Total	C	H	N	O	0	0
			137	40	65	2	30		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	2	Total	C	H	N	O	0	0
			54	16	26	2	10		

- Molecule 11 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



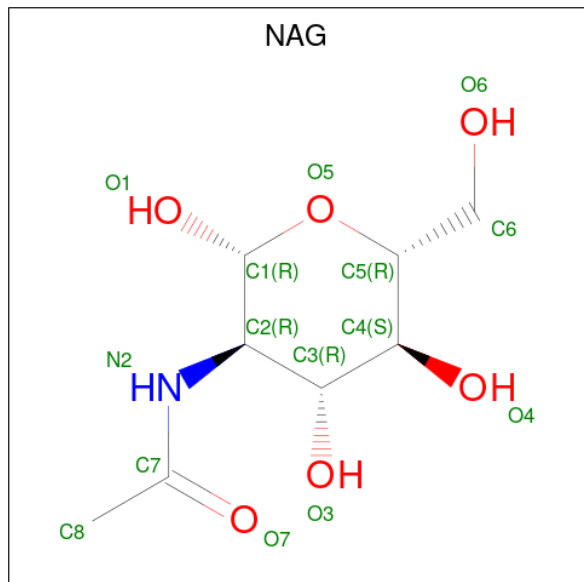
Mol	Chain	Residues	Atoms						AltConf
11	A	1	Total	C	H	N	O	P	0
			85	27	48	1	8	1	
11	E	1	Total	C	H	N	O	P	0
			79	25	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
11	E	1	Total	C	H	N	O	P
			79	25	44	1	8	1
11	E	1	Total	C	H	N	O	P
			79	25	44	1	8	1
11	C	1	Total	C	H	N	O	P
			85	27	48	1	8	1
11	C	1	Total	C	H	N	O	P
			70	22	38	1	8	1
11	D	1	Total	C	H	N	O	P
			116	37	69	1	8	1

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

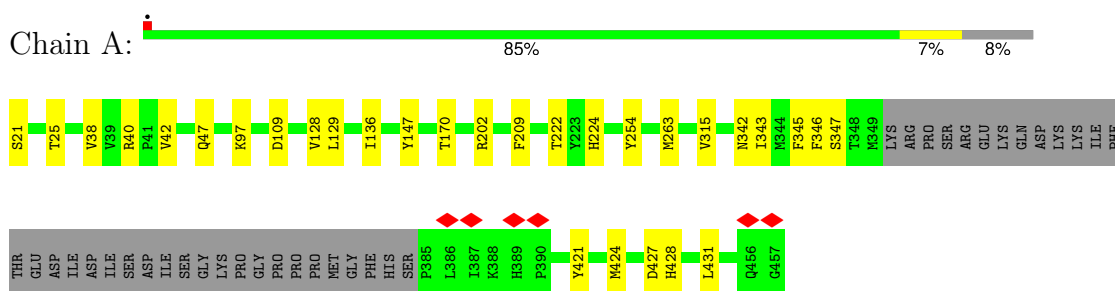


Mol	Chain	Residues	Atoms					AltConf
12	D	1	Total	C	H	N	O	
			27	8	13	1	5	0

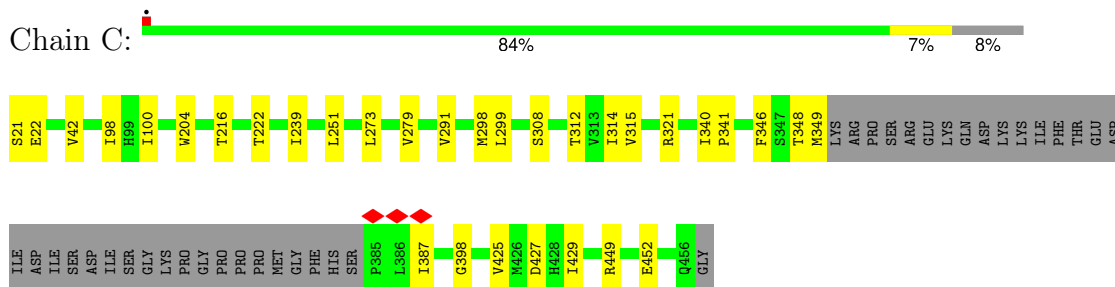
3 Residue-property plots [i](#)

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.

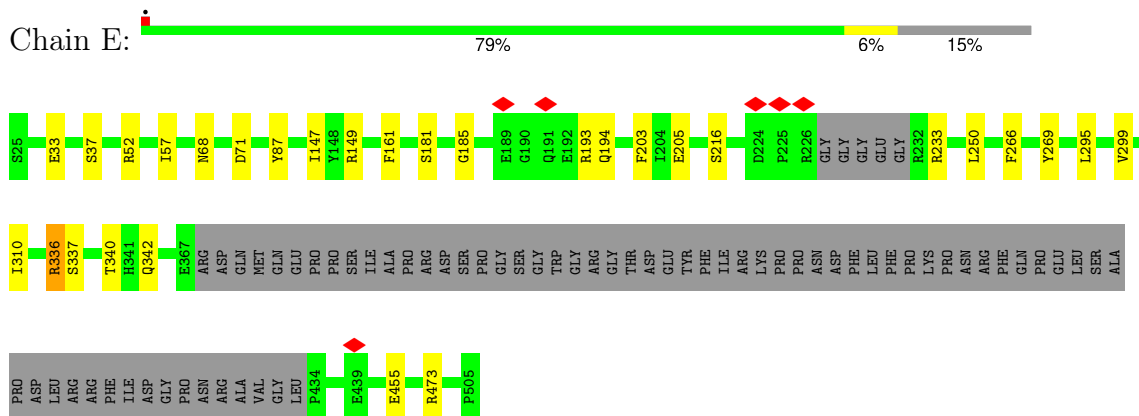
- Molecule 1: Acetylcholine receptor subunit alpha



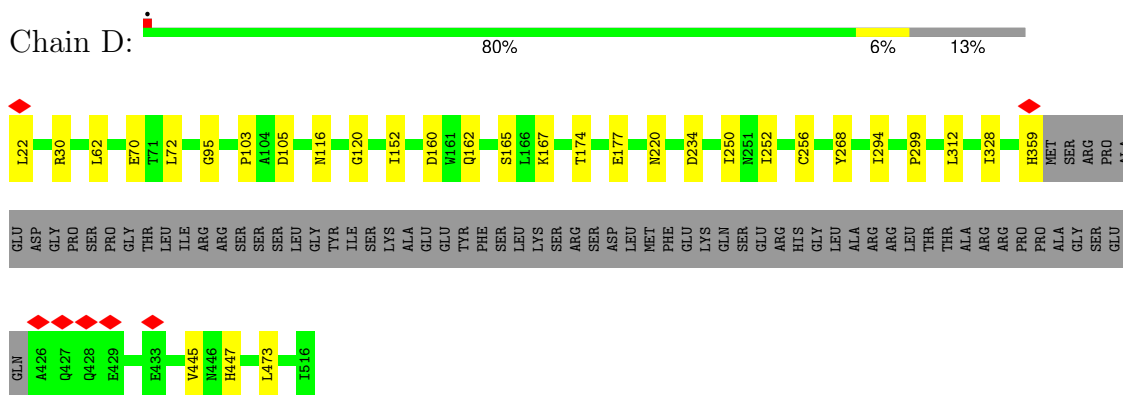
- Molecule 1: Acetylcholine receptor subunit alpha



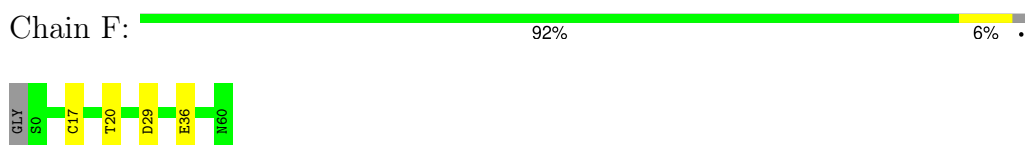
- Molecule 2: Acetylcholine receptor subunit beta



- Molecule 3: Acetylcholine receptor subunit delta



- Molecule 4: Toxin

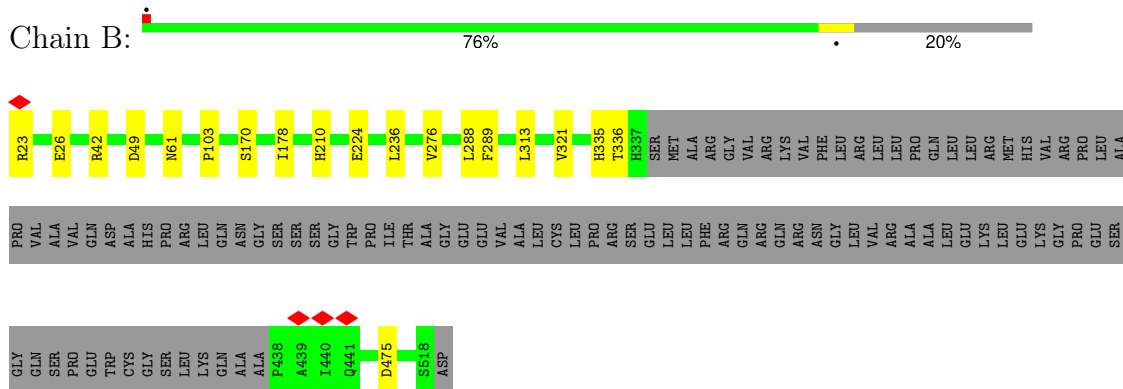


- Molecule 4: Toxin

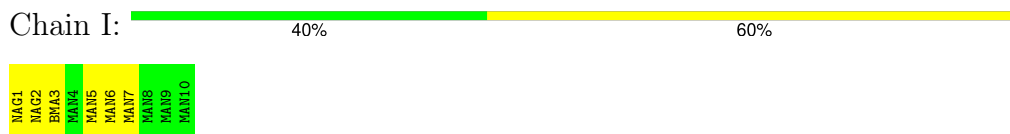


There are no outlier residues recorded for this chain.

- Molecule 5: Acetylcholine receptor subunit gamma



- 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



- 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

Chain J:  100%

MAG1
MAG2
BMA3
MAN4

- 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

Chain M:  100%

MAG1
MAG2
BMA3
MAN4

- 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

Chain K:  73% 18% 9%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10
MAN11

- 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

Chain L:  67% 33%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168720	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	1.083	Depositor
Minimum map value	-0.491	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.07	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

5.1 Standard geometry

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	0.30	0/3328	0.57	0/4540
1	C	0.31	0/3324	0.58	0/4535
2	E	0.28	0/3427	0.58	0/4674
3	D	0.30	0/3558	0.58	0/4854
4	F	0.32	0/485	0.69	1/651 (0.2%)
4	G	0.30	0/489	0.73	0/656
5	B	0.29	0/3243	0.59	0/4433
All	All	0.30	0/17854	0.59	1/24343 (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
2	E	0	3
3	D	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	29	ASP	CB-CG-OD1	5.27	123.05	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	30	ARG	Sidechain
2	E	149	ARG	Sidechain
2	E	233	ARG	Sidechain
2	E	336	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3241	3267	3260	31	0
1	C	3237	3264	3257	28	0
2	E	3337	3333	3327	23	0
3	D	3466	3483	3476	23	0
4	F	476	466	468	2	0
4	G	480	471	471	0	0
5	B	3159	3166	3157	16	0
6	I	116	104	97	5	0
7	J	50	46	43	0	0
7	M	50	46	43	0	0
8	K	127	114	106	6	0
9	L	72	65	61	2	0
10	N	28	26	25	0	0
11	A	37	48	48	11	0
11	C	69	86	86	8	0
11	D	47	69	69	6	0
11	E	105	132	132	14	0
12	D	14	13	13	1	0
All	All	18111	18199	18139	124	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 (124) 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)
2:E:161:PHE:CZ	11:E:601:POV:H23A	1.99	0.95
1:A:315:VAL:HG11	1:A:427:ASP:OD1	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:602:POV:O13	11:E:602:POV:C33	2.27	0.82
1:C:315:VAL:HG11	1:C:427:ASP:OD1	1.81	0.79
3:D:70:GLU:OE2	3:D:299:PRO:HG3	1.83	0.79
11:E:602:POV:O13	11:E:602:POV:H33	1.83	0.79
1:C:239:ILE:HG21	11:C:501:POV:H27A	1.67	0.76
1:C:204:TRP:HB2	8:K:2:NAG:H82	1.68	0.74
2:E:337:SER:HB3	2:E:340:THR:OG1	1.92	0.70
1:C:449:ARG:NH1	1:C:452:GLU:OE1	2.23	0.69
5:B:335:HIS:CD2	5:B:336:THR:HG23	2.27	0.69
2:E:269:TYR:CE1	11:E:603:POV:H1	2.30	0.67
3:D:174:THR:OG1	3:D:177:GLU:OE2	2.12	0.65
1:A:42:VAL:O	5:B:23:ARG:N	2.30	0.64
1:A:254:TYR:CE1	11:A:501:POV:H23A	2.31	0.64
2:E:473:ARG:HH22	11:E:603:POV:H15B	1.64	0.62
1:C:216:THR:HG23	1:C:216:THR:O	1.99	0.61
1:A:209:PHE:HE2	6:I:7:MAN:HO3	1.48	0.61
3:D:268:TYR:CD1	11:D:601:POV:H25A	2.35	0.61
8:K:1:NAG:H62	8:K:2:NAG:C7	2.31	0.61
2:E:68:ASN:ND2	2:E:71:ASP:OD2	2.35	0.60
1:A:209:PHE:HE2	6:I:7:MAN:O3	1.86	0.59
1:C:204:TRP:CZ3	8:K:3:BMA:H5	2.37	0.59
1:A:128:VAL:HG13	1:A:136:ILE:HG23	1.84	0.59
3:D:116:ASN:ND2	3:D:165:SER:O	2.35	0.58
3:D:70:GLU:OE1	3:D:152:ILE:HG12	2.05	0.57
1:A:428:HIS:HB3	11:A:501:POV:H13B	1.88	0.56
2:E:57:ILE:O	2:E:185:GLY:N	2.38	0.56
5:B:61:ASN:OD1	5:B:61:ASN:O	2.23	0.56
1:A:346:PHE:HZ	1:A:428:HIS:HD1	1.54	0.56
2:E:203:PHE:HE2	2:E:205:GLU:OE1	1.88	0.56
3:D:220:ASN:HB2	3:D:234:ASP:OD1	2.05	0.56
1:C:314:ILE:HG12	11:D:601:POV:H24A	1.88	0.56
2:E:161:PHE:CE2	11:E:601:POV:H25A	2.41	0.55
1:C:348:THR:O	1:C:349:MET:C	2.44	0.55
11:E:602:POV:O13	11:E:602:POV:H33A	2.03	0.55
11:A:501:POV:H33	11:A:501:POV:H3A	1.89	0.55
1:A:421:TYR:CD1	1:A:424:MET:HE1	2.42	0.54
1:A:254:TYR:CD2	11:A:501:POV:H27A	2.42	0.54
3:D:268:TYR:HE2	11:D:601:POV:H311	1.72	0.54
2:E:455:GLU:OE2	3:D:447:HIS:ND1	2.32	0.53
1:C:251:LEU:HD21	5:B:321:VAL:HG22	1.89	0.53
3:D:359:HIS:HB2	11:D:601:POV:H13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG13	5:B:103:PRO:HD3	1.91	0.52
1:A:315:VAL:CG1	1:A:427:ASP:OD1	2.54	0.51
3:D:167:LYS:HE2	3:D:234:ASP:OD2	2.11	0.51
1:C:321:ARG:NH2	11:D:601:POV:O22	2.44	0.51
3:D:95:GLY:HA2	12:D:602:NAG:H83	1.93	0.51
3:D:160:ASP:OD2	3:D:162:GLN:NE2	2.43	0.51
5:B:42:ARG:NH2	5:B:49:ASP:O	2.44	0.50
1:C:42:VAL:O	3:D:22:LEU:N	2.45	0.50
5:B:224:GLU:OE1	5:B:224:GLU:N	2.35	0.50
1:C:340:ILE:HG21	1:C:429:ILE:HD11	1.94	0.49
1:A:21:SER:N	2:E:87:TYR:HH	2.10	0.49
1:A:343:ILE:HG22	1:A:345:PHE:H	1.76	0.49
1:A:40:ARG:NH2	1:A:47:GLN:O	2.46	0.49
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.78	0.49
1:A:421:TYR:CD1	1:A:424:MET:CE	2.96	0.49
1:A:21:SER:O	1:A:25:THR:OG1	2.26	0.49
3:D:62:LEU:HD11	3:D:72:LEU:HD11	1.95	0.49
2:E:147:ILE:HD13	3:D:120:GLY:HA2	1.94	0.48
1:C:299:LEU:HG	11:C:502:POV:H36	1.96	0.48
6:I:1:NAG:H62	6:I:2:NAG:C7	2.43	0.48
1:C:308:SER:O	1:C:312:THR:OG1	2.27	0.48
11:C:502:POV:H22A	3:D:250:ILE:HD11	1.96	0.48
1:A:343:ILE:HB	11:A:501:POV:H14B	1.95	0.48
3:D:252:ILE:HG21	3:D:294:ILE:HD11	1.95	0.48
2:E:194:GLN:O	2:E:216:SER:N	2.46	0.47
2:E:266:PHE:CE2	11:E:603:POV:H3	2.49	0.47
3:D:268:TYR:CG	11:D:601:POV:H25A	2.50	0.47
11:A:501:POV:H3	2:E:336:ARG:NH1	2.30	0.46
2:E:161:PHE:HZ	11:E:601:POV:H23A	1.68	0.46
11:E:603:POV:H23	3:D:328:ILE:HD11	1.97	0.46
1:A:431:LEU:HD21	11:A:501:POV:H25	1.98	0.46
2:E:269:TYR:CD1	11:E:603:POV:H1	2.51	0.46
1:C:291:VAL:HG21	11:C:502:POV:H3A	1.98	0.46
11:C:502:POV:H32	11:C:502:POV:H35A	1.39	0.45
1:C:216:THR:O	1:C:216:THR:CG2	2.64	0.45
5:B:288:LEU:HD11	5:B:313:LEU:HD11	1.98	0.45
1:C:204:TRP:CD1	8:K:2:NAG:H2	2.51	0.45
1:C:387:ILE:HG22	1:C:387:ILE:O	2.17	0.45
1:C:98:ILE:HD12	1:C:100:ILE:HD11	1.99	0.45
11:E:602:POV:H32A	11:E:602:POV:H3A	1.65	0.45
3:D:268:TYR:OH	3:D:473:LEU:HD21	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:CD1	5:B:61:ASN:ND2	2.84	0.45
1:A:222:THR:HB	6:I:2:NAG:H81	1.99	0.45
1:C:398:GLY:HA3	3:D:445:VAL:HG21	1.99	0.45
1:A:202:ARG:HB3	1:A:224:HIS:NE2	2.32	0.44
2:E:33:GLU:O	2:E:37:SER:OG	2.33	0.44
4:F:36:GLU:HG3	6:I:5:MAN:O3	2.17	0.44
11:A:501:POV:H34A	11:A:501:POV:H38	2.00	0.44
1:C:346:PHE:HD1	5:B:336:THR:O	2.00	0.44
1:A:109:ASP:OD2	1:A:170:THR:OG1	2.24	0.44
4:F:20:THR:HG22	4:F:20:THR:O	2.18	0.44
1:C:341:PRO:HG3	1:C:425:VAL:HG21	1.98	0.44
1:C:21:SER:OG	1:C:22:GLU:N	2.50	0.43
11:C:501:POV:H39	11:C:501:POV:H36	1.76	0.43
2:E:52:ARG:HD3	2:E:181:SER:OG	2.18	0.43
1:C:222:THR:HB	8:K:2:NAG:H81	2.01	0.43
3:D:103:PRO:HB2	3:D:105:ASP:OD1	2.18	0.42
11:E:602:POV:H24	11:E:602:POV:H27	1.75	0.42
1:A:421:TYR:HD1	1:A:424:MET:HE1	1.81	0.42
1:C:204:TRP:CE3	8:K:3:BMA:H5	2.54	0.42
1:C:273:LEU:HD22	1:C:298:MET:CE	2.50	0.42
1:A:263:MET:HE2	5:B:276:VAL:HG21	2.01	0.42
5:B:335:HIS:NE2	5:B:336:THR:HG23	2.35	0.42
1:C:279:VAL:HG22	5:B:289:PHE:HA	2.01	0.42
1:C:291:VAL:CG2	11:C:502:POV:H1A	2.50	0.42
1:A:347:SER:HB3	2:E:340:THR:HA	2.01	0.42
11:A:501:POV:H3	2:E:336:ARG:NH2	2.35	0.42
2:E:250:LEU:HD22	11:E:601:POV:H2	2.02	0.42
1:A:97:LYS:HE3	1:A:129:LEU:HD11	2.02	0.41
11:C:502:POV:H13B	11:C:502:POV:H11	1.83	0.41
9:L:2:NAG:H83	9:L:2:NAG:H2	1.93	0.41
5:B:210:HIS:HB2	5:B:236:LEU:HD12	2.03	0.41
3:D:256:CYS:SG	3:D:312:LEU:HD21	2.61	0.41
2:E:295:LEU:O	2:E:299:VAL:HG23	2.21	0.41
1:A:40:ARG:NH1	5:B:26:GLU:OE2	2.53	0.41
1:A:342:ASN:HB3	11:A:501:POV:H14	2.03	0.41
9:L:1:NAG:H82	9:L:1:NAG:H2	1.97	0.41
2:E:299:VAL:HG21	2:E:310:ILE:HD11	2.03	0.40
5:B:170:SER:HB2	5:B:178:ILE:HD11	2.03	0.40
11:A:501:POV:H3A	11:A:501:POV:C33	2.43	0.40
1:A:128:VAL:CG1	1:A:136:ILE:HG23	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	398/437 (91%)	388 (98%)	10 (2%)	0	100	100
1	C	397/437 (91%)	386 (97%)	11 (3%)	0	100	100
2	E	404/481 (84%)	399 (99%)	5 (1%)	0	100	100
3	D	425/495 (86%)	421 (99%)	4 (1%)	0	100	100
4	F	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
4	G	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
5	B	392/497 (79%)	385 (98%)	7 (2%)	0	100	100
All	All	2135/2471 (86%)	2092 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	370/402 (92%)	370 (100%)	0	100	100
1	C	370/402 (92%)	370 (100%)	0	100	100
2	E	380/438 (87%)	378 (100%)	2 (0%)	86	90
3	D	395/451 (88%)	395 (100%)	0	100	100
4	F	57/57 (100%)	56 (98%)	1 (2%)	54	57
4	G	57/57 (100%)	57 (100%)	0	100	100
5	B	351/434 (81%)	350 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1980/2241 (88%)	1976 (100%)	4 (0%)	91	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	193	ARG
2	E	342	GLN
4	F	17	CYS
5	B	475	ASP

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

37 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	I	1	6	14,14,15	0.39	0	17,19,21	0.65	0
6	MAN	I	10	6	11,11,12	0.29	0	15,15,17	0.51	0
6	NAG	I	2	6	14,14,15	0.38	0	17,19,21	0.60	0
6	BMA	I	3	6	11,11,12	0.30	0	15,15,17	0.67	1 (6%)
6	MAN	I	4	6	11,11,12	0.26	0	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	I	5	6	11,11,12	0.38	0	15,15,17	0.52	0
6	MAN	I	6	6	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
6	MAN	I	7	6	11,11,12	0.41	0	15,15,17	0.56	0
6	MAN	I	8	6	11,11,12	0.30	0	15,15,17	0.52	0
6	MAN	I	9	6	11,11,12	0.43	0	15,15,17	0.59	0
7	NAG	J	1	2,7	14,14,15	0.37	0	17,19,21	0.55	0
7	NAG	J	2	7	14,14,15	0.38	0	17,19,21	0.53	0
7	BMA	J	3	7	11,11,12	0.31	0	15,15,17	0.46	0
7	MAN	J	4	7	11,11,12	0.30	0	15,15,17	0.51	0
8	NAG	K	1	8	14,14,15	0.42	0	17,19,21	0.76	0
8	MAN	K	10	8	11,11,12	0.45	0	15,15,17	0.57	0
8	MAN	K	11	8	11,11,12	0.33	0	15,15,17	0.54	0
8	NAG	K	2	8	14,14,15	0.40	0	17,19,21	0.69	0
8	BMA	K	3	8	11,11,12	0.31	0	15,15,17	0.71	1 (6%)
8	MAN	K	4	8	11,11,12	0.42	0	15,15,17	0.48	0
8	MAN	K	5	8	11,11,12	0.41	0	15,15,17	0.55	0
8	MAN	K	6	8	11,11,12	0.32	0	15,15,17	0.51	0
8	MAN	K	7	8	11,11,12	0.37	0	15,15,17	0.60	0
8	MAN	K	8	8	11,11,12	0.49	0	15,15,17	0.53	0
8	MAN	K	9	8	11,11,12	0.34	0	15,15,17	0.55	0
9	NAG	L	1	9,3	14,14,15	0.39	0	17,19,21	0.62	0
9	NAG	L	2	9	14,14,15	0.36	0	17,19,21	0.51	0
9	BMA	L	3	9	11,11,12	0.62	0	15,15,17	0.52	0
9	MAN	L	4	9	11,11,12	0.32	0	15,15,17	0.48	0
9	MAN	L	5	9	11,11,12	0.31	0	15,15,17	0.52	0
9	MAN	L	6	9	11,11,12	0.26	0	15,15,17	0.48	0
7	NAG	M	1	7	14,14,15	0.41	0	17,19,21	0.67	0
7	NAG	M	2	7	14,14,15	0.38	0	17,19,21	0.44	0
7	BMA	M	3	7	11,11,12	0.29	0	15,15,17	0.48	0
7	MAN	M	4	7	11,11,12	0.25	0	15,15,17	0.50	0
10	NAG	N	1	10,5	14,14,15	0.37	0	17,19,21	0.46	0
10	NAG	N	2	10	14,14,15	0.39	0	17,19,21	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. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1
6	MAN	I	6	6	-	0/2/19/22	0/1/1/1
6	MAN	I	7	6	-	1/2/19/22	0/1/1/1
6	MAN	I	8	6	-	0/2/19/22	0/1/1/1
6	MAN	I	9	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	0/2/19/22	0/1/1/1
7	MAN	J	4	7	-	1/2/19/22	0/1/1/1
8	NAG	K	1	8	-	2/6/23/26	0/1/1/1
8	MAN	K	10	8	-	0/2/19/22	0/1/1/1
8	MAN	K	11	8	-	0/2/19/22	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
8	MAN	K	4	8	-	0/2/19/22	0/1/1/1
8	MAN	K	5	8	-	0/2/19/22	0/1/1/1
8	MAN	K	6	8	-	0/2/19/22	0/1/1/1
8	MAN	K	7	8	-	0/2/19/22	0/1/1/1
8	MAN	K	8	8	-	0/2/19/22	0/1/1/1
8	MAN	K	9	8	-	0/2/19/22	0/1/1/1
9	NAG	L	1	9,3	-	2/6/23/26	0/1/1/1
9	NAG	L	2	9	-	2/6/23/26	0/1/1/1
9	BMA	L	3	9	-	0/2/19/22	0/1/1/1
9	MAN	L	4	9	-	0/2/19/22	0/1/1/1
9	MAN	L	5	9	-	0/2/19/22	0/1/1/1
9	MAN	L	6	9	-	0/2/19/22	0/1/1/1
7	NAG	M	1	7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	2/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
7	MAN	M	4	7	-	0/2/19/22	0/1/1/1
10	NAG	N	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	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	I	6	MAN	C1-O5-C5	2.37	115.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	K	3	BMA	C1-O5-C5	2.08	114.98	112.19
6	I	3	BMA	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

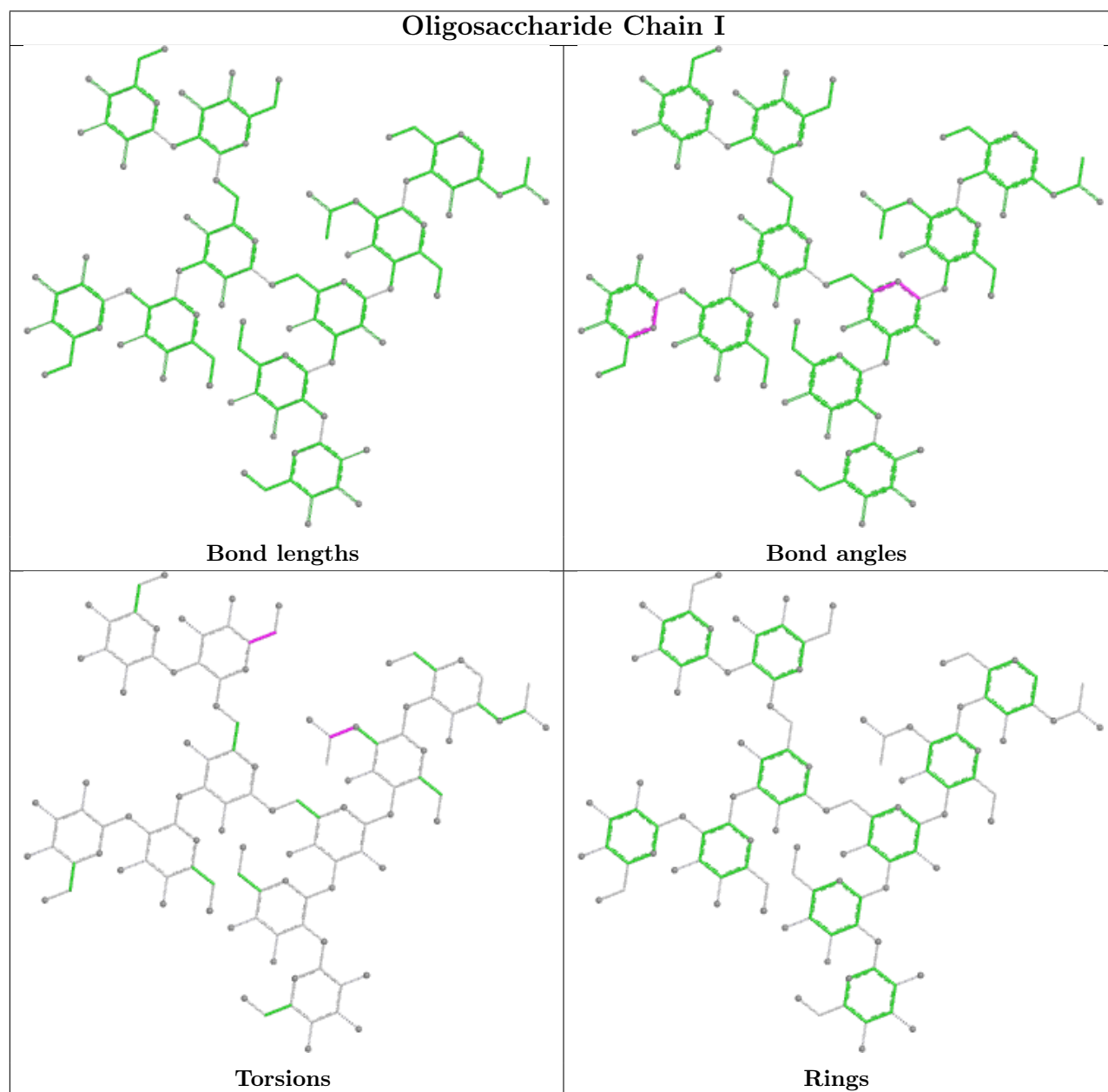
Mol	Chain	Res	Type	Atoms
7	M	1	NAG	C8-C7-N2-C2
9	L	2	NAG	C8-C7-N2-C2
9	L	2	NAG	O7-C7-N2-C2
6	I	2	NAG	C8-C7-N2-C2
7	M	1	NAG	O7-C7-N2-C2
10	N	2	NAG	C8-C7-N2-C2
10	N	2	NAG	O7-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
8	K	1	NAG	C8-C7-N2-C2
9	L	1	NAG	C8-C7-N2-C2
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
7	M	2	NAG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

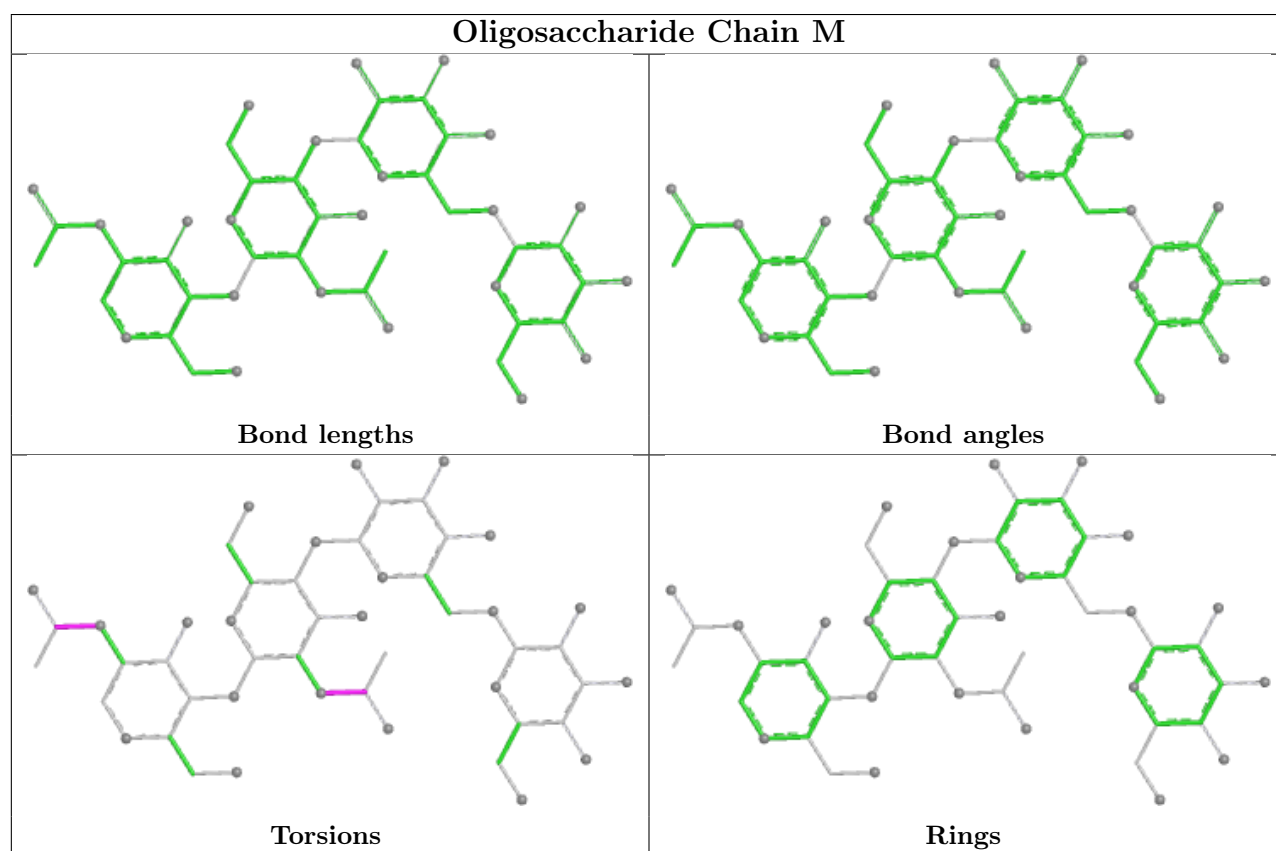
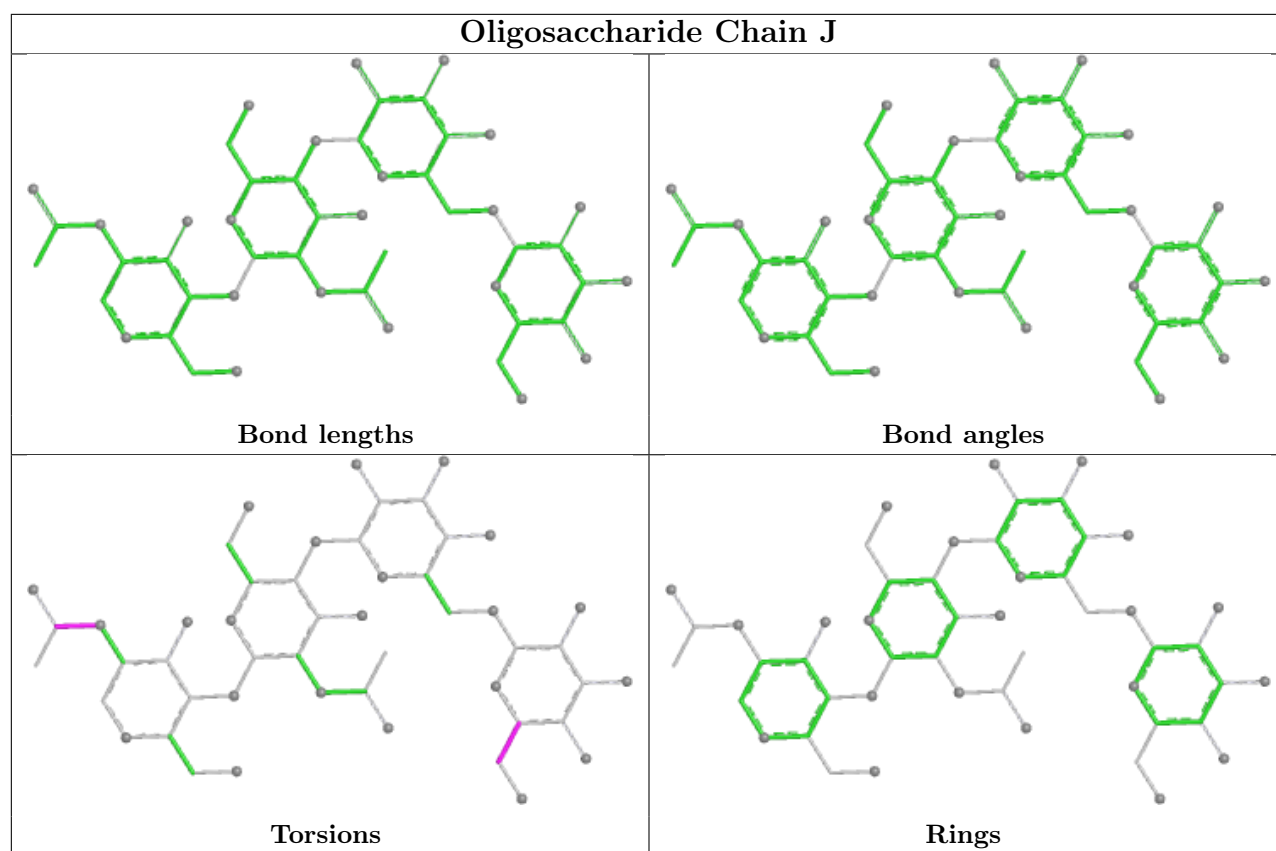
There are no ring outliers.

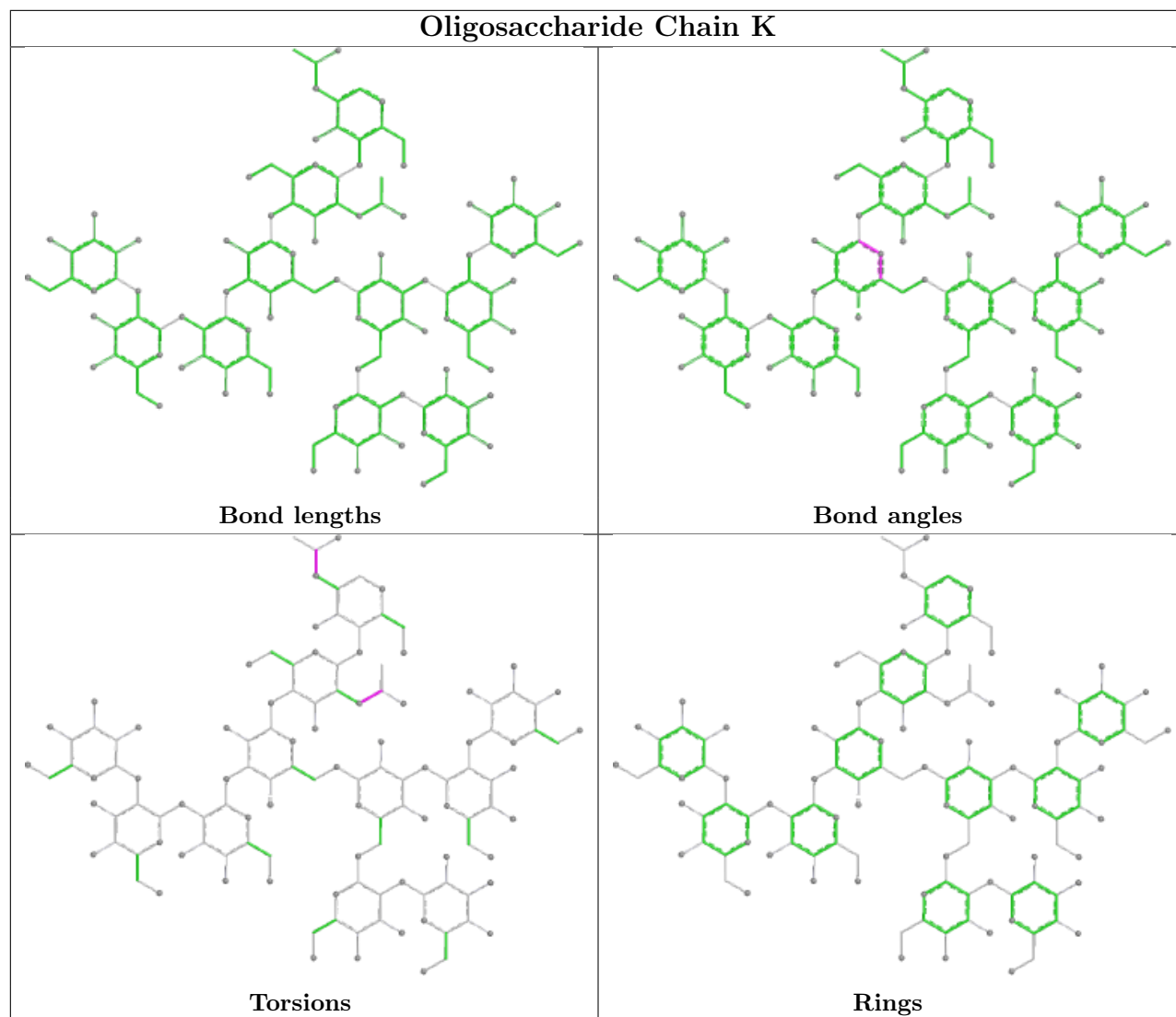
9 monomers are involved in 13 short contacts:

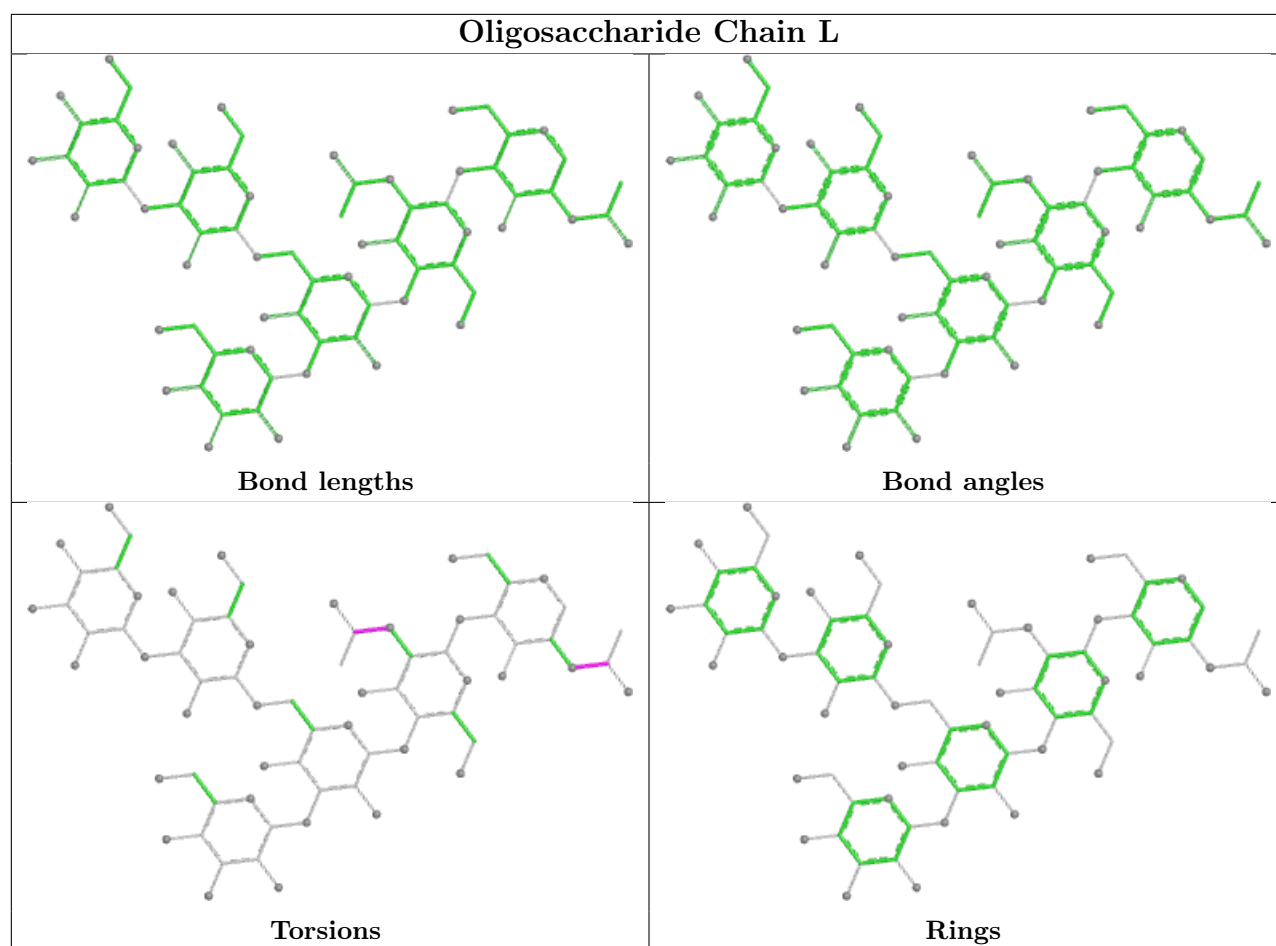
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	2	NAG	1	0
6	I	1	NAG	1	0
6	I	7	MAN	2	0
6	I	2	NAG	2	0
8	K	3	BMA	2	0
6	I	5	MAN	1	0
8	K	2	NAG	4	0
9	L	1	NAG	1	0
8	K	1	NAG	1	0

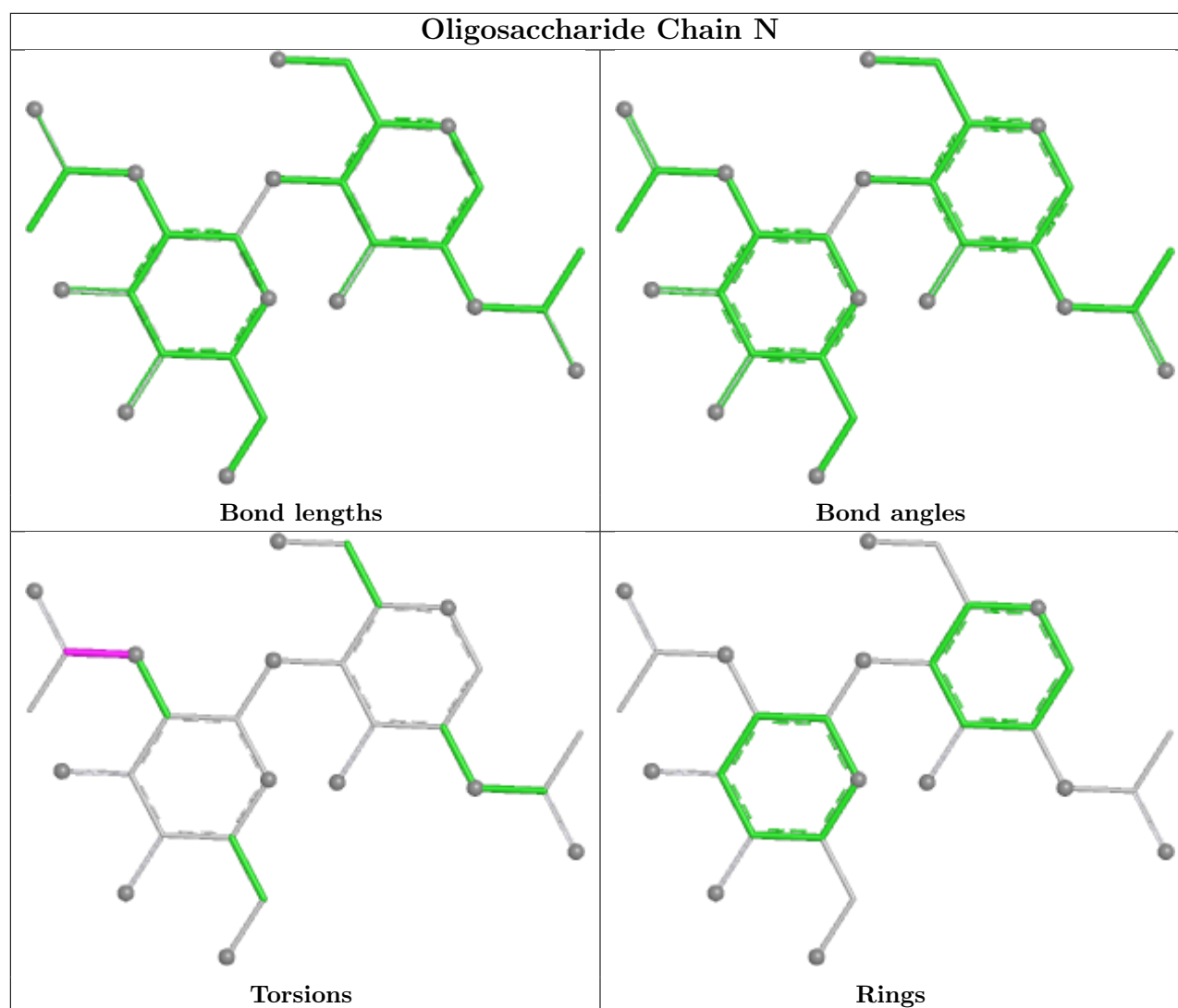
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
12	NAG	D	602	3	14,14,15	0.38	0	17,19,21	0.96	1 (5%)
11	POV	E	603	-	34,34,51	0.34	0	40,42,59	0.35	0
11	POV	C	502	-	31,31,51	0.34	0	37,39,59	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	POV	D	601	-	46,46,51	0.30	0	52,54,59	0.33	0
11	POV	E	602	-	34,34,51	0.34	0	40,42,59	0.37	0
11	POV	E	601	-	34,34,51	0.34	0	40,42,59	0.36	0
11	POV	C	501	-	36,36,51	0.32	0	42,44,59	0.35	0
11	POV	A	501	-	36,36,51	0.32	0	42,44,59	0.41	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
12	NAG	D	602	3	-	3/6/23/26	0/1/1/1
11	POV	E	603	-	-	9/38/38/55	-
11	POV	C	502	-	-	23/35/35/55	-
11	POV	D	601	-	-	14/50/50/55	-
11	POV	E	602	-	-	30/38/38/55	-
11	POV	E	601	-	-	15/38/38/55	-
11	POV	C	501	-	-	17/40/40/55	-
11	POV	A	501	-	-	13/40/40/55	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	602	NAG	C2-N2-C7	3.40	127.45	122.90

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	POV	C11-O12-P-O11
11	A	501	POV	C11-O12-P-O13
11	A	501	POV	C22-C21-O21-C2
11	A	501	POV	O22-C21-O21-C2
11	A	501	POV	C32-C31-O31-C3
11	E	601	POV	C22-C21-O21-C2
11	E	602	POV	C1-O11-P-O12
11	E	602	POV	C1-O11-P-O13

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

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Mol	Chain	Res	Type	Atoms
11	C	502	POV	C22-C23-C24-C25
11	E	602	POV	C22-C23-C24-C25
11	E	602	POV	C25-C26-C27-C28
11	E	602	POV	C11-C12-N-C13
11	D	601	POV	O32-C31-O31-C3
11	E	601	POV	C36-C37-C38-C39
11	C	501	POV	C25-C26-C27-C28
11	E	603	POV	C22-C21-O21-C2
11	C	501	POV	C22-C21-O21-C2
11	E	602	POV	C11-C12-N-C15
11	C	501	POV	C23-C24-C25-C26
11	C	502	POV	C31-C32-C33-C34
11	E	602	POV	O21-C2-C3-O31
11	E	601	POV	C33-C34-C35-C36
11	C	501	POV	C35-C36-C37-C38
11	E	602	POV	C26-C27-C28-C29
11	C	502	POV	C34-C35-C36-C37
11	C	501	POV	O22-C21-O21-C2
11	E	601	POV	C31-C32-C33-C34
11	D	601	POV	C22-C21-O21-C2
11	E	601	POV	C34-C35-C36-C37
11	E	601	POV	C311-C310-C39-C38
12	D	602	NAG	O5-C5-C6-O6
11	E	603	POV	O22-C21-O21-C2
11	E	601	POV	C37-C38-C39-C310
11	A	501	POV	C34-C35-C36-C37
11	E	602	POV	C23-C24-C25-C26
11	E	602	POV	C24-C25-C26-C27
11	C	501	POV	O11-C1-C2-C3
11	C	501	POV	C311-C310-C39-C38
11	E	602	POV	C1-C2-C3-O31
11	E	602	POV	C21-C22-C23-C24
11	C	501	POV	O11-C1-C2-O21
11	E	603	POV	O21-C2-C3-O31
11	D	601	POV	O22-C21-O21-C2
12	D	602	NAG	C1-C2-N2-C7
11	E	602	POV	C32-C33-C34-C35
11	A	501	POV	O12-C11-C12-N
11	E	603	POV	O12-C11-C12-N
11	C	502	POV	O12-C11-C12-N
11	D	601	POV	O12-C11-C12-N
11	D	601	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
11	D	601	POV	C29-C210-C211-C212
11	C	501	POV	C33-C34-C35-C36
11	E	602	POV	C11-O12-P-O13
11	C	501	POV	C1-O11-P-O14
11	C	501	POV	C11-O12-P-O14
11	C	502	POV	C1-O11-P-O12
11	C	502	POV	C11-O12-P-O11
12	D	602	NAG	C3-C2-N2-C7
11	E	603	POV	C33-C34-C35-C36
11	C	502	POV	C2-C1-O11-P
11	A	501	POV	C35-C36-C37-C38
11	A	501	POV	C1-C2-O21-C21
11	D	601	POV	C3-C2-O21-C21
11	D	601	POV	C24-C25-C26-C27
11	A	501	POV	C22-C23-C24-C25
11	D	601	POV	C1-C2-C3-O31
11	E	601	POV	C23-C24-C25-C26
11	E	602	POV	C2-C1-O11-P
11	C	502	POV	O11-C1-C2-O21
11	A	501	POV	C25-C26-C27-C28
11	E	603	POV	C1-C2-C3-O31
11	E	603	POV	C12-C11-O12-P
11	D	601	POV	O11-C1-C2-C3
11	E	602	POV	O31-C31-C32-C33
11	C	502	POV	O31-C31-C32-C33
11	E	602	POV	O11-C1-C2-O21
11	C	502	POV	O21-C21-C22-C23
11	E	602	POV	O21-C21-C22-C23
11	A	501	POV	C3-C2-O21-C21
11	E	602	POV	O32-C31-C32-C33
11	C	502	POV	O32-C31-C32-C33
11	E	602	POV	O22-C21-C22-C23

There are no ring outliers.

8 monomers are involved in 40 short contacts:

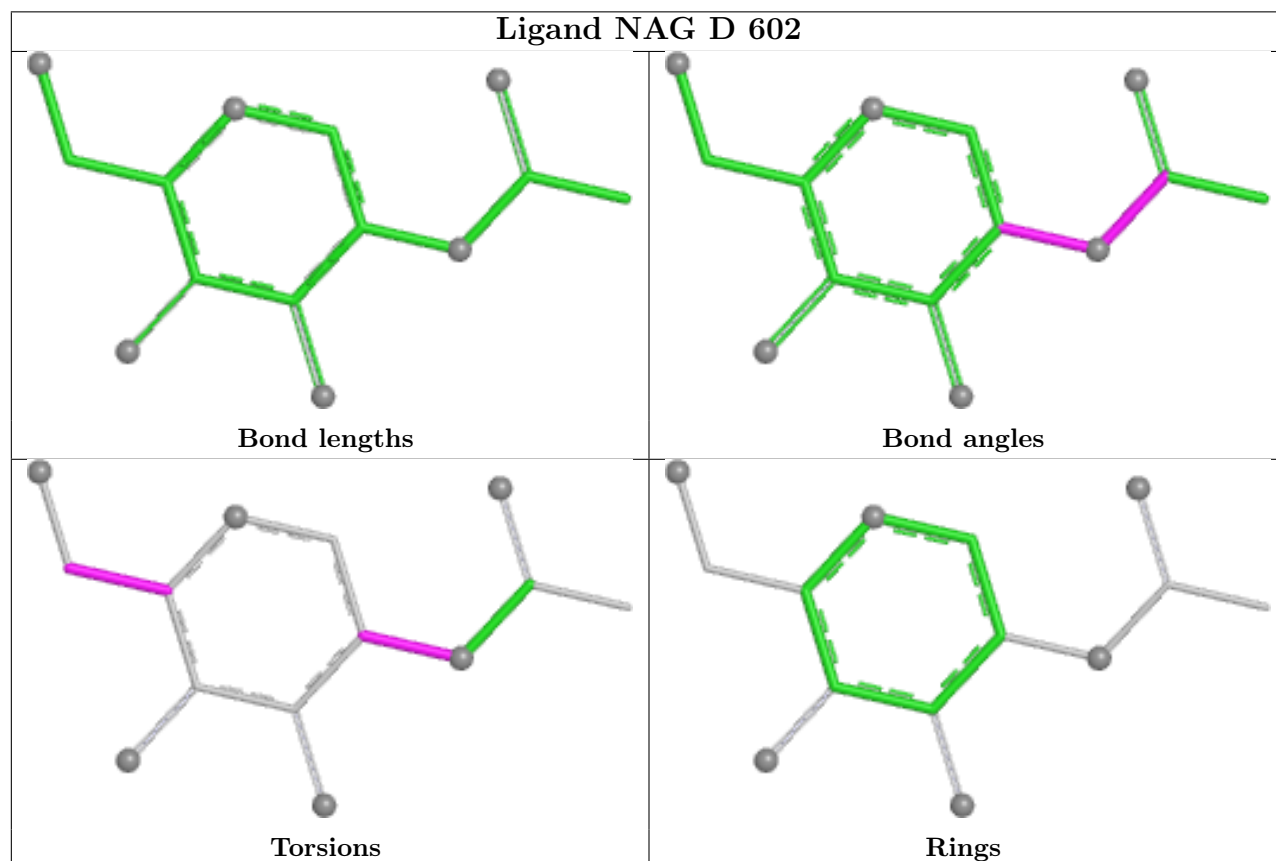
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	602	NAG	1	0
11	E	603	POV	5	0
11	C	502	POV	6	0
11	D	601	POV	6	0
11	E	602	POV	5	0

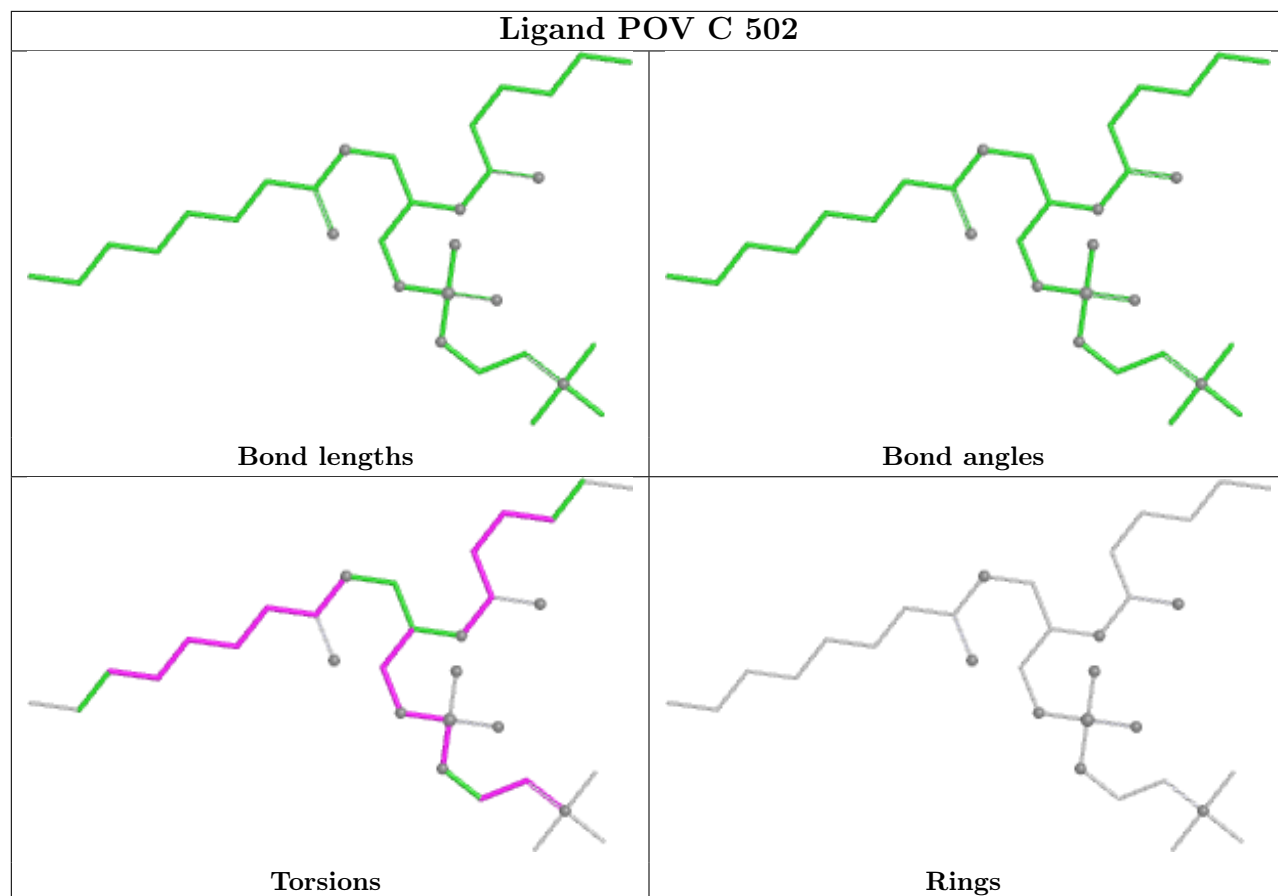
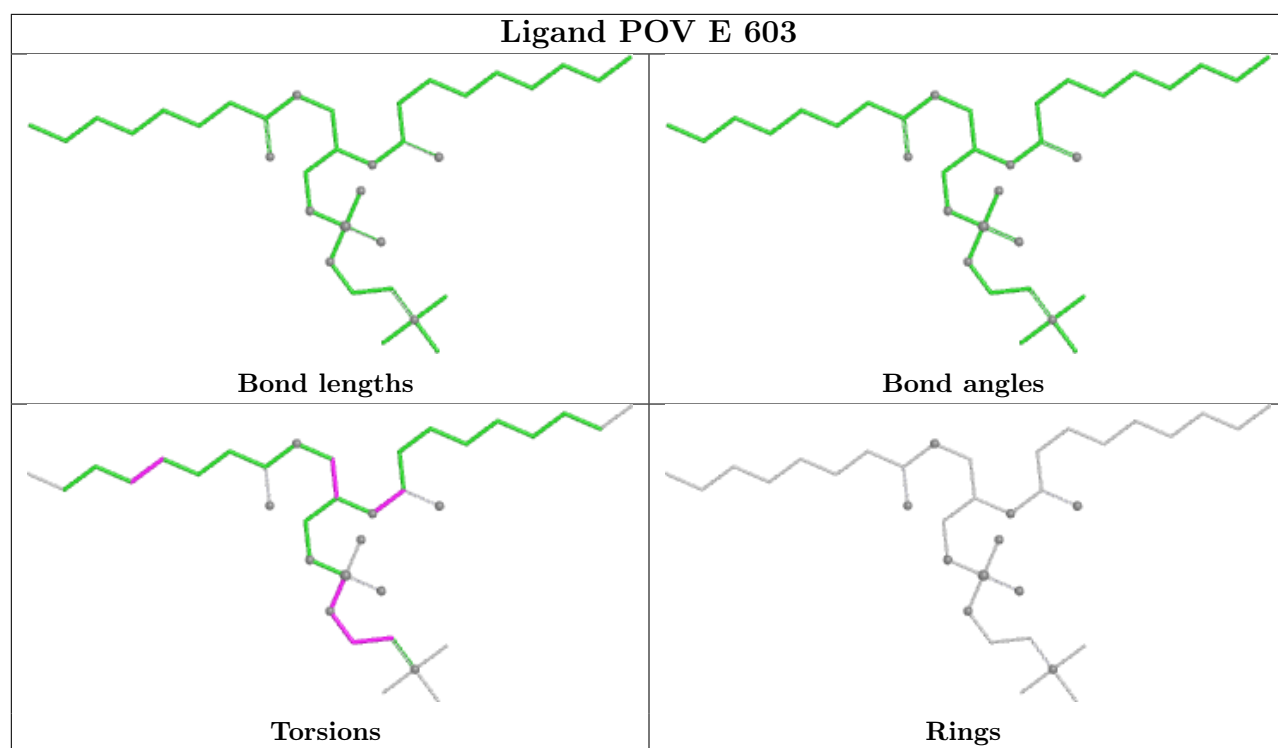
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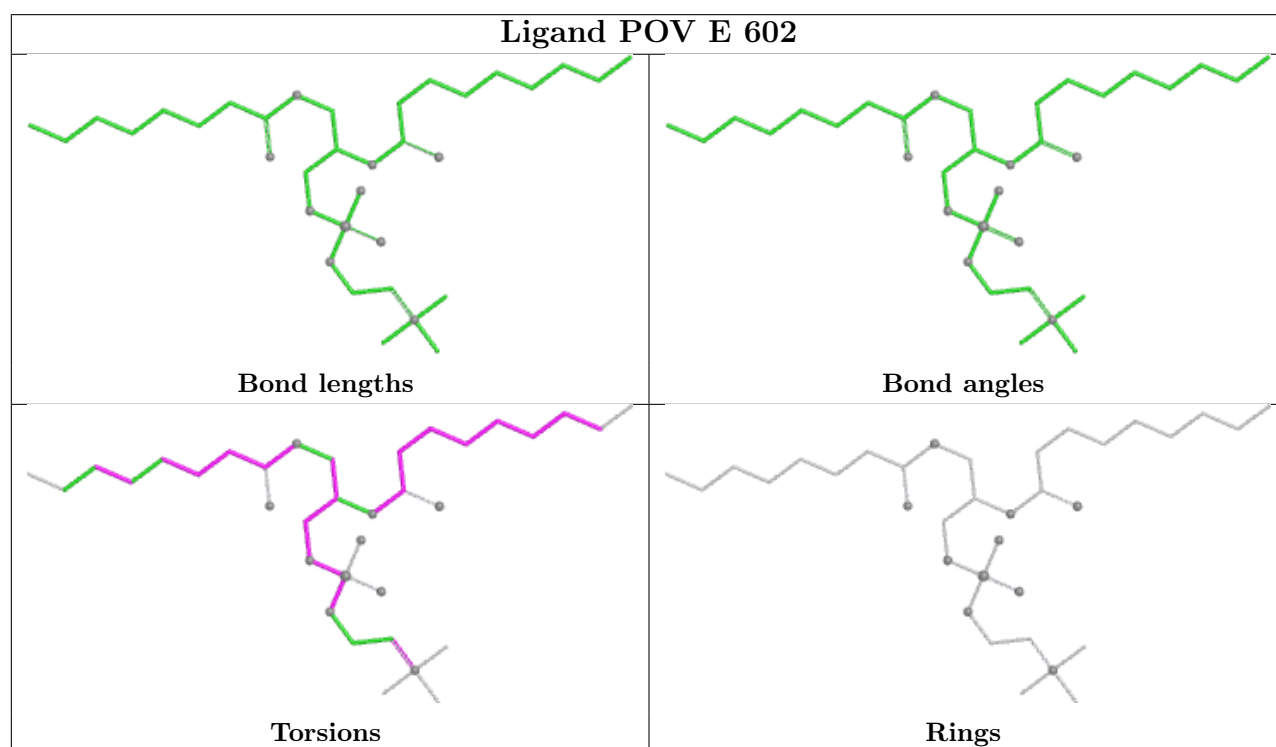
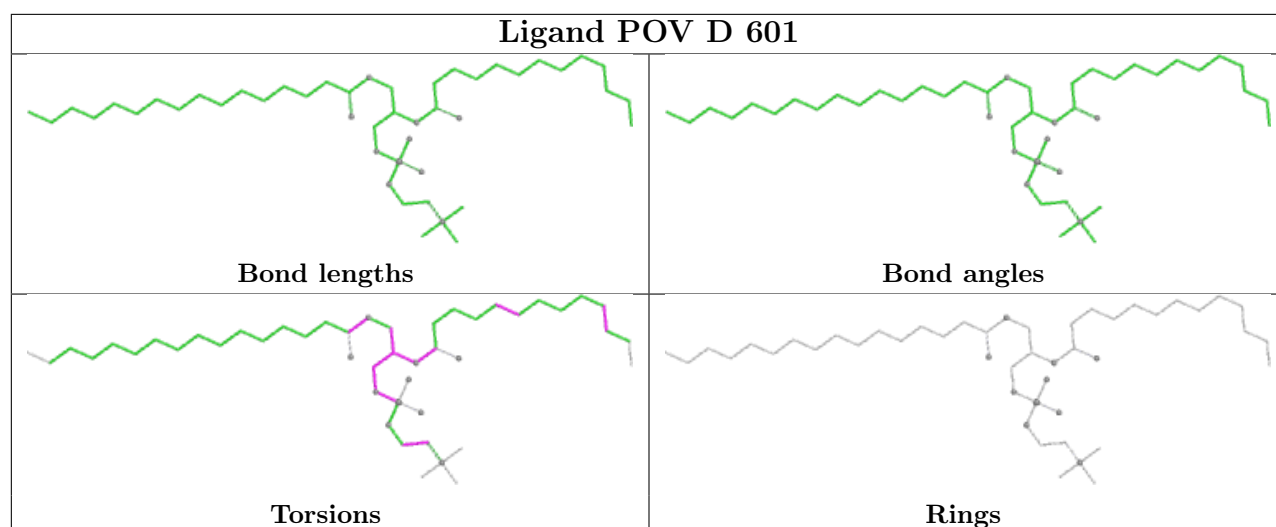
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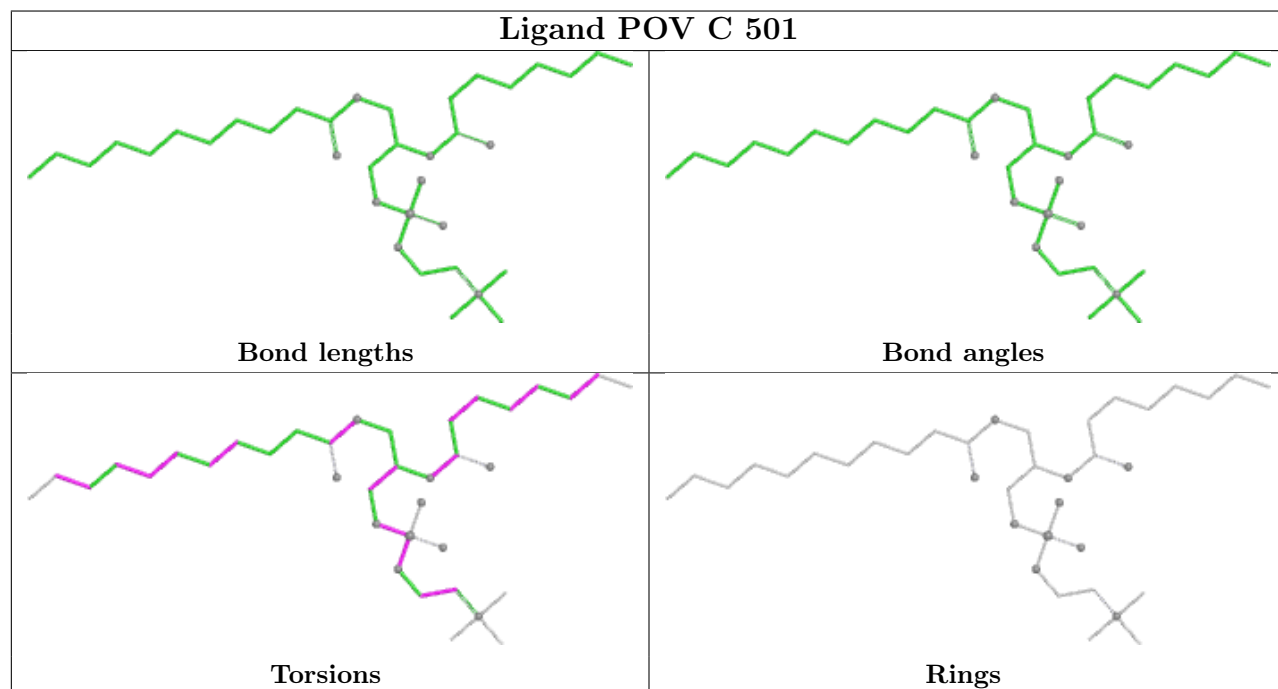
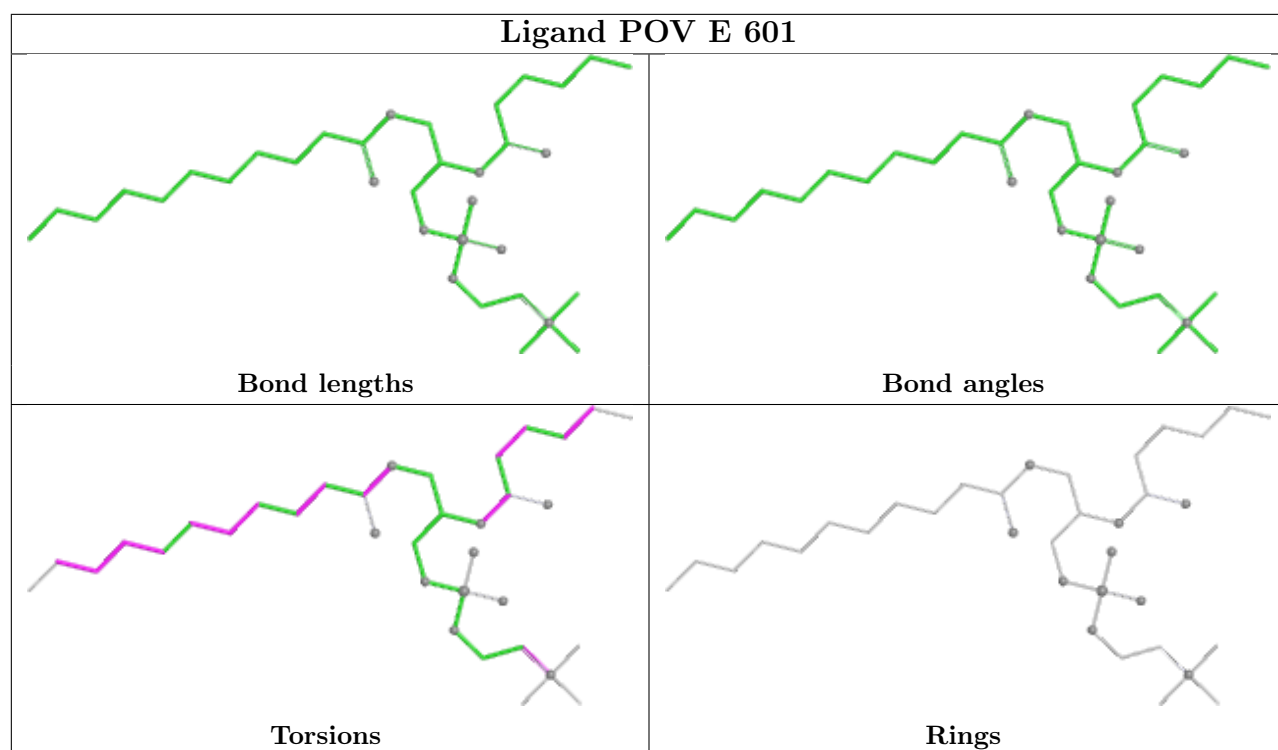
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	601	POV	4	0
11	C	501	POV	2	0
11	A	501	POV	11	0

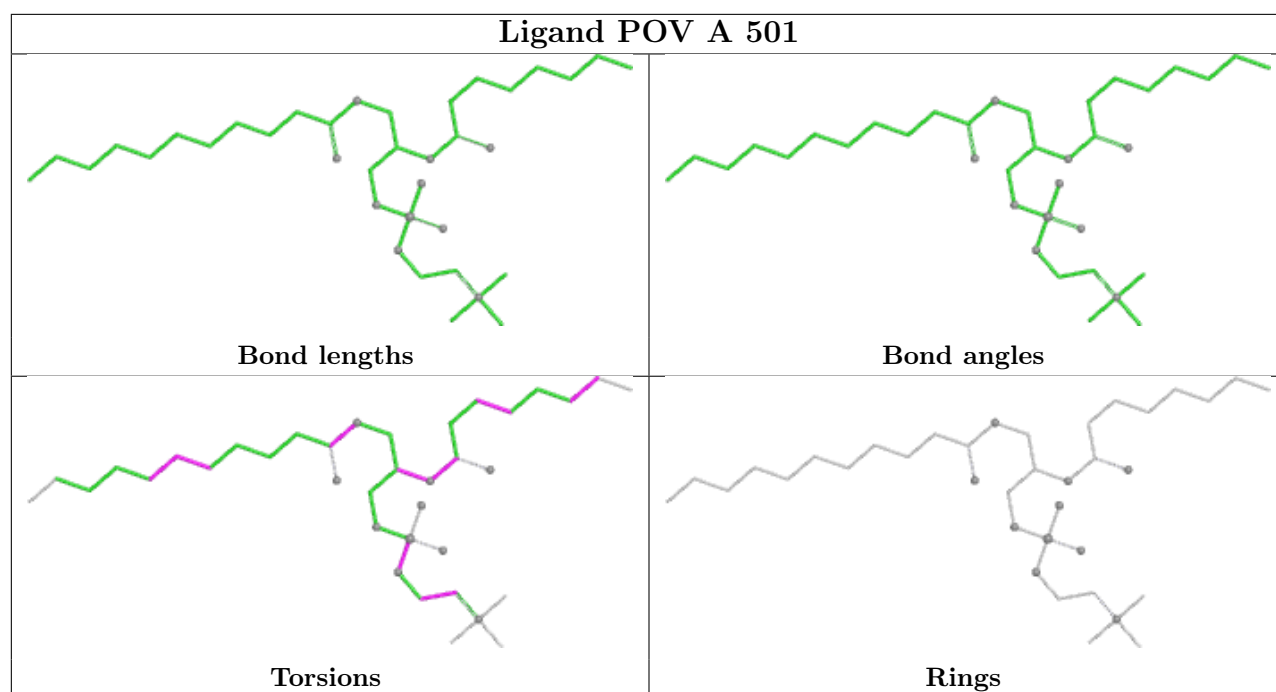
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

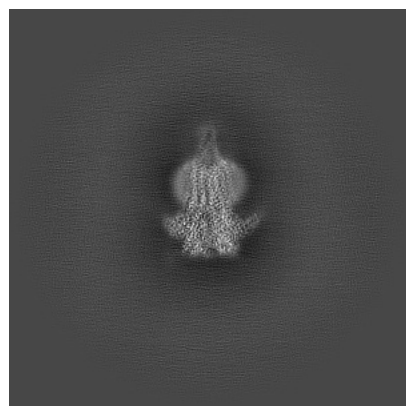
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43926. These allow visual inspection of the internal detail of the map and identification of artifacts.

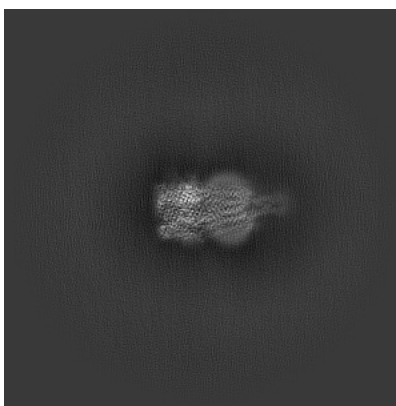
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

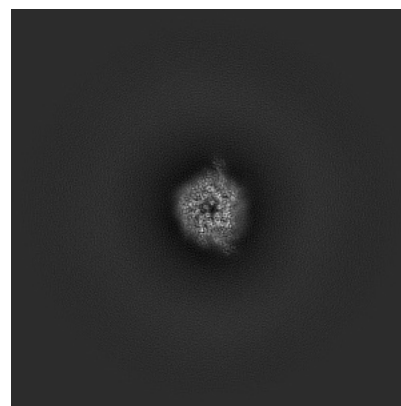
6.1.1 Primary map



X

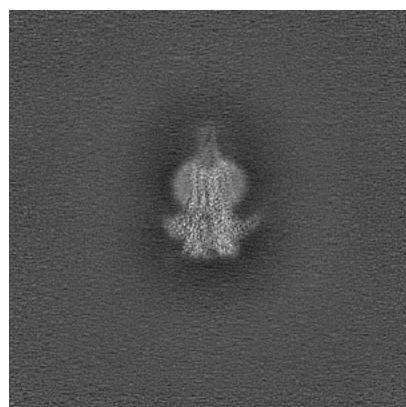


Y

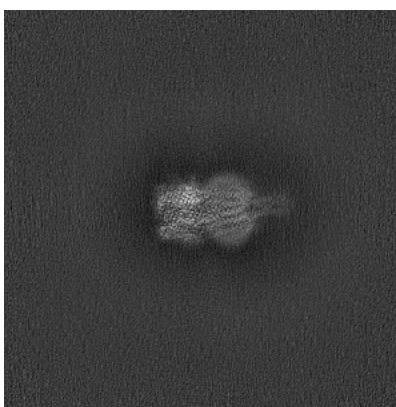


Z

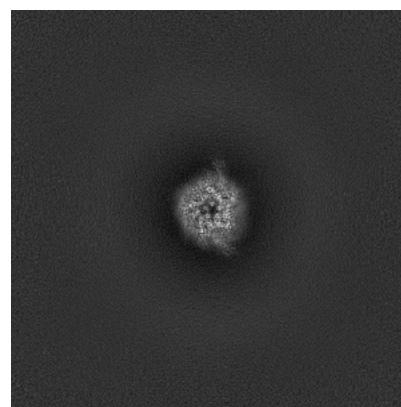
6.1.2 Raw map



X



Y



Z

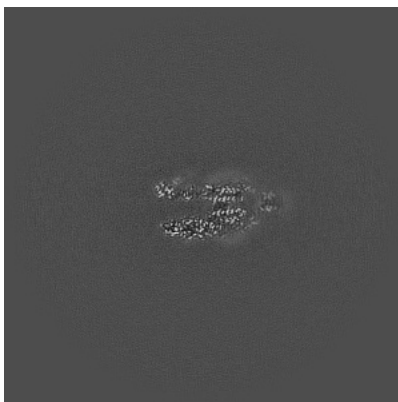
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256

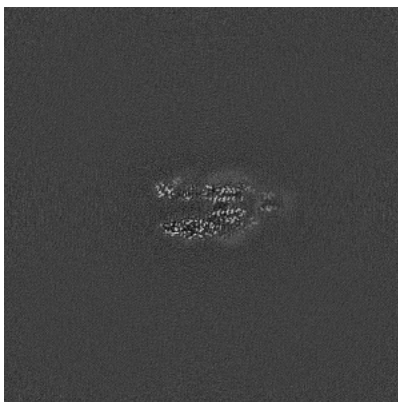


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

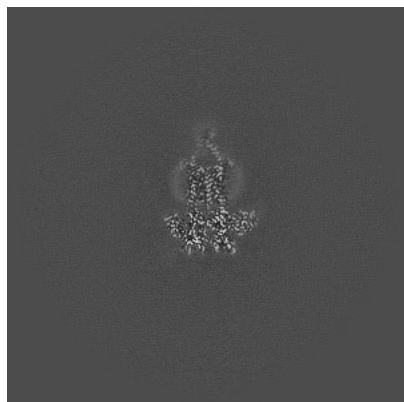


Z Index: 256

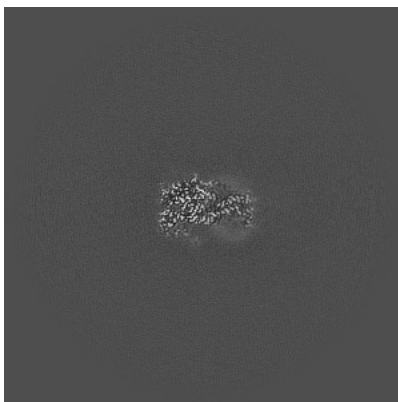
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

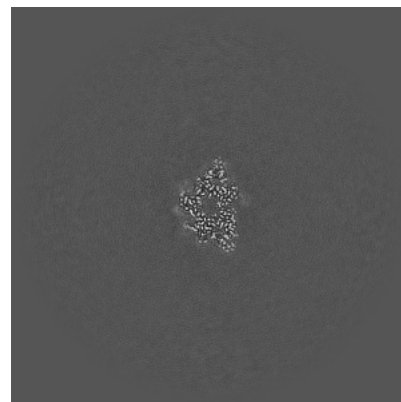
6.3.1 Primary map



X Index: 267



Y Index: 274

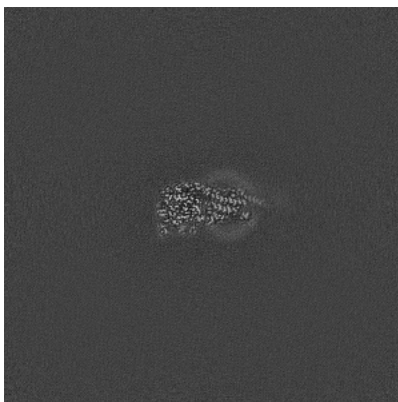


Z Index: 233

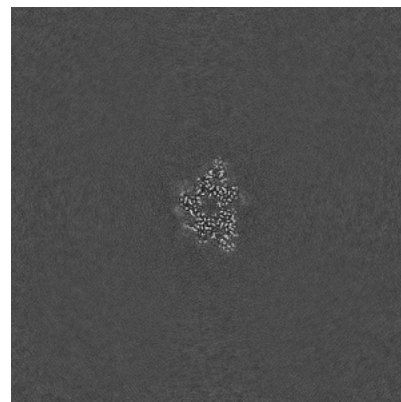
6.3.2 Raw map



X Index: 267



Y Index: 239

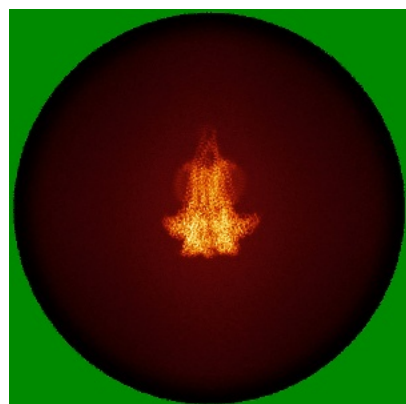


Z Index: 233

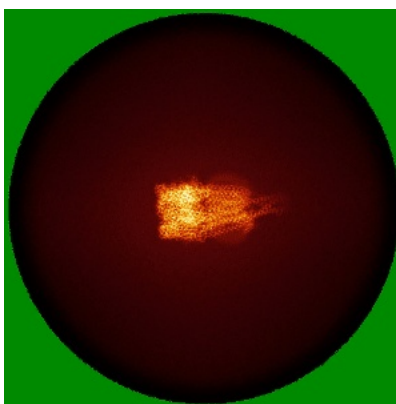
The images above show the largest variance slices of the map in three orthogonal directions.

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

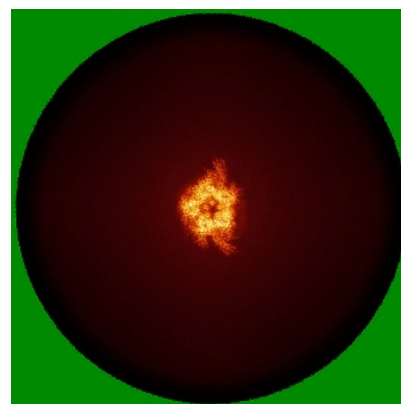
6.4.1 Primary map



X

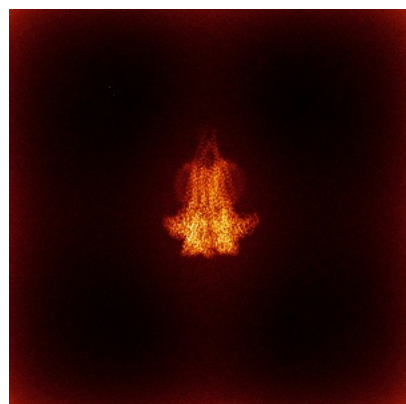


Y

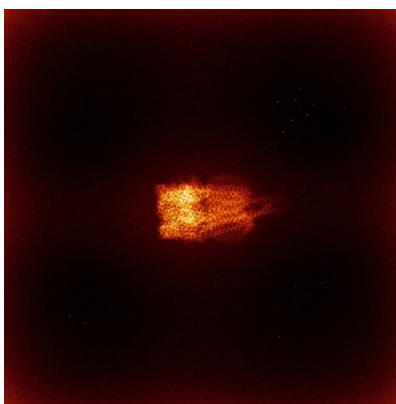


Z

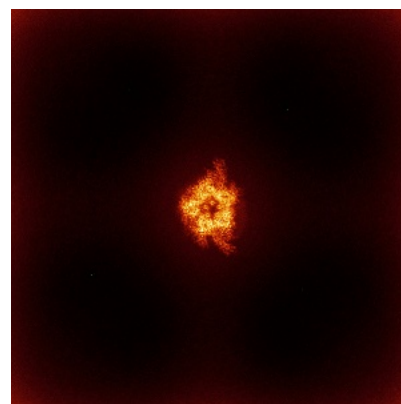
6.4.2 Raw map



X



Y

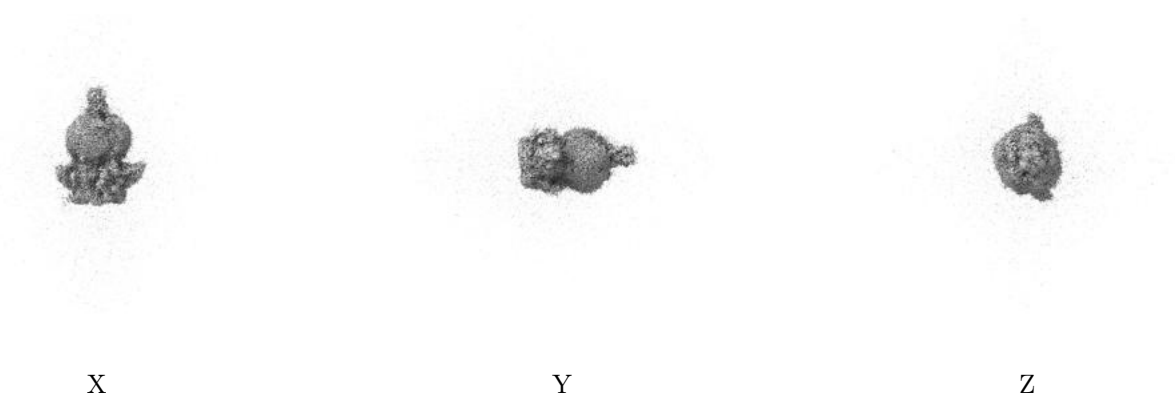


Z

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

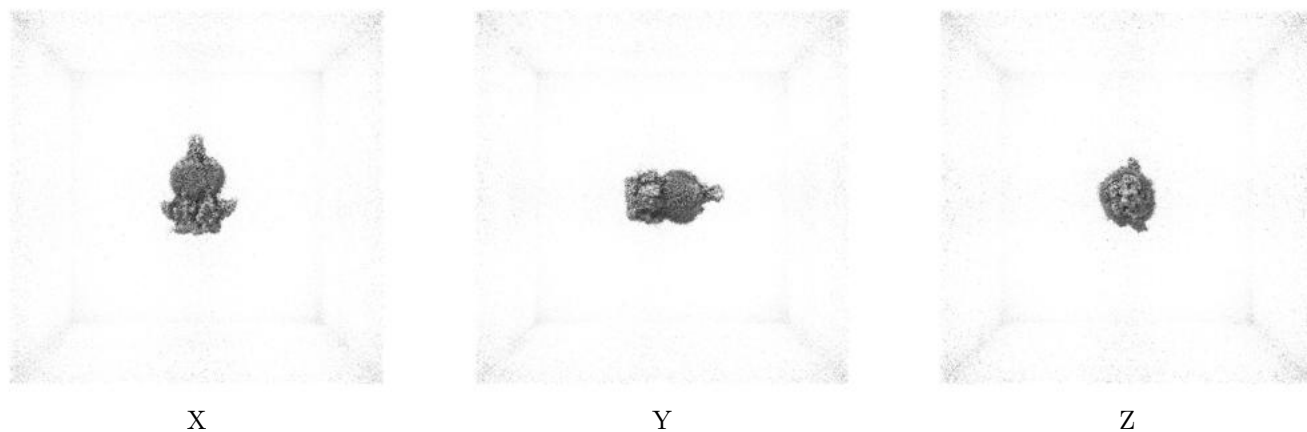
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

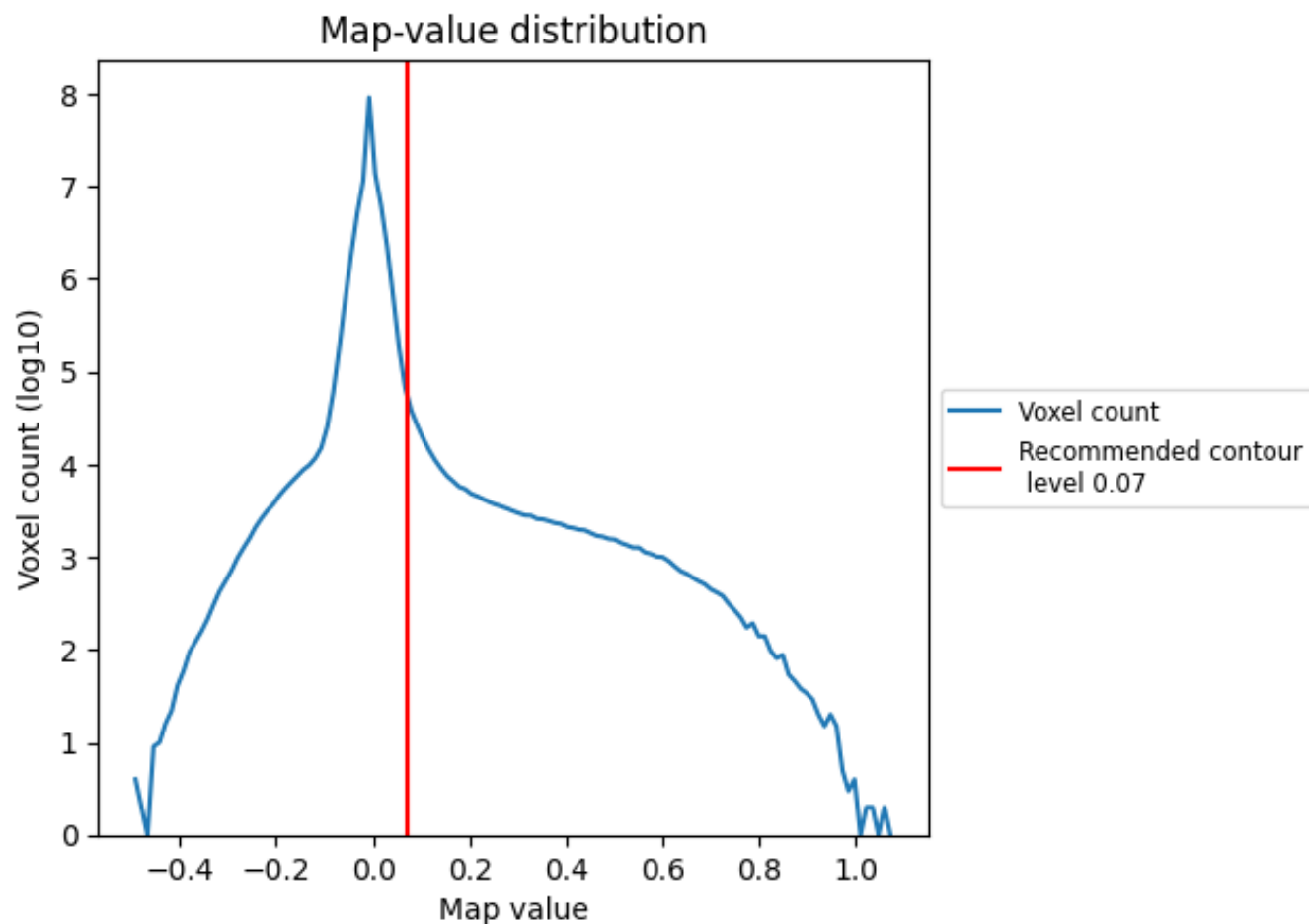
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

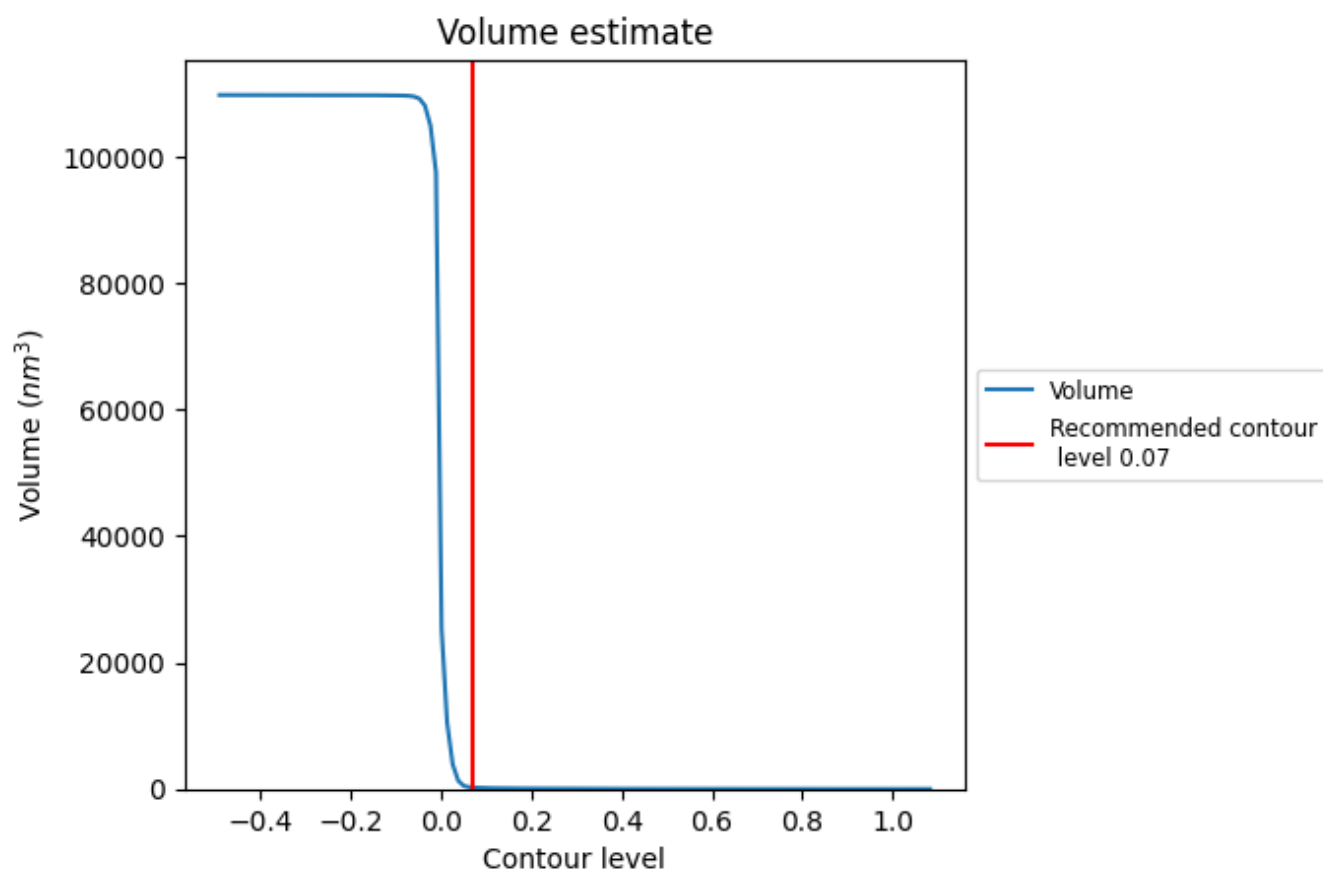
This section contains the results of statistical analysis of the map.

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.

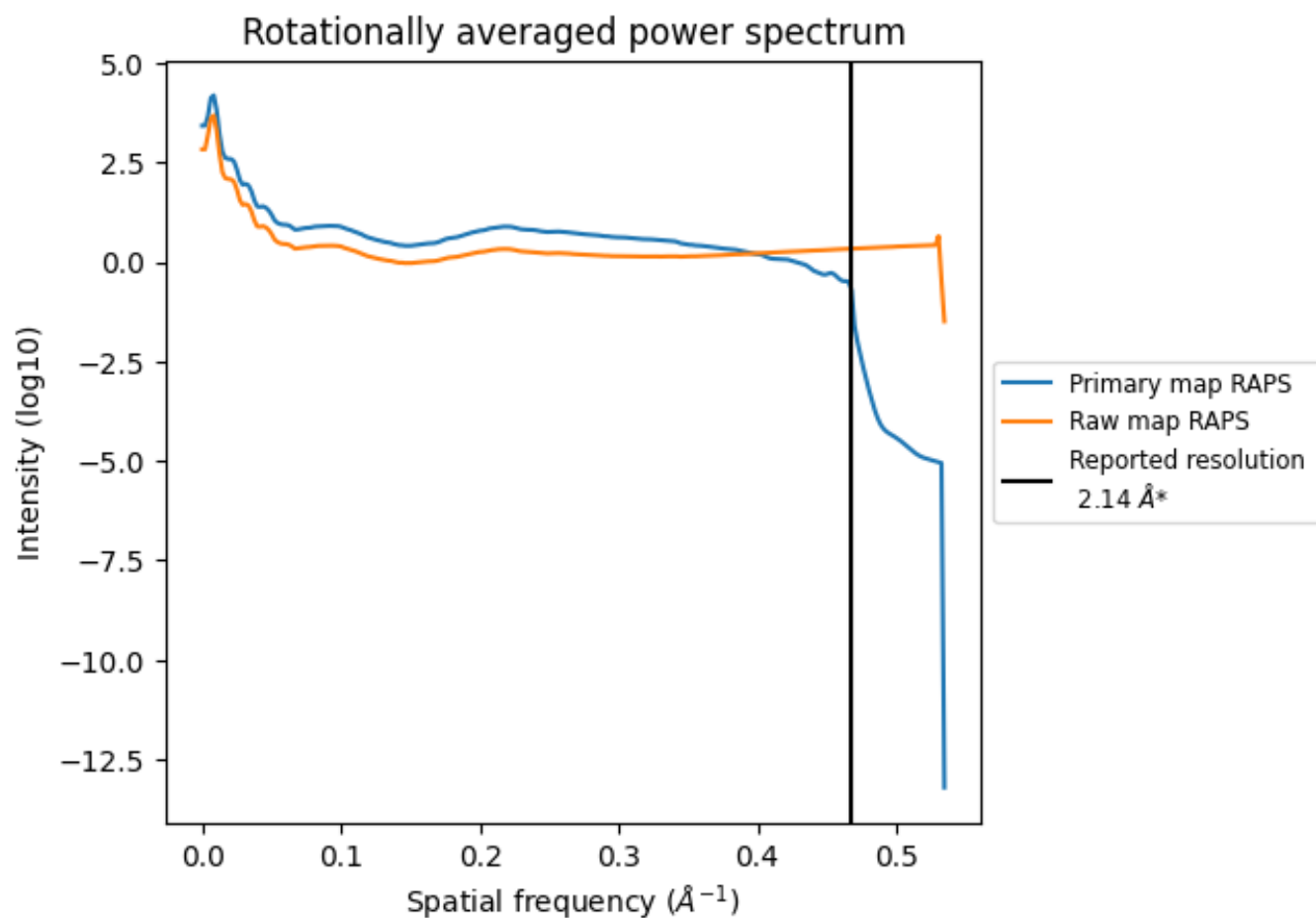
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 231 nm^3 ; this corresponds to an approximate mass of 208 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 ⓘ

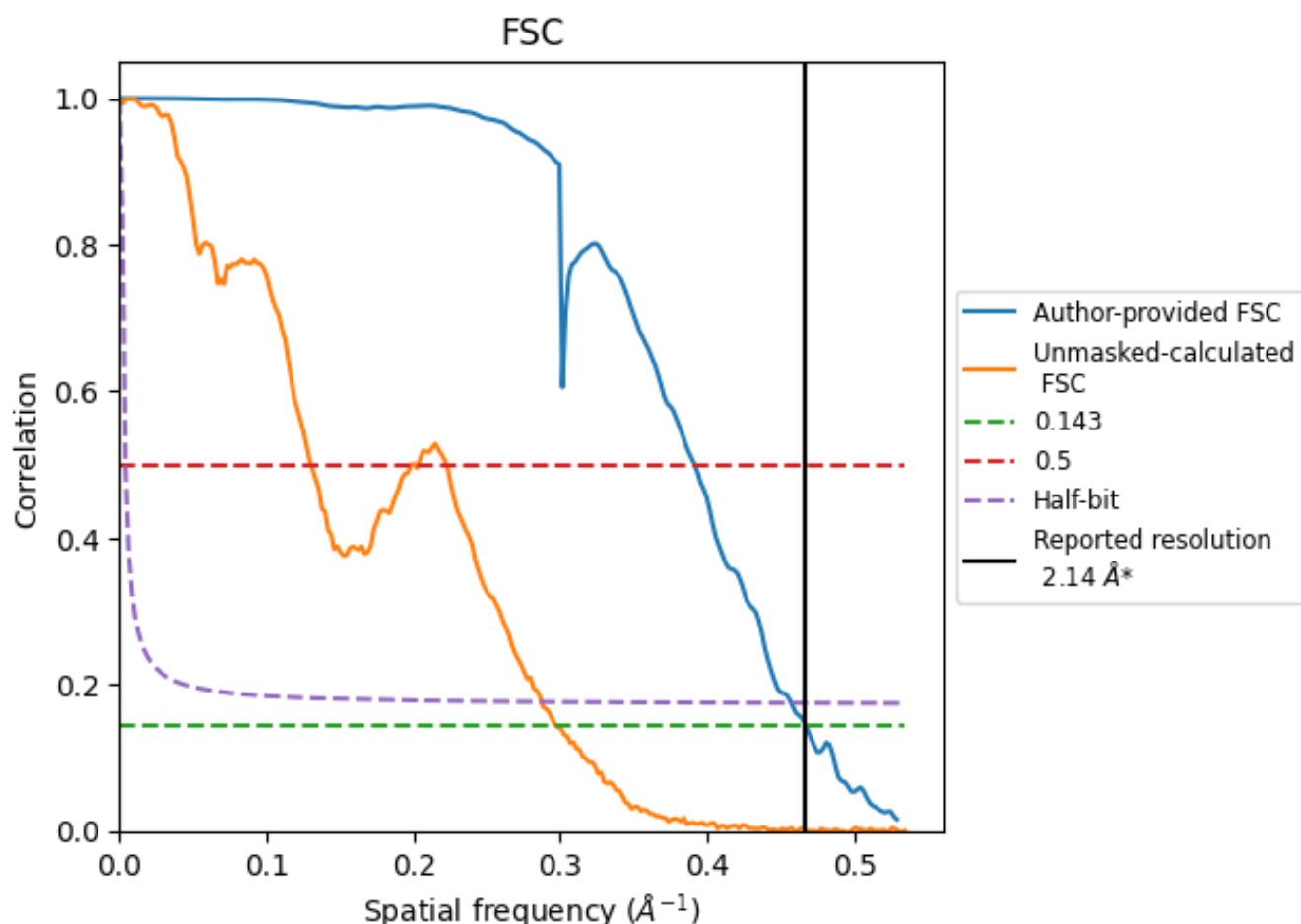


*Reported resolution corresponds to spatial frequency of 0.467 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.467 \AA^{-1}

8.2 Resolution estimates [i](#)

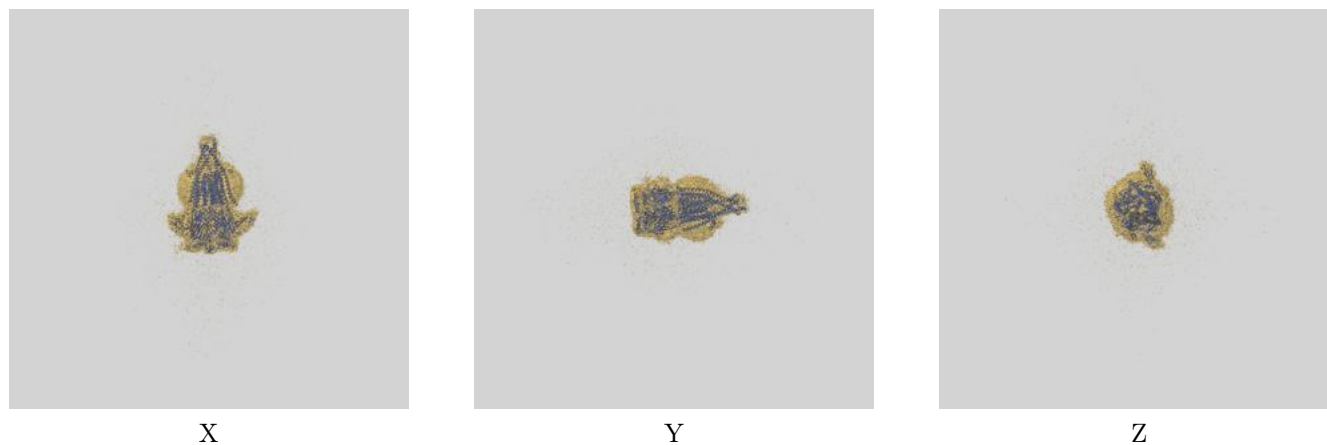
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.14	2.55	2.19
Unmasked-calculated*	3.36	7.67	3.48

*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 3.36 differs from the reported value 2.14 by more than 10 %

9 Map-model fit [i](#)

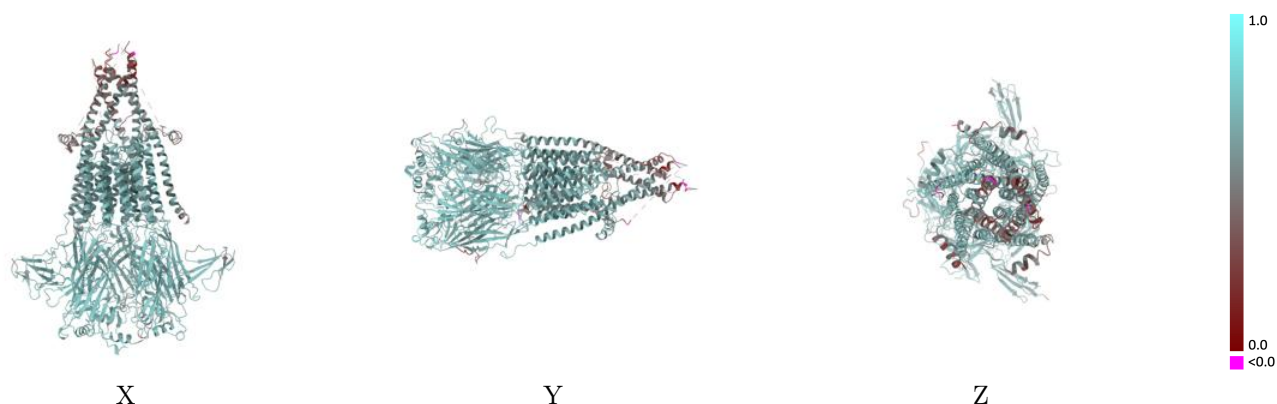
This section contains information regarding the fit between EMDB map EMD-43926 and PDB model 9AWK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



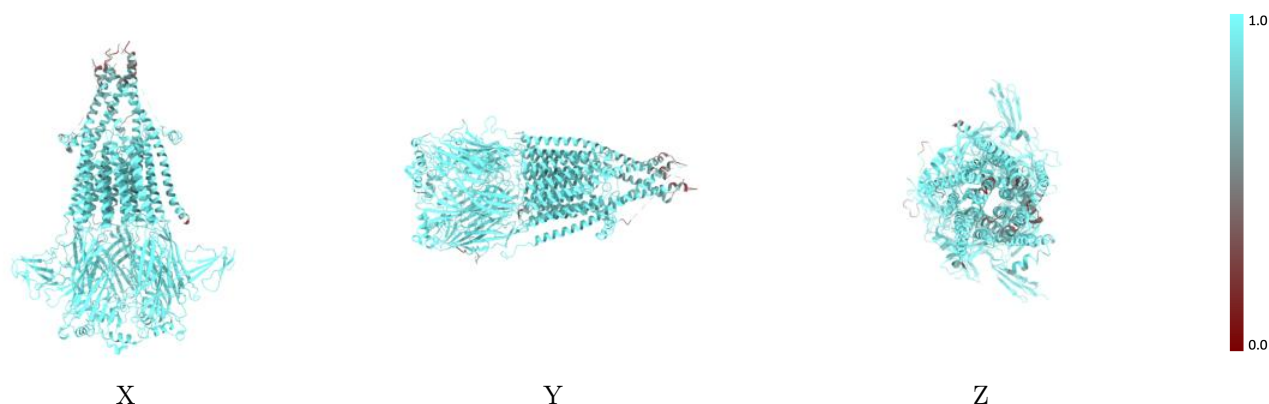
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



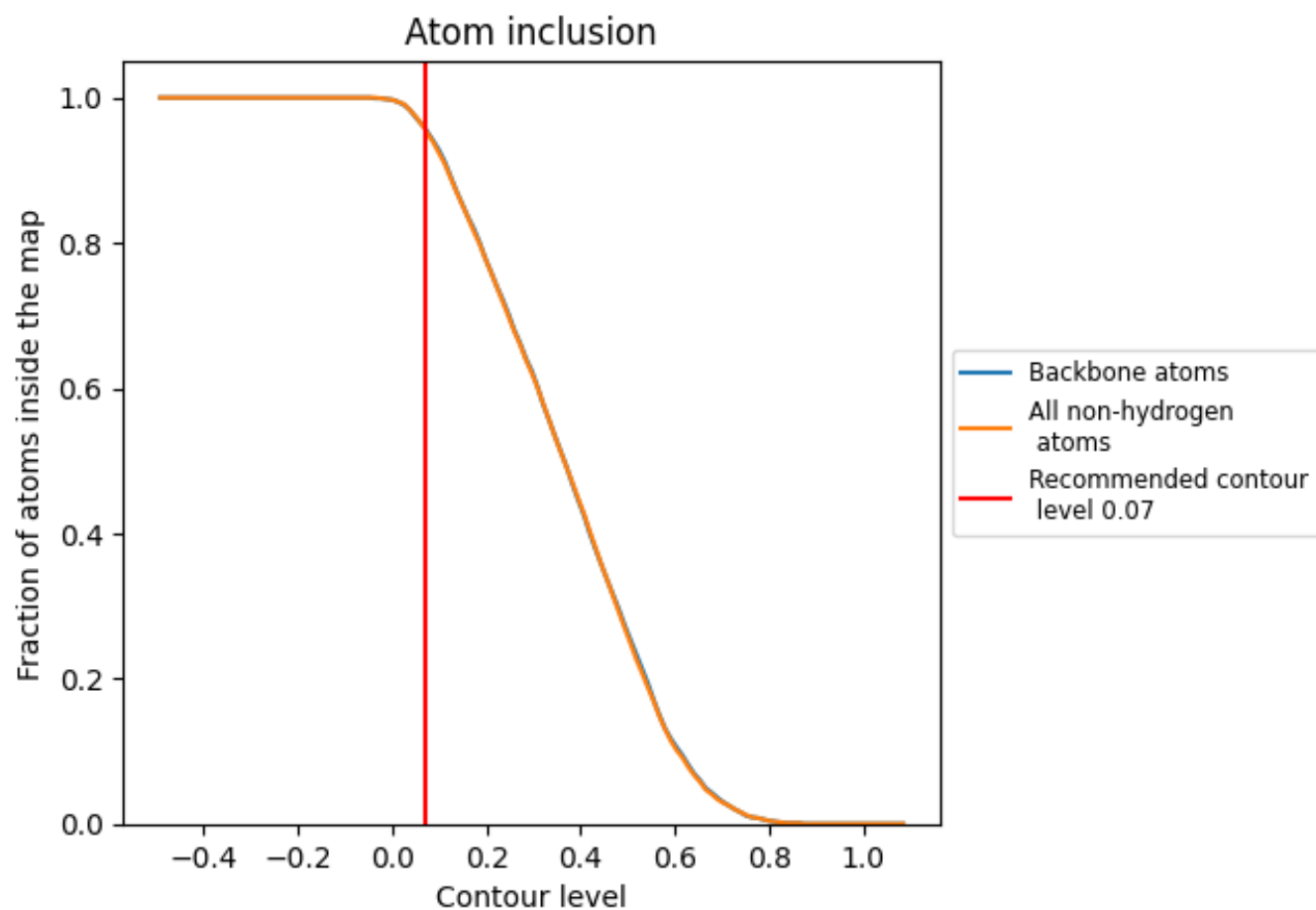
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9570</div>	<div><div></div>0.6340</div>
A	<div><div></div>0.9530</div>	<div><div></div>0.6330</div>
B	<div><div></div>0.9610</div>	<div><div></div>0.6340</div>
C	<div><div></div>0.9550</div>	<div><div></div>0.6330</div>
D	<div><div></div>0.9610</div>	<div><div></div>0.6420</div>
E	<div><div></div>0.9580</div>	<div><div></div>0.6370</div>
F	<div><div></div>0.9810</div>	<div><div></div>0.6280</div>
G	<div><div></div>0.9960</div>	<div><div></div>0.6500</div>
I	<div><div></div>0.9910</div>	<div><div></div>0.6260</div>
J	<div><div></div>0.8600</div>	<div><div></div>0.4350</div>
K	<div><div></div>0.9450</div>	<div><div></div>0.5800</div>
L	<div><div></div>0.8890</div>	<div><div></div>0.5050</div>
M	<div><div></div>0.8800</div>	<div><div></div>0.4450</div>
N	<div><div></div>0.8930</div>	<div><div></div>0.5230</div>

1.0

0.0

<0.0