



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:20 AM UTC

PDB ID : 9OUO / pdb\_00009ouo  
EMDB ID : EMD-70874  
Title : Native GABA-A receptor from rat cerebella, beta1-alpha1-beta1-alpha1-gamma2 subtype, in complex with GABA and PZ-II-029  
Authors : Sun, C.; Gouaux, E.  
Deposited on : 2025-05-29  
Resolution : 2.92 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

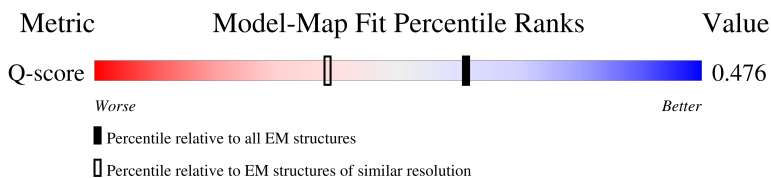
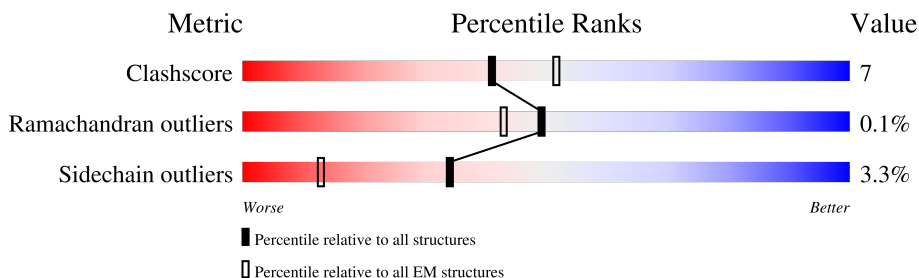
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.92 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 ( 2.42 - 3.42 )

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	D	466	
2	H	223	
2	J	223	
3	K	213	

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Mol	Chain	Length	Quality of chain
3	L	213	
4	A	455	
4	C	455	
5	B	474	
5	E	474	
6	F	2	
6	M	2	
6	O	2	
7	G	7	
8	I	3	
8	N	3	
8	P	3	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 24261 atoms, of which 11926 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 Gamma-aminobutyric acid receptor subunit gamma-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	D	208	Total	C	H	N	O	S	0	0
			3417	1105	1692	298	314	8		

- Molecule 2 is a protein called 8E3 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	117	Total	C	H	N	O	S	0	0
			1783	587	863	152	177	4		
2	J	117	Total	C	H	N	O	S	0	0
			1783	587	863	152	177	4		

- Molecule 3 is a protein called 8E3 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	105	Total	C	H	N	O	S	0	0
			1552	505	756	132	155	4		
3	K	105	Total	C	H	N	O	S	0	0
			1552	505	756	132	155	4		

- Molecule 4 is a protein called Gamma-aminobutyric acid receptor subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	213	Total	C	H	N	O	S	0	0
			3424	1094	1697	301	321	11		
4	C	212	Total	C	H	N	O	S	0	0
			3414	1090	1695	300	318	11		

- Molecule 5 is a protein called Gamma-aminobutyric acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	210	Total	C	H	N	O	S	0	0
			3382	1084	1681	286	320	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace	
5	E	210	Total	C	H	N	O	S	0	0
			3365	1081	1670	283	320	11		

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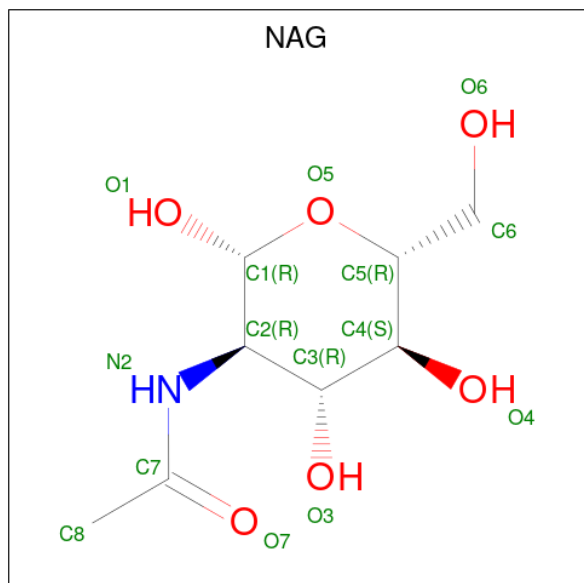
A diagram of a 1D chain consisting of a green circle followed by two blue squares, with a wavy line indicating the chain continues. The segments are labeled with  $\beta$  and 4 below the chain.



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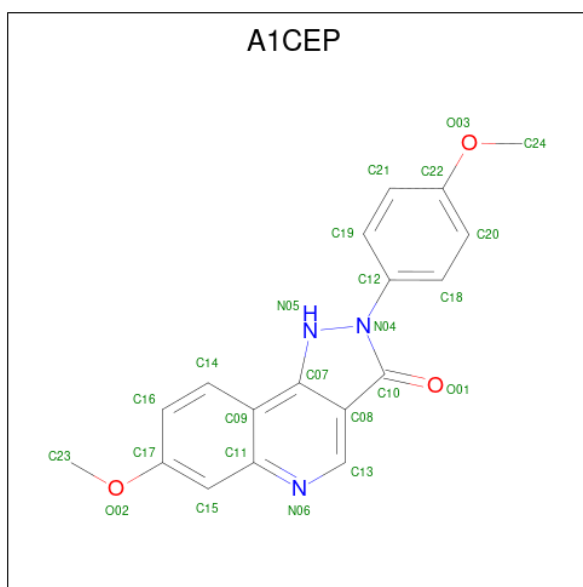
Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	3	Total	C	H	N	O	0
			73	22	34	2	15	
8	P	3	Total	C	H	N	O	0
			73	22	34	2	15	

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



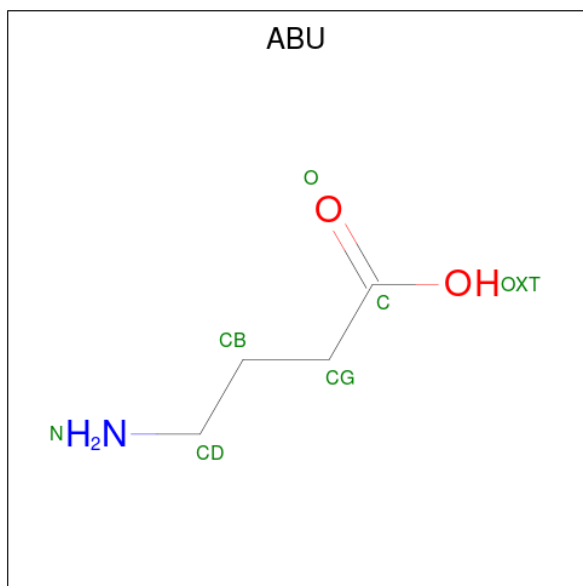
Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 10 is 7-methoxy-2-(4-methoxyphenyl)-1,2-dihydro-3H-pyrazolo[4,3-c]quinolin-3-one (CCD ID: A1CEP) (formula:  $C_{18}H_{15}N_3O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	H	N	O	0
			39	18	15	3	3	

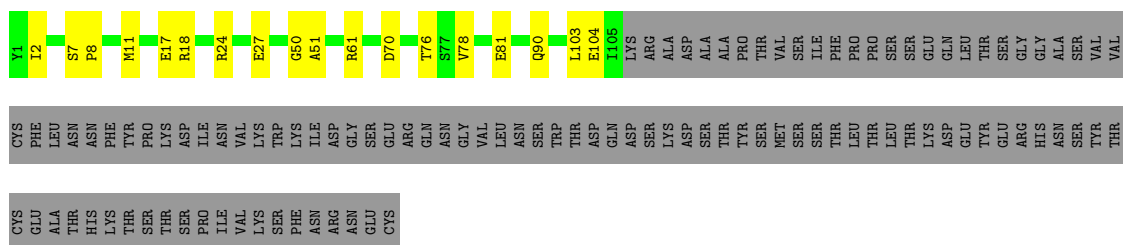
- Molecule 11 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula:  $C_4H_9NO_2$ ) (labeled as "Ligand of Interest" by depositor).



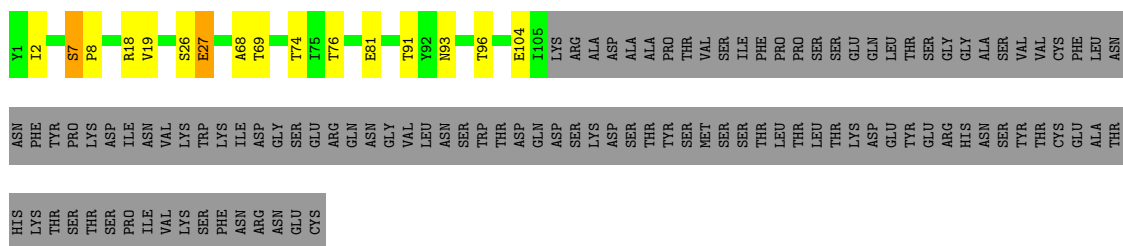
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	H	N	O	0
			16	4	9	1	2	
11	E	1	Total	C	H	N	O	0
			16	4	9	1	2	



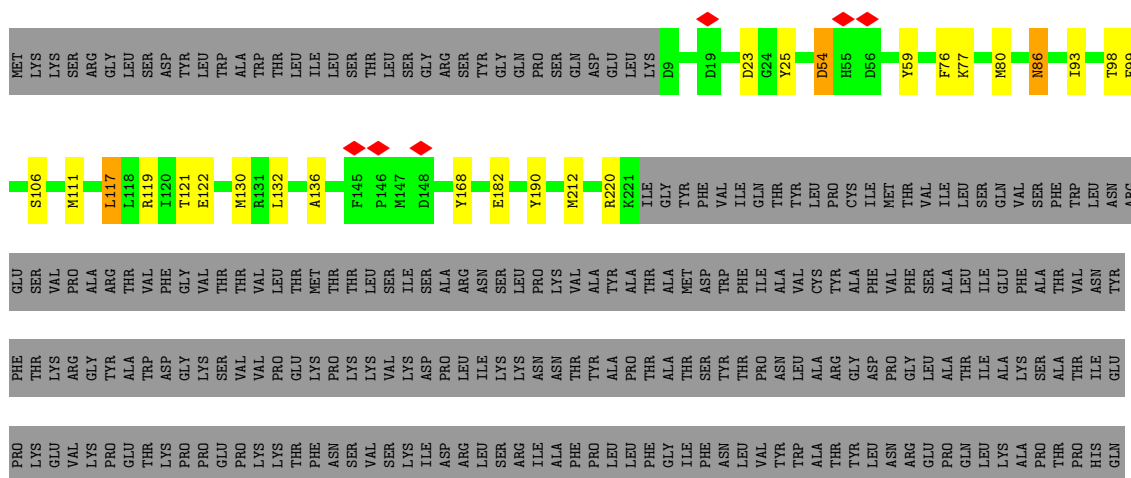
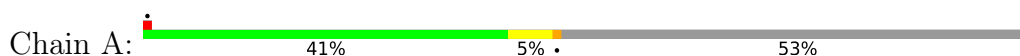
- Molecule 3: 8E3 Fab light chain



- Molecule 3: 8E3 Fab light chain



- Molecule 4: Gamma-aminobutyric acid receptor subunit alpha-1





[illegible]

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

Chain F:  100%

NAG1  
NAG2

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

Chain M: 

NAG1  
NAG2

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

Chain O:  100%

NAG1  
NAG2

- Molecule 7:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain G:  14% 71% 14%

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7
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- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%

NAG1  
NAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%

MAG1  
MAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

MAG1  
MAG2  
BMA3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.713	Depositor
Minimum map value	-0.341	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	344.16, 344.16, 344.16	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95600003, 0.95600003, 0.95600003	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, ABU, MAN, NAG, A1CEP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	D	0.19	0/1769	0.31	0/2403
2	H	0.18	0/946	0.35	0/1284
2	J	0.19	0/946	0.33	0/1284
3	K	0.18	0/815	0.34	0/1108
3	L	0.19	0/815	0.39	0/1108
4	A	0.19	0/1767	0.32	0/2393
4	C	0.21	0/1759	0.41	2/2382 (0.1%)
5	B	0.21	0/1738	0.41	0/2354
5	E	0.20	0/1732	0.35	0/2347
All	All	0.20	0/12287	0.36	2/16663 (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
5	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	100	PHE	CA-C-N	8.99	133.98	120.31
4	C	100	PHE	C-N-CA	8.99	133.98	120.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	109	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1725	1692	1693	33	0
2	H	920	863	863	10	0
2	J	920	863	863	18	0
3	K	796	756	756	9	0
3	L	796	756	756	11	0
4	A	1727	1697	1698	17	0
4	C	1719	1695	1694	27	0
5	B	1701	1681	1682	22	0
5	E	1695	1670	1671	21	0
6	F	28	0	25	6	0
6	M	28	25	25	0	0
6	O	28	25	25	0	0
7	G	83	70	70	1	0
8	I	39	32	34	0	0
8	N	39	34	34	3	0
8	P	39	34	34	5	0
9	D	14	0	13	2	0
10	C	24	15	0	4	0
11	C	7	9	0	0	0
11	E	7	9	0	0	0
All	All	12335	11926	11936	168	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 7.

All (168) 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)
10:C:501:A1CEP:C12	10:C:501:A1CEP:N04	1.67	1.55
1:D:194:ARG:O	1:D:194:ARG:NE	2.05	0.88
1:D:208:ASN:OD1	6:F:1:NAG:N2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:2:NAG:O3	8:N:3:BMA:O5	1.93	0.86
4:C:15:THR:OG1	5:B:24:ASP:OD2	1.95	0.85
4:C:101:HIS:NE2	10:C:501:A1CEP:O02	2.11	0.84
4:A:182:GLU:N	4:A:182:GLU:OE1	2.11	0.84
1:D:159:PRO:O	1:D:231:ARG:NH1	2.11	0.82
5:E:28:ARG:NH2	5:E:30:ASP:O	2.13	0.81
4:C:43:ASP:OD2	4:C:172:ARG:NH2	2.14	0.80
2:J:105:GLN:NE2	2:J:106:GLY:O	2.15	0.80
3:L:27:GLU:N	3:L:27:GLU:OE1	2.15	0.80
2:J:28:SER:OG	2:J:31:ASP:OD2	1.99	0.79
2:J:48:ILE:HG21	2:J:80:MET:HE3	1.62	0.78
2:J:48:ILE:HD13	2:J:80:MET:HE1	1.65	0.78
1:D:161:ASP:OD1	1:D:162:GLU:N	2.17	0.77
2:J:94:ARG:NH2	2:J:101:ASP:OD2	2.17	0.77
5:B:28:ARG:NH1	5:B:30:ASP:O	2.19	0.76
2:H:10:GLU:OE1	2:H:10:GLU:N	2.17	0.76
6:F:2:NAG:H83	6:F:2:NAG:H3	1.68	0.73
4:A:106:SER:OG	5:B:109:VAL:HG11	1.88	0.72
3:K:104:GLU:N	3:K:104:GLU:OE1	2.23	0.72
5:E:213:ARG:NH1	8:P:1:NAG:O7	2.24	0.71
1:D:197:ARG:NH1	4:C:137:GLU:OE2	2.24	0.71
5:E:155:GLU:OE1	5:E:207:ARG:NH2	2.23	0.71
5:B:190:ASP:OD1	5:B:191:TYR:N	2.27	0.67
4:C:198:ASP:OD1	4:C:199:SER:N	2.28	0.67
5:B:41:ARG:C	5:B:42:ILE:HD12	2.21	0.66
3:K:2:ILE:O	3:K:96:THR:HG21	1.95	0.66
3:L:17:GLU:N	3:L:17:GLU:OE1	2.29	0.65
2:H:94:ARG:NH2	2:H:101:ASP:OD2	2.30	0.64
1:D:190:VAL:HG13	1:D:196:TRP:CZ2	2.32	0.64
1:D:69:ASN:ND2	1:D:71:GLU:OE1	2.31	0.64
1:D:199:TYR:OH	4:C:57:MET:SD	2.56	0.63
2:J:48:ILE:HD13	2:J:80:MET:CE	2.28	0.62
5:B:41:ARG:NH2	5:B:169:ASN:OD1	2.32	0.62
5:B:189:VAL:HG21	5:B:215:LYS:CE	2.31	0.61
1:D:141:TYR:OH	1:D:143:LEU:HD23	2.00	0.60
3:K:68:ALA:O	3:K:69:THR:OG1	2.15	0.60
1:D:70:MET:SD	1:D:153:LEU:N	2.73	0.60
1:D:90:ASN:HB2	9:D:501:NAG:H2	1.83	0.60
1:D:70:MET:HE1	1:D:153:LEU:O	2.02	0.59
5:B:189:VAL:HG21	5:B:215:LYS:HE3	1.84	0.59
1:D:185:ARG:HG2	6:F:2:NAG:HN2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:102:ASN:N	4:C:102:ASN:OD1	2.35	0.59
2:H:54:ASN:ND2	2:H:56:ASP:OD1	2.35	0.59
3:K:27:GLU:OE1	3:K:27:GLU:N	2.37	0.58
3:L:24:ARG:NH1	3:L:70:ASP:OD1	2.37	0.58
1:D:32:ASN:OD1	4:C:28:ARG:NH2	2.37	0.57
7:G:2:NAG:H83	7:G:2:NAG:H3	1.87	0.57
4:C:48:SER:OG	4:C:186:ARG:NE	2.38	0.56
3:K:18:ARG:HH12	3:K:76:THR:HG22	1.70	0.56
4:A:130:MET:HE3	4:A:132:LEU:HD21	1.88	0.55
4:C:190:TYR:OH	4:C:220:ARG:NH2	2.40	0.55
1:D:207:ARG:NH1	1:D:228:ASP:OD2	2.40	0.55
3:K:81:GLU:N	3:K:81:GLU:OE1	2.40	0.55
5:E:172:GLU:N	5:E:172:GLU:OE1	2.40	0.54
8:N:2:NAG:HO3	8:N:3:BMA:C1	2.15	0.54
4:A:190:TYR:OH	4:A:220:ARG:NH2	2.42	0.53
4:C:111:MET:HG3	4:C:112:THR:HA	1.90	0.53
1:D:142:THR:HG21	10:C:501:A1CEP:O01	2.09	0.53
4:C:11:THR:HG22	4:C:11:THR:O	2.09	0.52
5:B:85:ASN:O	5:B:114:ARG:NH1	2.41	0.52
4:A:111:MET:HE1	5:E:106:VAL:HG23	1.92	0.52
5:E:44:VAL:HG11	5:E:181:ILE:HD11	1.91	0.52
3:K:91:THR:HG22	3:K:91:THR:O	2.10	0.51
5:B:199:GLU:OE1	5:B:199:GLU:N	2.36	0.51
4:C:154:LEU:C	4:C:154:LEU:HD23	2.35	0.51
4:C:176:ARG:NH1	3:K:93:ASN:OD1	2.43	0.51
1:D:193:THR:HG22	1:D:193:THR:O	2.10	0.51
5:E:189:VAL:HG12	5:E:189:VAL:O	2.11	0.51
5:E:189:VAL:O	5:E:190:ASP:HB2	2.12	0.50
5:E:53:VAL:HG23	5:E:54:ASN:OD1	2.12	0.50
1:D:188:VAL:HG11	1:D:206:LEU:CD1	2.42	0.50
5:E:52:GLU:OE1	5:E:138:MET:HE1	2.11	0.50
1:D:99:ASN:OD1	1:D:99:ASN:N	2.43	0.49
4:C:117:LEU:HD13	4:C:119:ARG:HE	1.77	0.49
4:C:187:LEU:HD12	4:C:187:LEU:H	1.76	0.49
5:E:44:VAL:CG1	5:E:181:ILE:HD11	2.42	0.49
1:D:170:SER:OG	1:D:171:SER:N	2.46	0.49
2:J:51:ILE:HG12	2:J:71:VAL:HG23	1.94	0.49
2:H:51:ILE:HD13	2:H:71:VAL:HG13	1.95	0.48
2:J:48:ILE:HG21	2:J:80:MET:CE	2.37	0.48
5:B:196:LYS:NZ	8:N:2:NAG:O7	2.37	0.48
1:D:120:ASP:N	1:D:120:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:16:THR:HG22	2:J:17:SER:H	1.79	0.48
5:B:107:HIS:NE2	5:B:131:THR:OG1	2.39	0.47
1:D:130:MET:HE1	4:C:206:THR:HG21	1.96	0.47
4:C:100:PHE:HE2	4:C:154:LEU:HD21	1.80	0.47
5:E:87:VAL:HG12	5:E:87:VAL:O	2.14	0.47
2:J:16:THR:HG22	2:J:17:SER:N	2.30	0.47
5:E:189:VAL:O	5:E:190:ASP:CB	2.63	0.46
8:P:1:NAG:O3	8:P:1:NAG:H82	2.15	0.46
1:D:190:VAL:HG12	1:D:191:GLY:O	2.15	0.46
3:L:18:ARG:HE	3:L:76:THR:HA	1.79	0.46
5:B:142:ARG:O	5:B:143:TYR:C	2.59	0.46
5:E:169:ASN:O	5:E:174:ALA:HB2	2.15	0.46
4:A:59:TYR:CE1	4:A:136:ALA:HB3	2.50	0.46
5:B:114:ARG:CB	5:B:128:LEU:HD23	2.46	0.46
4:A:54:ASP:N	4:A:54:ASP:OD1	2.49	0.46
3:K:7:SER:CB	3:K:8:PRO:HD3	2.45	0.46
1:D:65:VAL:HG23	1:D:65:VAL:O	2.16	0.46
5:B:114:ARG:HB3	5:B:128:LEU:HD23	1.97	0.46
6:F:2:NAG:H3	6:F:2:NAG:C8	2.42	0.46
6:F:1:NAG:H61	6:F:2:NAG:C7	2.46	0.46
1:D:208:ASN:OD1	1:D:208:ASN:N	2.49	0.45
3:L:11:MET:CG	3:L:103:LEU:HD12	2.46	0.45
4:A:117:LEU:C	4:A:117:LEU:HD12	2.42	0.45
2:H:109:LEU:HD13	2:H:109:LEU:C	2.42	0.45
4:A:86:ASN:OD1	4:A:86:ASN:N	2.43	0.45
4:C:120:ILE:HD12	4:C:120:ILE:N	2.32	0.45
5:B:109:VAL:O	5:B:109:VAL:HG13	2.16	0.45
2:J:12:VAL:HG23	2:J:111:VAL:HG12	1.99	0.45
1:D:150:GLU:N	1:D:150:GLU:OE1	2.50	0.45
1:D:90:ASN:HB2	9:D:501:NAG:H83	1.98	0.44
2:H:16:THR:HG22	2:H:17:SER:H	1.82	0.44
4:A:121:THR:HG22	4:A:122:GLU:N	2.31	0.44
4:A:98:THR:HG22	4:A:99:PHE:N	2.32	0.44
5:B:109:VAL:O	5:B:109:VAL:HG22	2.17	0.44
4:C:187:LEU:HD12	4:C:187:LEU:N	2.32	0.44
1:D:118:LYS:NZ	1:D:148:ASP:OD2	2.35	0.43
2:H:60:ASN:OD1	2:H:61:ARG:N	2.51	0.43
3:L:104:GLU:N	3:L:104:GLU:OE1	2.51	0.43
4:A:25:TYR:CE1	4:A:93:ILE:HA	2.53	0.43
5:B:178:VAL:HG21	5:B:191:TYR:CE2	2.53	0.43
5:E:9:MET:SD	5:E:9:MET:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:128:TYR:CE2	4:C:130:MET:HE3	2.54	0.43
5:B:84:ASP:OD1	5:B:85:ASN:N	2.52	0.43
4:C:43:ASP:OD1	4:C:44:ILE:N	2.52	0.43
2:H:6:GLN:N	2:H:105:GLN:OE1	2.50	0.43
4:A:77:LYS:HA	4:A:122:GLU:OE2	2.18	0.43
4:C:193:LEU:HD11	4:C:219:LYS:HB2	2.00	0.43
5:E:99:LEU:C	5:E:99:LEU:HD13	2.44	0.42
2:H:4:LEU:HD22	2:H:34:MET:HE1	2.02	0.42
1:D:176:ARG:HG3	1:D:221:VAL:HG23	2.01	0.42
4:C:118:LEU:HD23	4:C:120:ILE:HD11	2.01	0.42
3:L:2:ILE:HD12	3:L:90:GLN:OE1	2.19	0.42
2:H:13:LYS:NZ	2:H:112:SER:OG	2.42	0.42
8:P:1:NAG:H82	8:P:1:NAG:C3	2.49	0.42
3:L:7:SER:CB	3:L:8:PRO:HD2	2.49	0.42
3:L:50:GLY:O	3:L:51:ALA:HB3	2.20	0.42
5:E:161:THR:HG21	5:E:197:LYS:HG2	2.01	0.42
1:D:188:VAL:HG11	1:D:206:LEU:HD11	2.01	0.41
4:A:98:THR:O	5:B:110:THR:HB	2.20	0.41
8:P:1:NAG:O3	8:P:1:NAG:C8	2.68	0.41
2:J:109:LEU:C	2:J:109:LEU:HD13	2.45	0.41
4:A:168:TYR:O	4:A:212:MET:HE3	2.21	0.41
4:C:101:HIS:HE2	10:C:501:A1CEP:C23	2.25	0.41
1:D:201:PHE:HB3	1:D:229:LEU:HD13	2.03	0.41
3:L:7:SER:CB	3:L:8:PRO:CD	2.99	0.41
8:P:2:NAG:C6	8:P:3:BMA:C1	2.98	0.41
1:D:65:VAL:HG21	1:D:201:PHE:CE2	2.56	0.41
2:J:51:ILE:HD13	2:J:57:THR:HG22	2.01	0.41
3:L:81:GLU:OE1	3:L:81:GLU:N	2.43	0.41
4:C:105:LYS:HE3	4:C:105:LYS:HA	2.03	0.41
5:B:185:GLN:O	5:B:185:GLN:HG3	2.20	0.41
5:E:52:GLU:HA	5:E:138:MET:HE1	2.02	0.41
5:B:76:GLY:O	5:B:77:ILE:C	2.62	0.41
1:D:217:SER:OG	5:E:117:ARG:NH1	2.54	0.40
2:J:84:SER:HA	2:J:111:VAL:CG2	2.51	0.40
2:J:107:THR:O	2:J:107:THR:HG23	2.20	0.40
5:E:189:VAL:HG21	5:E:215:LYS:HE2	2.03	0.40
6:F:1:NAG:O7	6:F:1:NAG:H3	2.20	0.40
2:J:18:VAL:HG22	2:J:19:LYS:N	2.37	0.40
2:J:97:ASN:HB2	4:C:169:GLU:OE2	2.21	0.40
2:J:83:THR:O	2:J:111:VAL:HG21	2.21	0.40
4:A:76:PHE:O	4:A:122:GLU:OE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:119:ARG:NH2	5:E:205:TYR:OH	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	206/466 (44%)	196 (95%)	10 (5%)	0	100	100
2	H	115/223 (52%)	107 (93%)	8 (7%)	0	100	100
2	J	115/223 (52%)	105 (91%)	10 (9%)	0	100	100
3	K	103/213 (48%)	91 (88%)	12 (12%)	0	100	100
3	L	103/213 (48%)	94 (91%)	9 (9%)	0	100	100
4	A	211/455 (46%)	203 (96%)	8 (4%)	0	100	100
4	C	210/455 (46%)	201 (96%)	9 (4%)	0	100	100
5	B	208/474 (44%)	193 (93%)	15 (7%)	0	100	100
5	E	208/474 (44%)	198 (95%)	9 (4%)	1 (0%)	24	53
All	All	1479/3196 (46%)	1388 (94%)	90 (6%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	190	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	193/428 (45%)	184 (95%)	9 (5%)	23	55
2	H	98/195 (50%)	94 (96%)	4 (4%)	27	60
2	J	98/195 (50%)	97 (99%)	1 (1%)	68	87
3	K	83/188 (44%)	78 (94%)	5 (6%)	17	45
3	L	83/188 (44%)	81 (98%)	2 (2%)	43	73
4	A	192/404 (48%)	187 (97%)	5 (3%)	40	72
4	C	191/404 (47%)	186 (97%)	5 (3%)	40	72
5	B	190/423 (45%)	182 (96%)	8 (4%)	26	59
5	E	189/423 (45%)	184 (97%)	5 (3%)	40	72
All	All	1317/2848 (46%)	1273 (97%)	44 (3%)	34	65

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	43	ARG
1	D	69	ASN
1	D	99	ASN
1	D	124	ILE
1	D	168	GLU
1	D	206	LEU
1	D	209	THR
1	D	228	ASP
1	D	231	ARG
2	H	16	THR
2	H	68	THR
2	H	105	GLN
2	H	109	LEU
2	J	69	LEU
3	L	61	ARG
3	L	78	VAL
4	A	23	ASP
4	A	54	ASP
4	A	80	MET
4	A	86	ASN
4	A	117	LEU
4	C	10	ASN
4	C	102	ASN

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Mol	Chain	Res	Type
4	C	187	LEU
4	C	195	GLN
4	C	214	THR
3	K	7	SER
3	K	19	VAL
3	K	26	SER
3	K	27	GLU
3	K	74	THR
5	B	13	LYS
5	B	24	ASP
5	B	59	LEU
5	B	101	ASP
5	B	114	ARG
5	B	141	ARG
5	B	151	THR
5	B	202	THR
5	E	13	LYS
5	E	28	ARG
5	E	85	ASN
5	E	183	LEU
5	E	202	THR

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

Mol	Chain	Res	Type
2	H	97	ASN
2	J	82(A)	ASN
4	A	87	ASN
4	C	203	GLN
5	E	85	ASN

### 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

22 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	F	1	1,6	14,14,15	0.79	0	17,19,21	1.43	2 (11%)
6	NAG	F	2	6	14,14,15	0.74	0	17,19,21	1.22	1 (5%)
7	NAG	G	1	7,4	14,14,15	0.67	0	17,19,21	1.19	2 (11%)
7	NAG	G	2	7	14,14,15	0.66	0	17,19,21	1.57	2 (11%)
7	BMA	G	3	7	11,11,12	0.75	0	15,15,17	2.82	4 (26%)
7	MAN	G	4	7	11,11,12	0.68	0	15,15,17	1.76	2 (13%)
7	MAN	G	5	7	11,11,12	0.74	0	15,15,17	1.20	1 (6%)
7	MAN	G	6	7	11,11,12	0.78	0	15,15,17	1.00	1 (6%)
7	MAN	G	7	7	11,11,12	0.77	0	15,15,17	0.92	0
8	NAG	I	1	8,4	14,14,15	0.79	0	17,19,21	1.05	1 (5%)
8	NAG	I	2	8	14,14,15	0.74	0	17,19,21	0.83	0
8	BMA	I	3	8	11,11,12	0.81	0	15,15,17	1.62	2 (13%)
6	NAG	M	1	5,6	14,14,15	0.76	0	17,19,21	1.09	1 (5%)
6	NAG	M	2	6	14,14,15	0.74	0	17,19,21	0.92	1 (5%)
8	NAG	N	1	5,8	14,14,15	0.86	0	17,19,21	1.31	1 (5%)
8	NAG	N	2	8	14,14,15	0.84	0	17,19,21	1.17	1 (5%)
8	BMA	N	3	8	11,11,12	0.85	0	15,15,17	1.89	3 (20%)
6	NAG	O	1	5,6	14,14,15	0.76	0	17,19,21	1.15	2 (11%)
6	NAG	O	2	6	14,14,15	0.70	0	17,19,21	1.18	2 (11%)
8	NAG	P	1	5,8	14,14,15	1.00	1 (7%)	17,19,21	2.21	8 (47%)
8	NAG	P	2	8	14,14,15	0.69	0	17,19,21	2.29	5 (29%)
8	BMA	P	3	8	11,11,12	0.81	0	15,15,17	2.91	7 (46%)

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	F	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	4/6/23/26	0/1/1/1
7	NAG	G	1	7,4	-	1/6/23/26	0/1/1/1
7	NAG	G	2	7	-	4/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	1/1/1/1
7	MAN	G	6	7	-	1/2/19/22	0/1/1/1
7	MAN	G	7	7	-	1/2/19/22	0/1/1/1
8	NAG	I	1	8,4	-	1/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	BMA	I	3	8	-	1/2/19/22	0/1/1/1
6	NAG	M	1	5,6	-	1/6/23/26	0/1/1/1
6	NAG	M	2	6	-	1/6/23/26	0/1/1/1
8	NAG	N	1	5,8	-	3/6/23/26	0/1/1/1
8	NAG	N	2	8	-	0/6/23/26	0/1/1/1
8	BMA	N	3	8	-	1/2/19/22	0/1/1/1
6	NAG	O	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
8	NAG	P	1	5,8	-	3/6/23/26	0/1/1/1
8	NAG	P	2	8	-	0/6/23/26	0/1/1/1
8	BMA	P	3	8	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	1	NAG	O5-C1	-2.11	1.40	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	3	BMA	C1-O5-C5	8.90	124.11	112.19
8	P	3	BMA	C1-O5-C5	8.07	123.00	112.19
7	G	4	MAN	C1-O5-C5	5.67	119.79	112.19
8	P	2	NAG	C1-O5-C5	5.61	119.70	112.19
8	N	3	BMA	C1-O5-C5	5.47	119.52	112.19
8	P	1	NAG	C2-N2-C7	5.45	130.21	122.90
7	G	2	NAG	C2-N2-C7	4.88	129.43	122.90
8	I	3	BMA	C1-O5-C5	4.32	117.97	112.19
8	N	1	NAG	C2-N2-C7	4.13	128.44	122.90
6	F	1	NAG	C2-N2-C7	3.97	128.22	122.90
8	P	2	NAG	C1-C2-N2	-3.94	104.23	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	3	BMA	C2-C3-C4	3.89	117.70	110.86
8	P	2	NAG	C2-N2-C7	3.76	127.94	122.90
6	F	2	NAG	C2-N2-C7	3.67	127.82	122.90
8	P	3	BMA	C1-C2-C3	3.56	114.83	109.64
7	G	3	BMA	C3-C4-C5	3.41	116.42	110.23
8	P	1	NAG	C4-C3-C2	3.27	115.81	111.02
6	O	2	NAG	C2-N2-C7	3.26	127.27	122.90
8	I	1	NAG	O5-C1-C2	-3.19	106.35	111.29
7	G	5	MAN	C1-O5-C5	3.14	116.39	112.19
7	G	3	BMA	O4-C4-C3	-2.99	103.34	110.38
8	P	1	NAG	C8-C7-N2	2.93	120.98	116.12
8	P	3	BMA	C3-C4-C5	2.78	115.27	110.23
8	P	3	BMA	O3-C3-C2	-2.77	104.40	110.05
7	G	1	NAG	C2-N2-C7	2.72	126.54	122.90
6	M	1	NAG	C1-O5-C5	2.67	115.76	112.19
8	P	1	NAG	O5-C5-C4	-2.66	104.36	110.83
7	G	3	BMA	O5-C5-C4	2.62	117.19	110.83
8	P	3	BMA	O5-C1-C2	2.57	116.92	110.79
7	G	6	MAN	C1-O5-C5	2.49	115.52	112.19
6	O	1	NAG	O4-C4-C3	-2.40	104.71	110.38
8	P	3	BMA	O4-C4-C3	-2.37	104.79	110.38
8	P	1	NAG	C1-C2-N2	-2.36	106.71	110.43
8	N	3	BMA	C3-C4-C5	2.36	114.50	110.23
6	M	2	NAG	O5-C1-C2	-2.34	107.67	111.29
6	F	1	NAG	O5-C1-C2	-2.32	107.71	111.29
7	G	1	NAG	O5-C1-C2	-2.30	107.73	111.29
8	P	2	NAG	O5-C5-C6	-2.30	103.19	107.66
8	P	1	NAG	O5-C5-C6	2.29	112.11	107.66
8	P	1	NAG	C1-O5-C5	-2.26	109.16	112.19
7	G	2	NAG	C8-C7-N2	2.20	119.77	116.12
8	P	1	NAG	O7-C7-C8	-2.18	118.17	122.05
6	O	1	NAG	O5-C1-C2	-2.14	107.98	111.29
8	N	3	BMA	O4-C4-C3	-2.10	105.42	110.38
8	N	2	NAG	C2-N2-C7	2.10	125.71	122.90
8	P	2	NAG	O5-C1-C2	2.07	114.50	111.29
6	O	2	NAG	O5-C1-C2	-2.03	108.15	111.29
7	G	4	MAN	O2-C2-C1	-2.01	104.62	109.22
8	I	3	BMA	O4-C4-C3	-2.01	105.64	110.38

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C3-C2-N2-C7
7	G	1	NAG	C1-C2-N2-C7
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
6	O	2	NAG	C8-C7-N2-C2
6	O	2	NAG	O7-C7-N2-C2
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
8	N	1	NAG	C8-C7-N2-C2
8	N	1	NAG	O7-C7-N2-C2
8	P	1	NAG	C8-C7-N2-C2
8	P	1	NAG	O7-C7-N2-C2
6	O	1	NAG	O5-C5-C6-O6
8	I	3	BMA	O5-C5-C6-O6
8	I	1	NAG	O5-C5-C6-O6
7	G	7	MAN	O5-C5-C6-O6
7	G	6	MAN	O5-C5-C6-O6
8	P	3	BMA	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
8	N	1	NAG	O5-C5-C6-O6
8	P	1	NAG	C3-C2-N2-C7
6	F	2	NAG	C3-C2-N2-C7
7	G	2	NAG	C3-C2-N2-C7
8	N	3	BMA	O5-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	F	2	NAG	C1-C2-N2-C7
7	G	2	NAG	C1-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	5	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 15 short contacts:

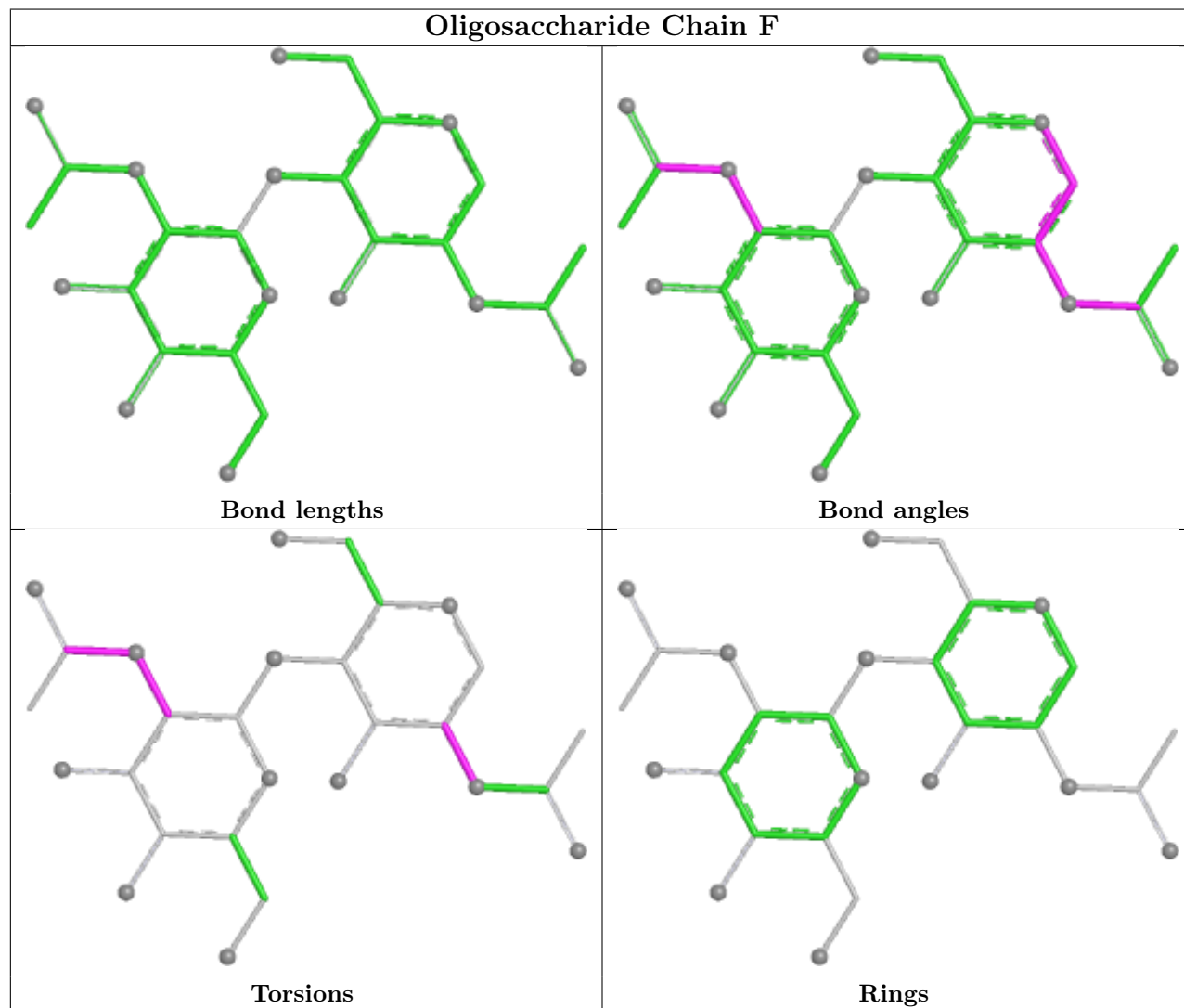
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	P	2	NAG	1	0
8	N	3	BMA	2	0
8	N	2	NAG	3	0
8	P	3	BMA	1	0
6	F	1	NAG	3	0
7	G	2	NAG	1	0

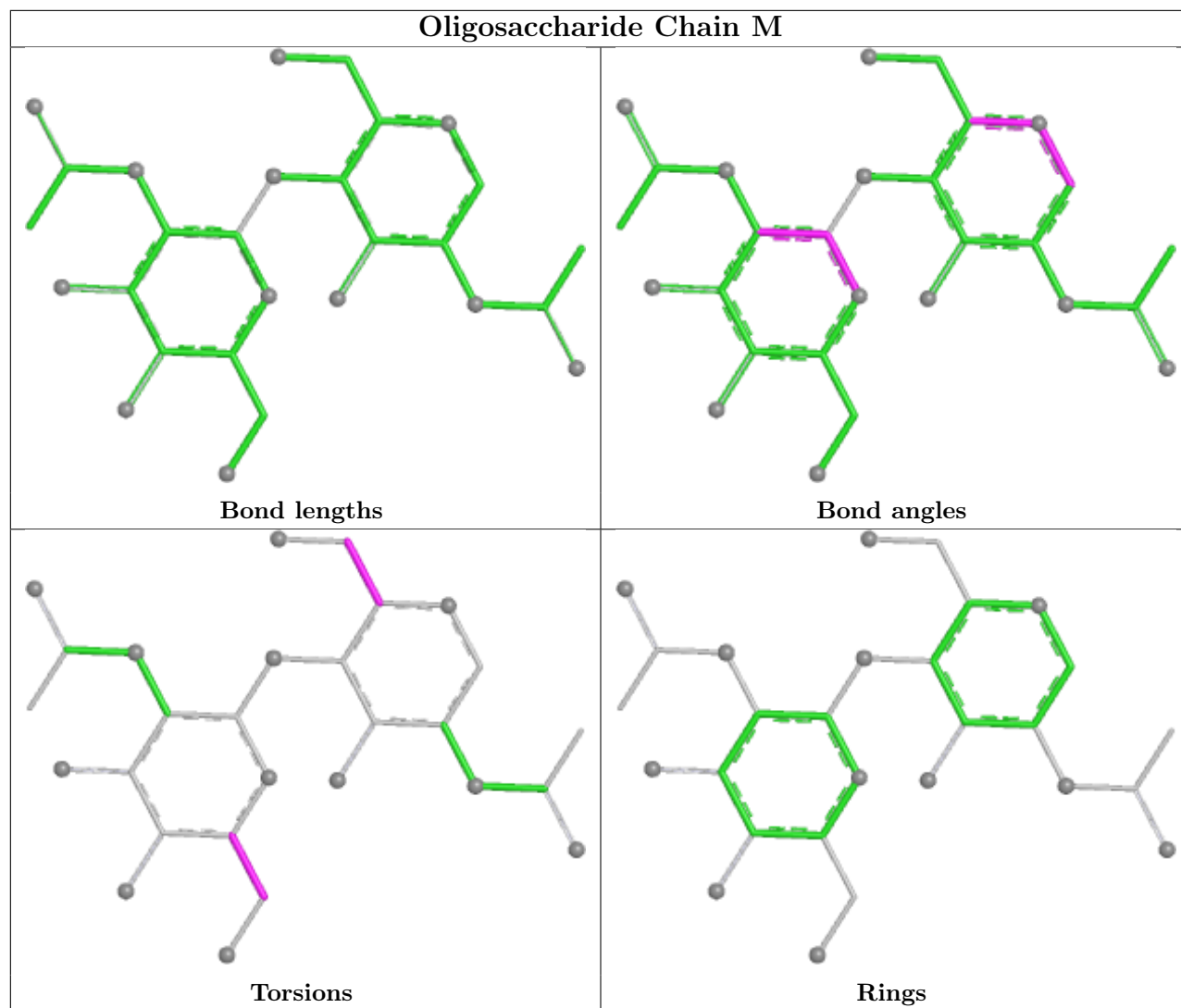
*Continued on next page...*

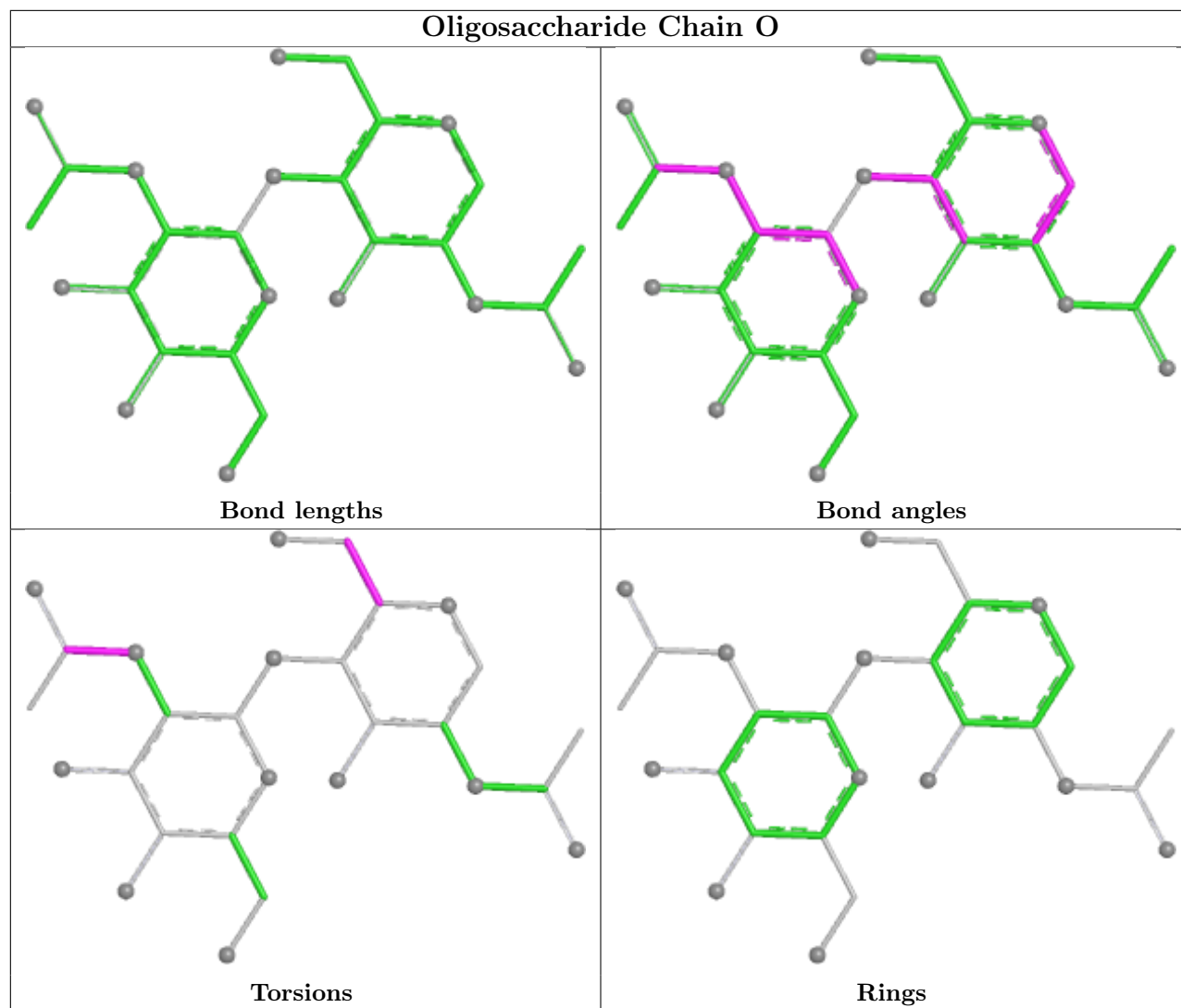
*Continued from previous page...*

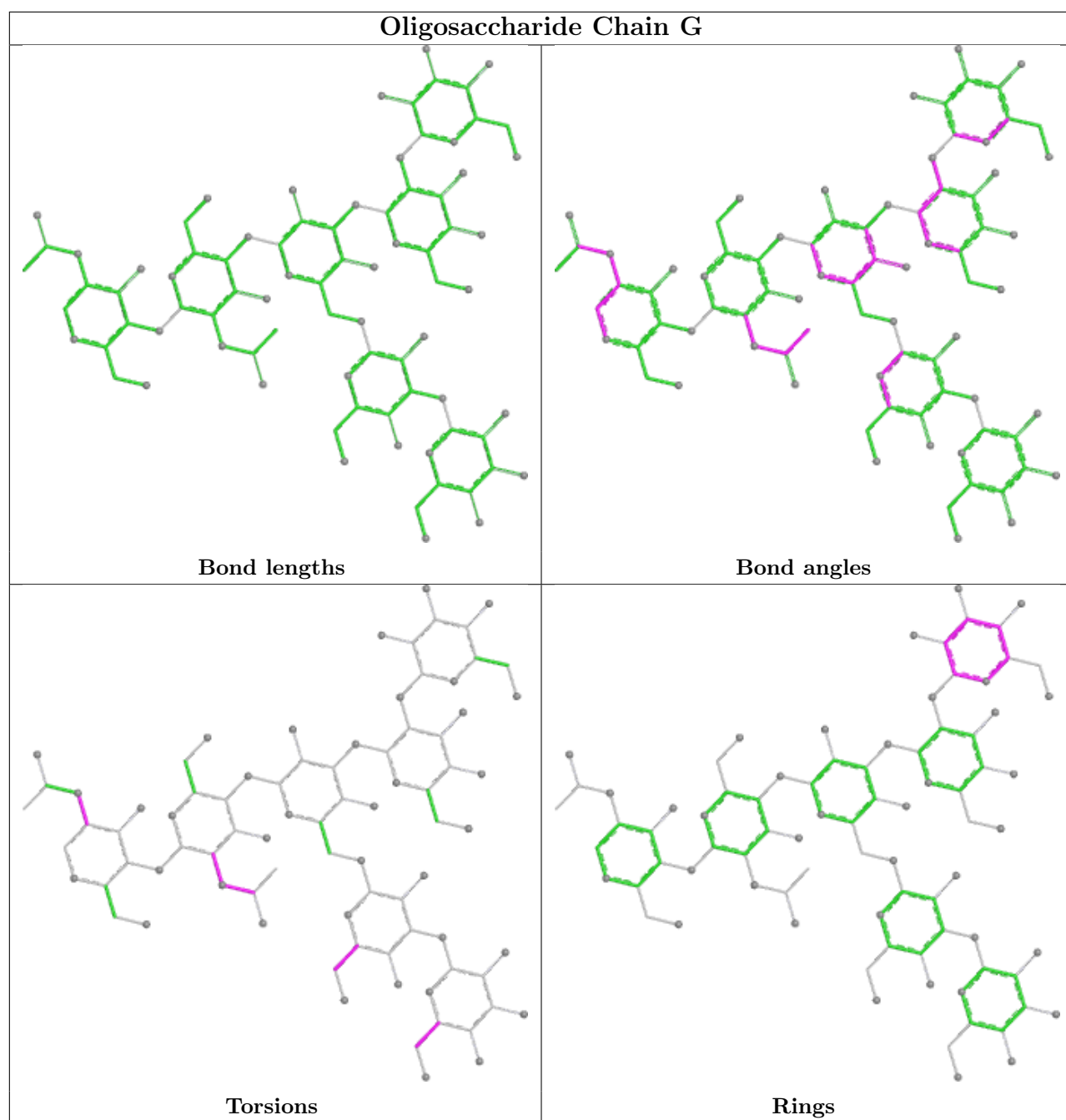
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	NAG	4	0
8	P	1	NAG	4	0

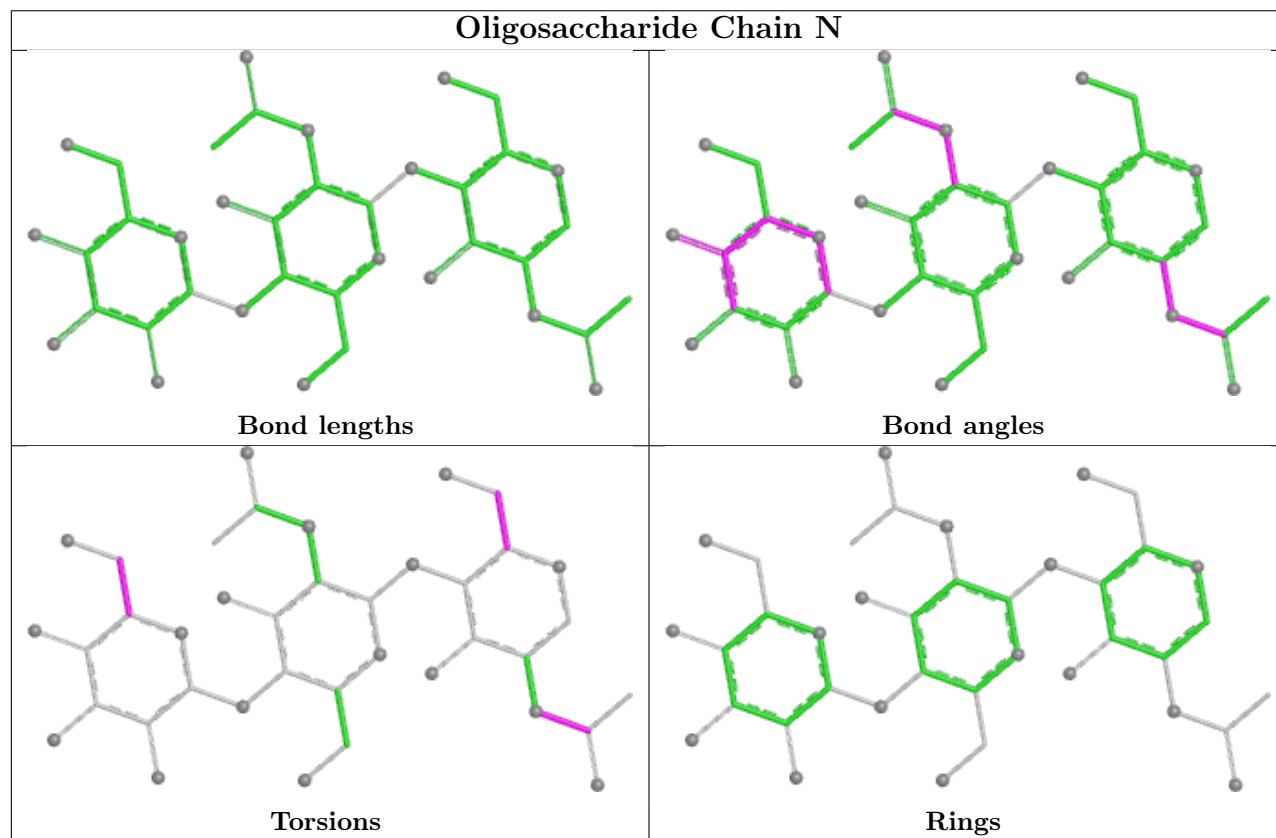
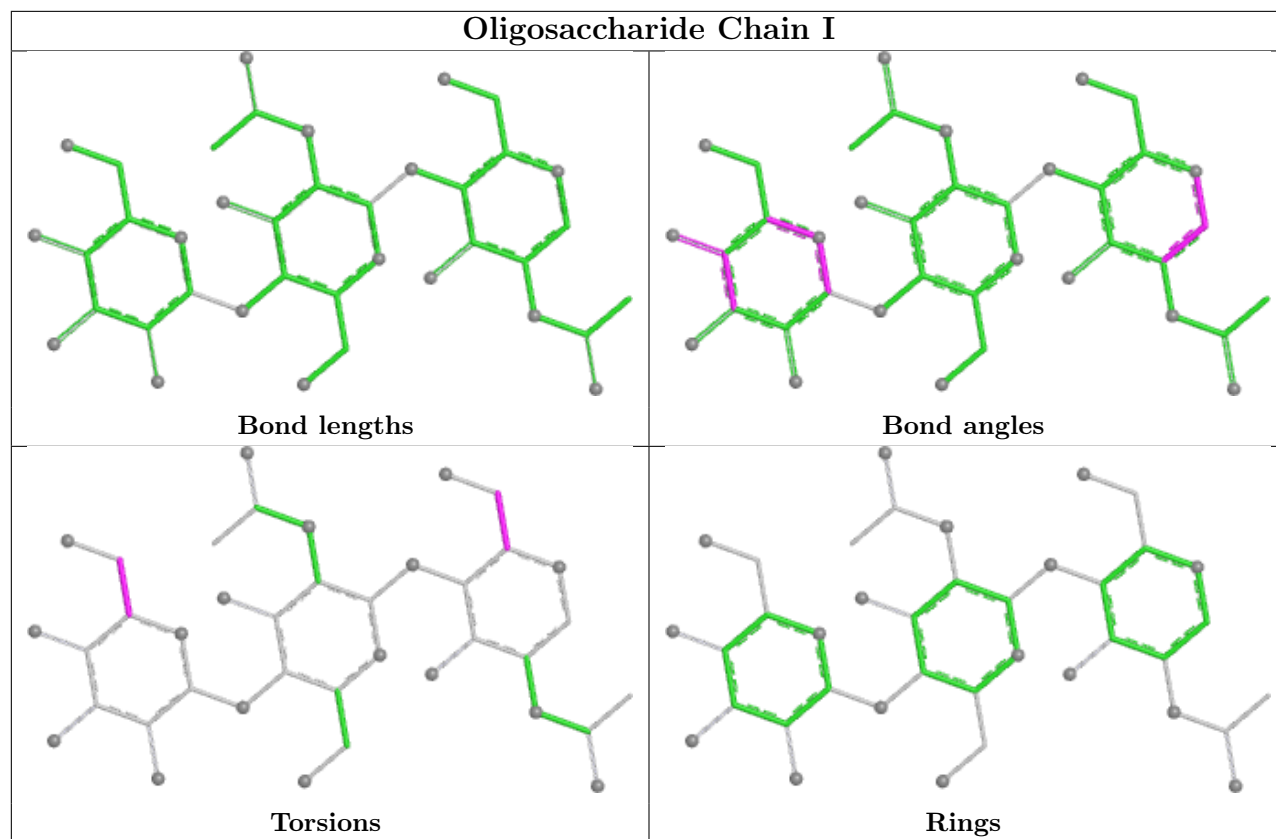
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

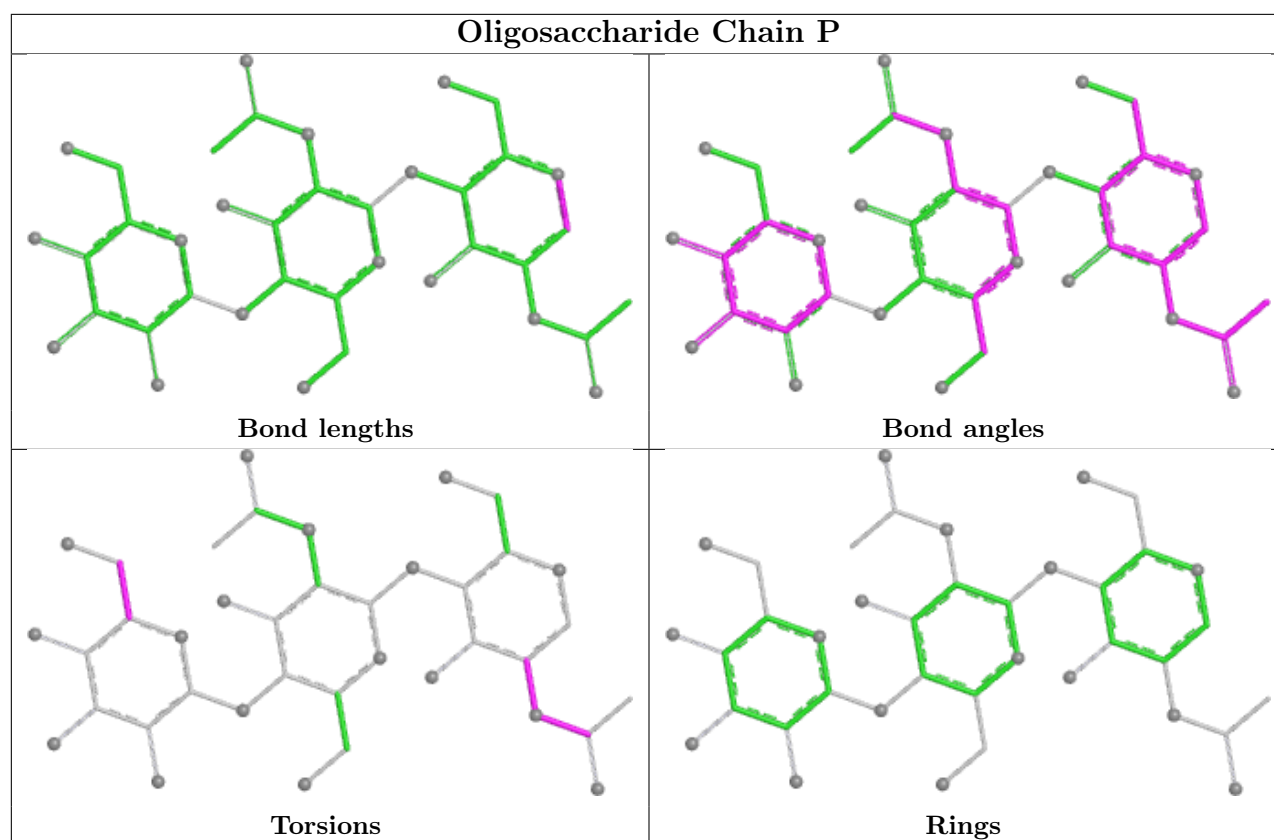












## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
9	NAG	D	501	1	14,14,15	0.72	0	17,19,21	0.75	0
11	ABU	E	501	-	6,6,6	2.14	2 (33%)	6,6,6	0.95	0
10	A1CEP	C	501	-	24,27,27	6.69	15 (62%)	31,39,39	2.98	14 (45%)
11	ABU	C	502	-	6,6,6	2.14	2 (33%)	6,6,6	0.94	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
9	NAG	D	501	1	-	3/6/23/26	0/1/1/1
11	ABU	E	501	-	-	0/4/4/4	-
10	A1CEP	C	501	-	-	2/8/8/8	0/4/4/4
11	ABU	C	502	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	501	A1CEP	C12-N04	19.39	1.67	1.42
10	C	501	A1CEP	C07-C09	15.22	1.69	1.43
10	C	501	A1CEP	C15-C11	13.87	1.63	1.41
10	C	501	A1CEP	C11-N06	9.39	1.53	1.37
10	C	501	A1CEP	C16-C17	5.76	1.49	1.38
10	C	501	A1CEP	C13-C08	5.55	1.50	1.40
10	C	501	A1CEP	C14-C09	4.91	1.52	1.42
11	C	502	ABU	CG-C	4.41	1.60	1.50
11	E	501	ABU	CG-C	4.39	1.60	1.50
10	C	501	A1CEP	C08-C10	4.22	1.55	1.48
10	C	501	A1CEP	C21-C19	3.91	1.45	1.38
10	C	501	A1CEP	C20-C18	3.77	1.44	1.38
10	C	501	A1CEP	O02-C17	3.74	1.45	1.37
10	C	501	A1CEP	O03-C22	2.68	1.42	1.37
11	C	502	ABU	O-C	2.46	1.30	1.22
11	E	501	ABU	O-C	2.46	1.30	1.22
10	C	501	A1CEP	C21-C22	2.41	1.43	1.38
10	C	501	A1CEP	C19-C12	2.33	1.43	1.39
10	C	501	A1CEP	C18-C12	2.25	1.43	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	501	A1CEP	C08-C10-N04	10.48	111.37	104.84
10	C	501	A1CEP	C13-N06-C11	6.18	124.12	116.96
10	C	501	A1CEP	C15-C11-N06	5.33	124.13	118.01
10	C	501	A1CEP	C09-C11-N06	-3.94	118.65	122.82
10	C	501	A1CEP	C16-C14-C09	3.03	125.40	121.15
10	C	501	A1CEP	C08-C07-C09	-2.89	119.04	122.09
10	C	501	A1CEP	C17-C15-C11	2.71	122.66	119.12
10	C	501	A1CEP	C24-O03-C22	2.48	122.81	117.50
10	C	501	A1CEP	C16-C17-C15	-2.42	117.68	120.83
10	C	501	A1CEP	C21-C22-C20	-2.28	116.84	120.16
10	C	501	A1CEP	C23-O02-C17	2.25	122.33	117.50

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	501	A1CEP	C19-C12-N04	2.21	122.21	119.84
10	C	501	A1CEP	C15-C11-C09	-2.12	117.22	119.58
10	C	501	A1CEP	C07-C08-C10	-2.10	106.13	108.16

There are no chirality outliers.

All (7) torsion outliers are listed below:

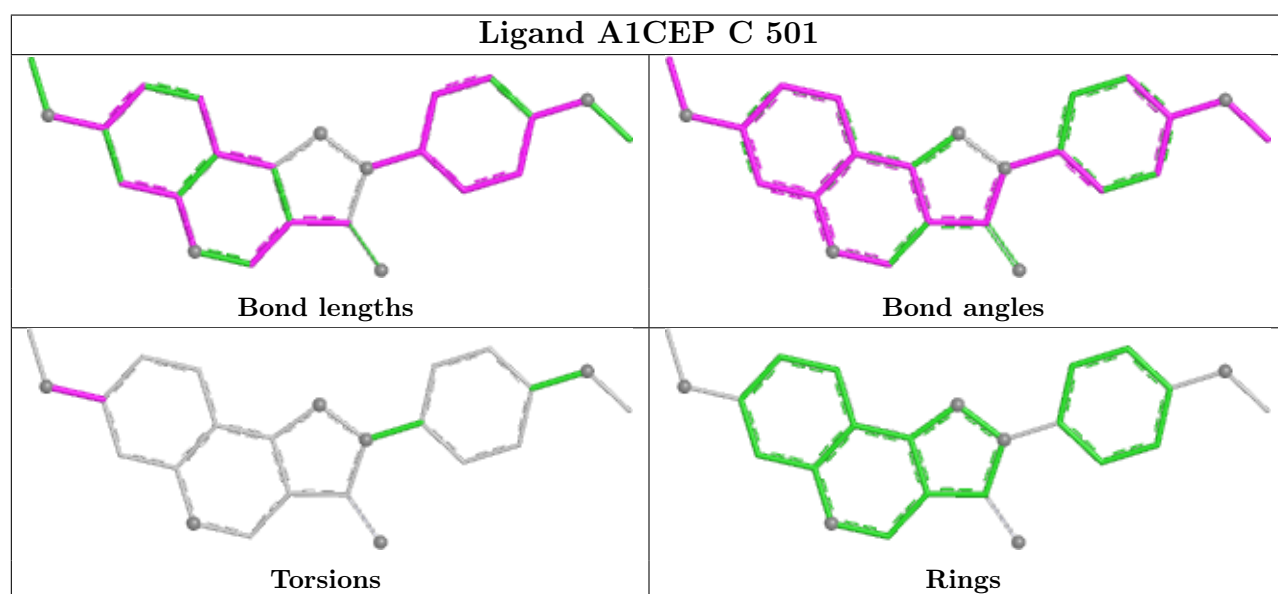
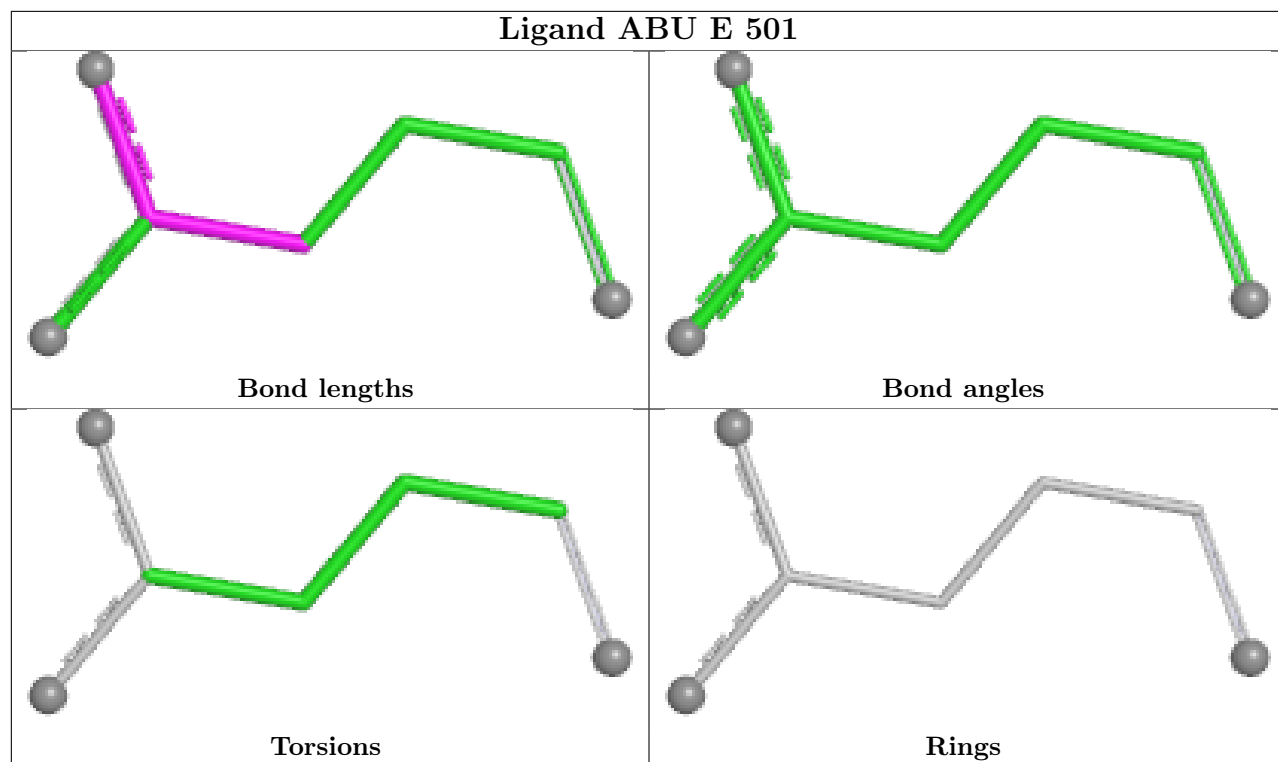
Mol	Chain	Res	Type	Atoms
10	C	501	A1CEP	C16-C17-O02-C23
10	C	501	A1CEP	C15-C17-O02-C23
9	D	501	NAG	C8-C7-N2-C2
9	D	501	NAG	O7-C7-N2-C2
9	D	501	NAG	O5-C5-C6-O6
11	C	502	ABU	O-C-CG-CB
11	C	502	ABU	OXT-C-CG-CB

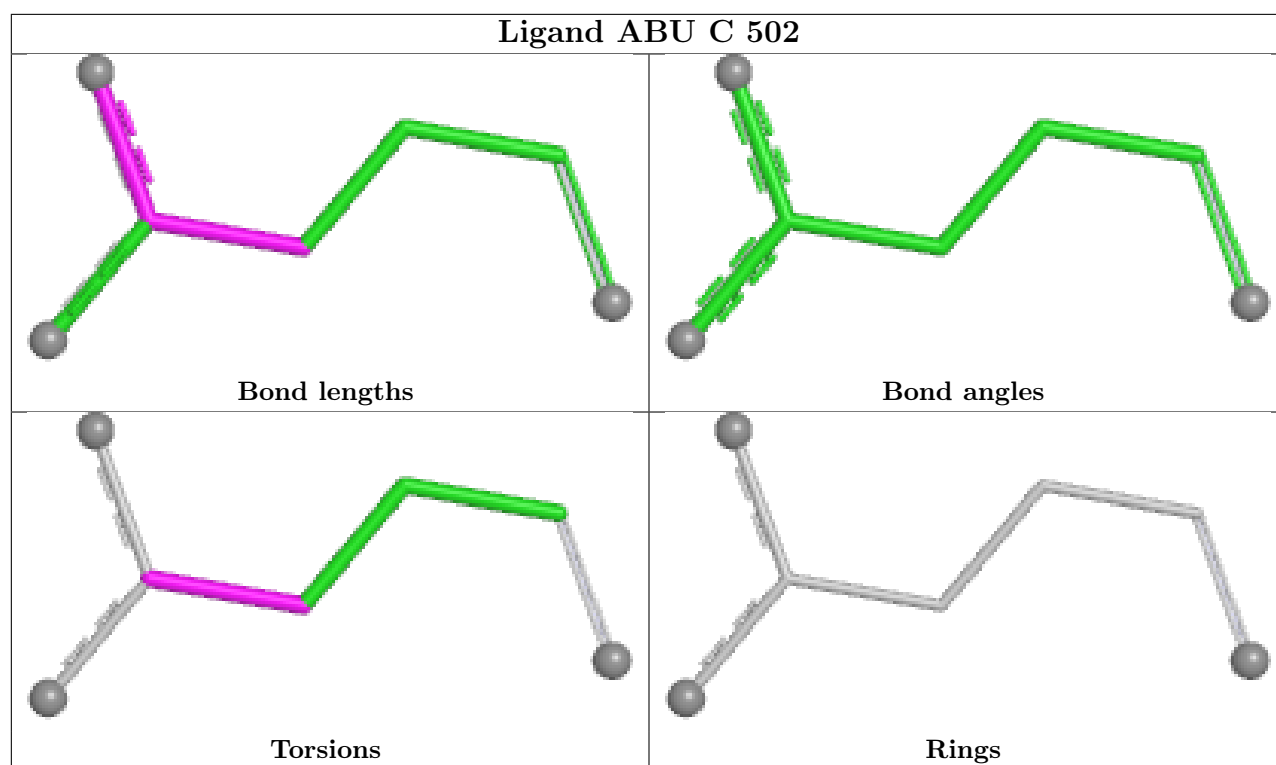
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	NAG	2	0
10	C	501	A1CEP	4	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.

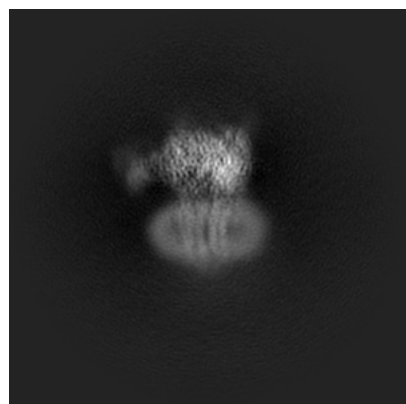
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70874. These allow visual inspection of the internal detail of the map and identification of artifacts.

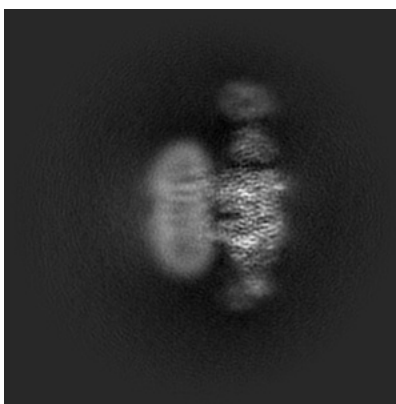
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

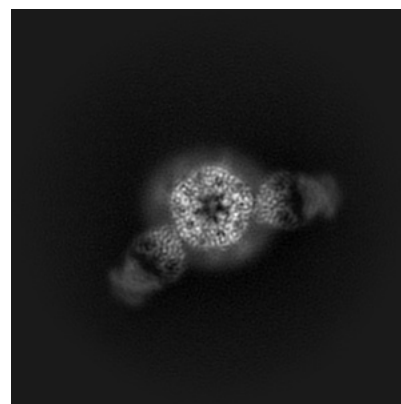
#### 6.1.1 Primary map



X

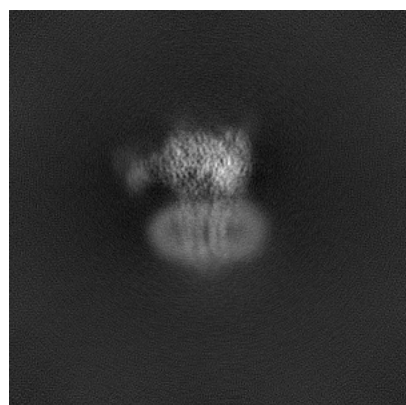


Y

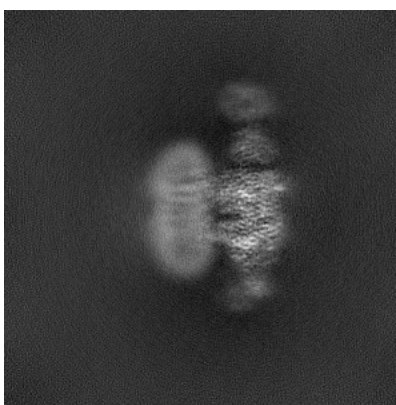


Z

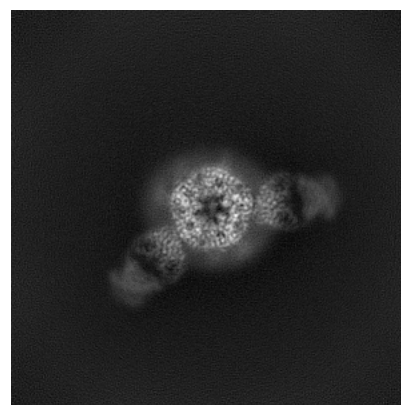
#### 6.1.2 Raw map



X



Y

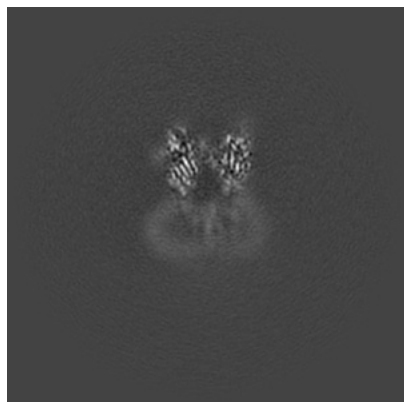


Z

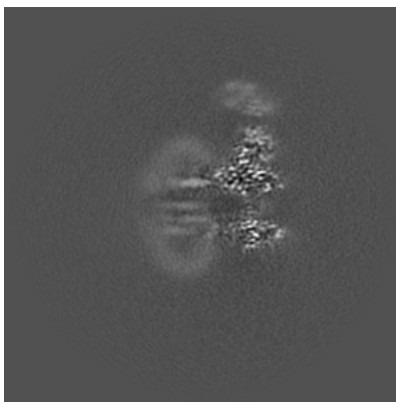
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

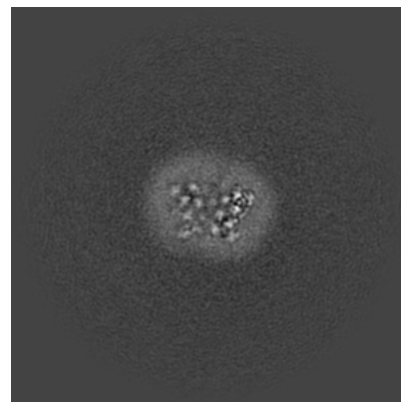
### 6.2.1 Primary map



X Index: 180

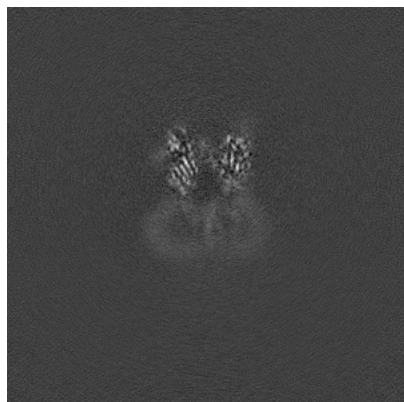


Y Index: 180

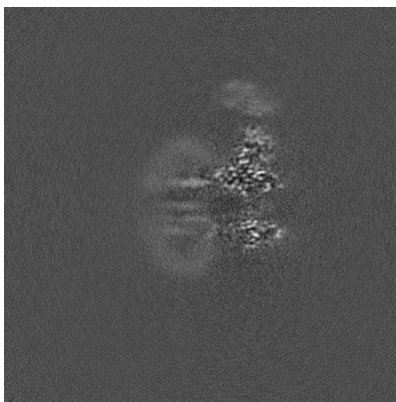


Z Index: 180

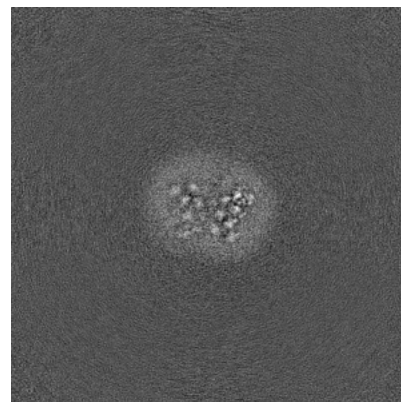
### 6.2.2 Raw map



X Index: 180



Y Index: 180

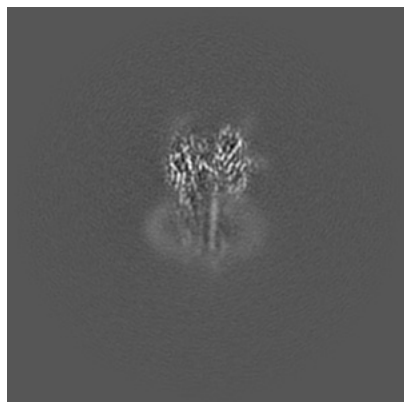


Z Index: 180

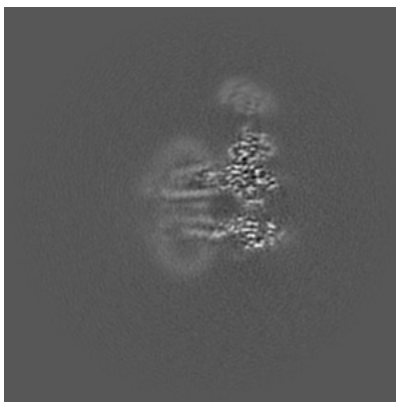
The images above show central slices of the map in three orthogonal directions.

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

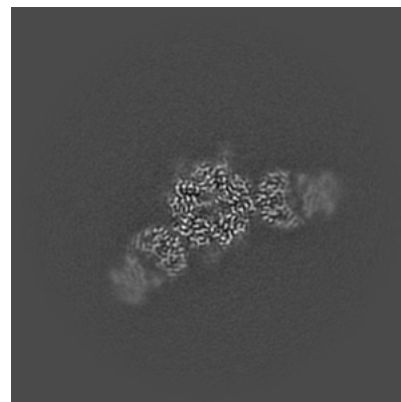
### 6.3.1 Primary map



X Index: 193

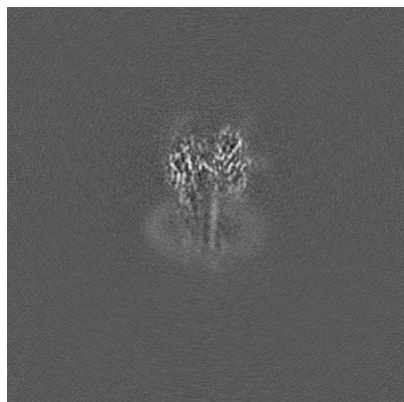


Y Index: 185

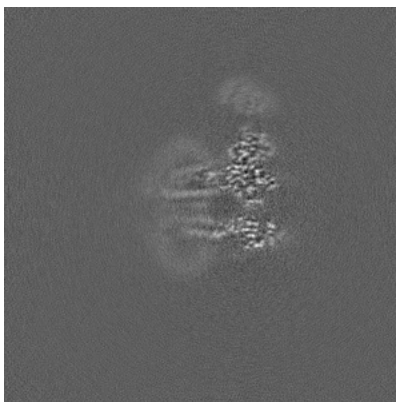


Z Index: 222

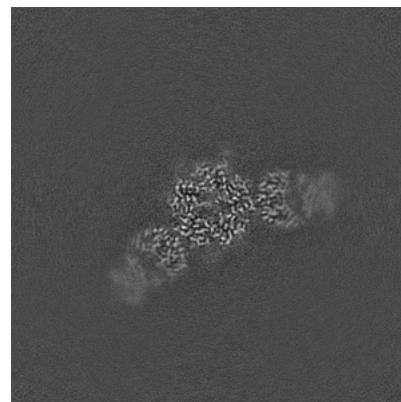
### 6.3.2 Raw map



X Index: 193



Y Index: 185

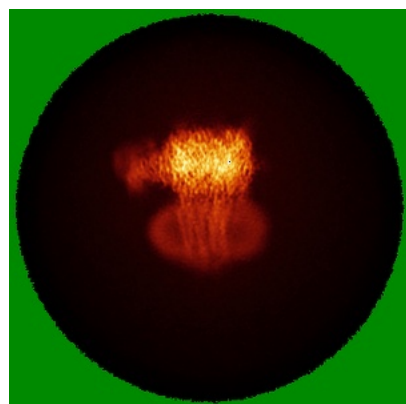


Z Index: 222

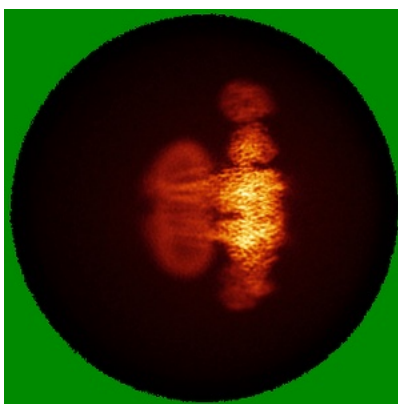
The images above show the largest variance slices of the map in three orthogonal directions.

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

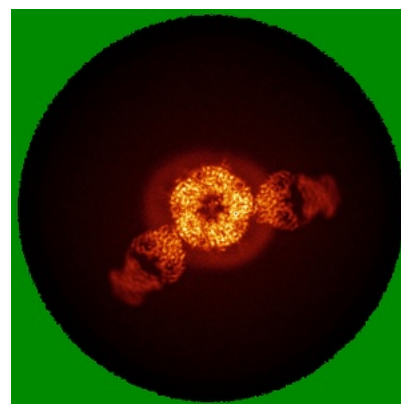
### 6.4.1 Primary map



X

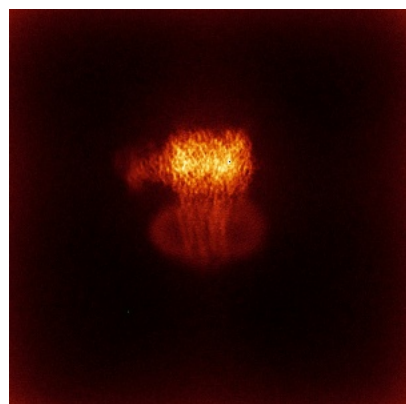


Y

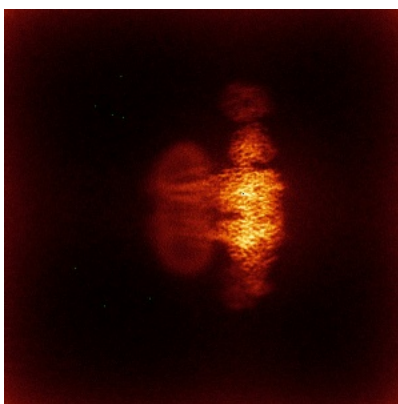


Z

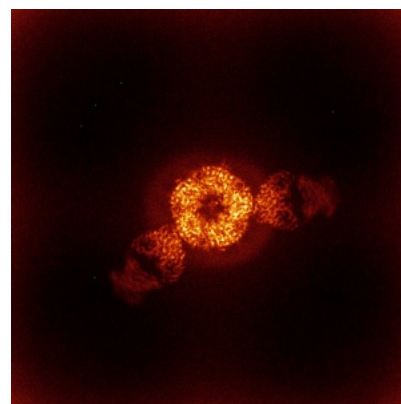
### 6.4.2 Raw map



X



Y

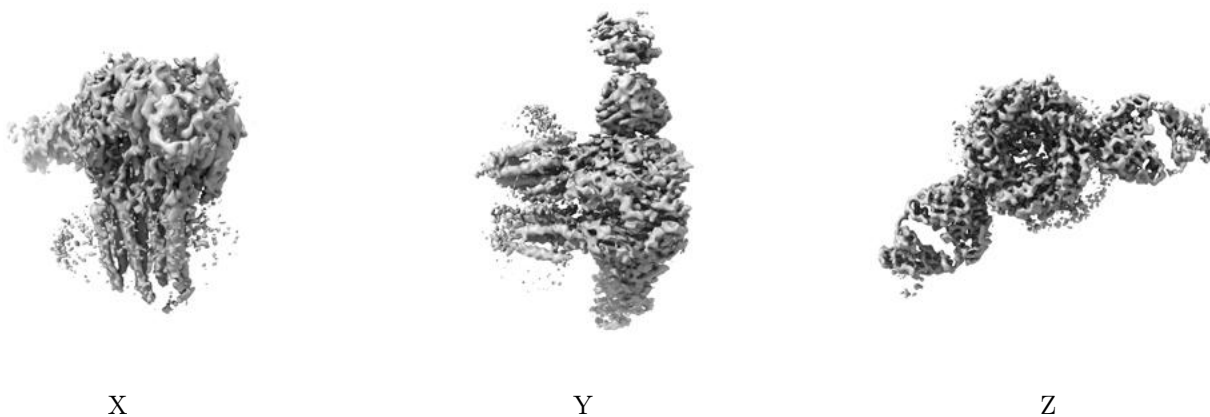


Z

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.

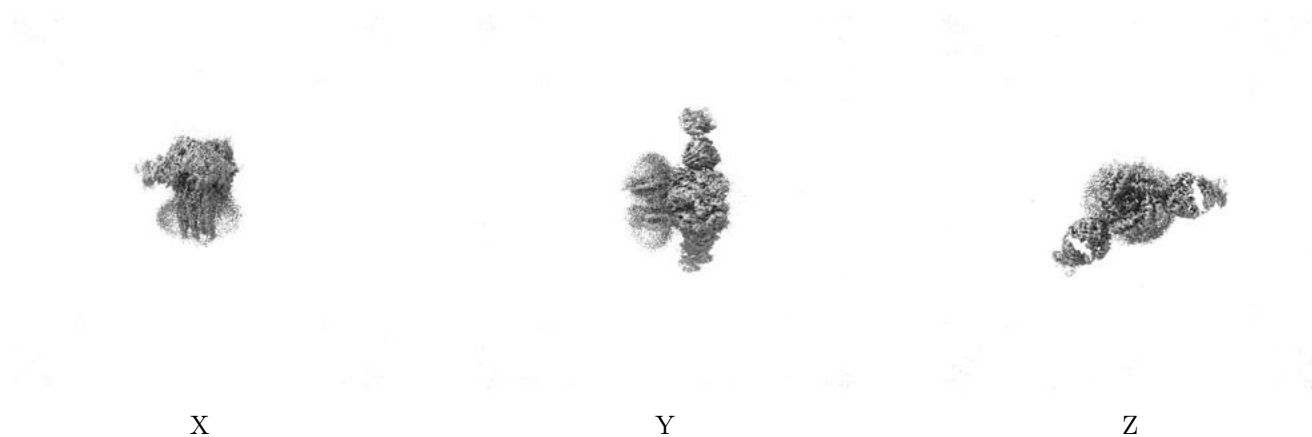
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

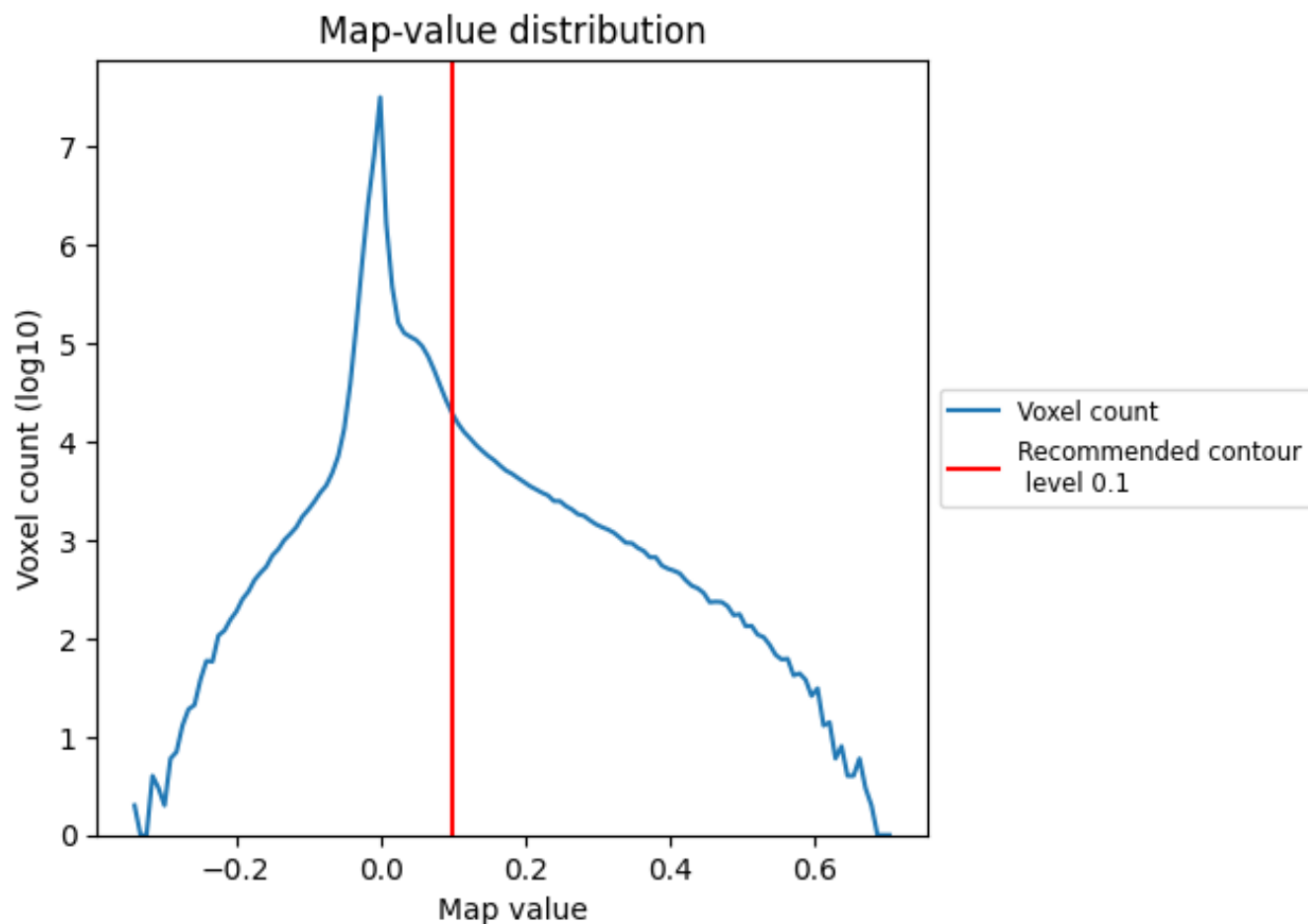
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

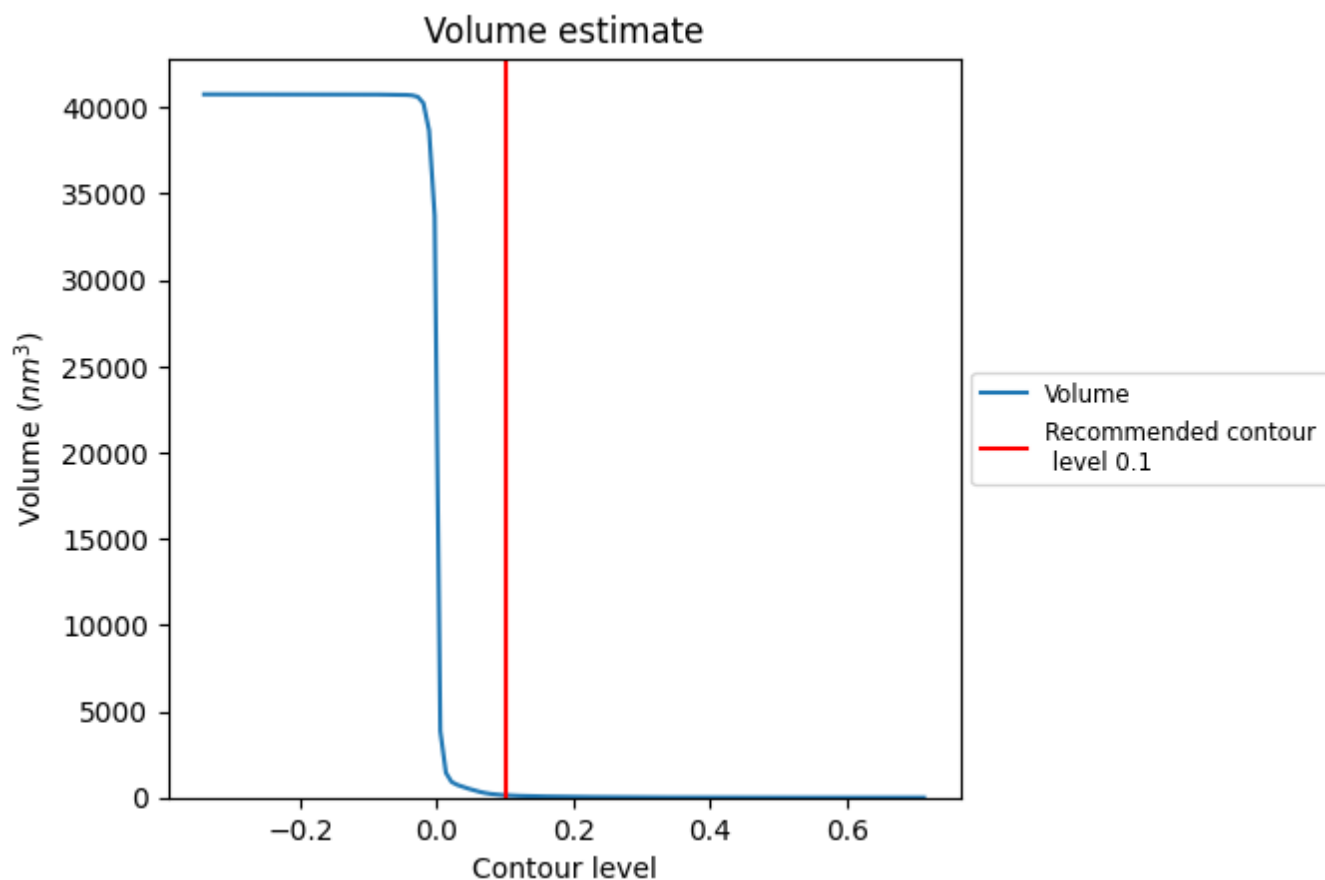
This section contains the results of statistical analysis of the map.

### 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.

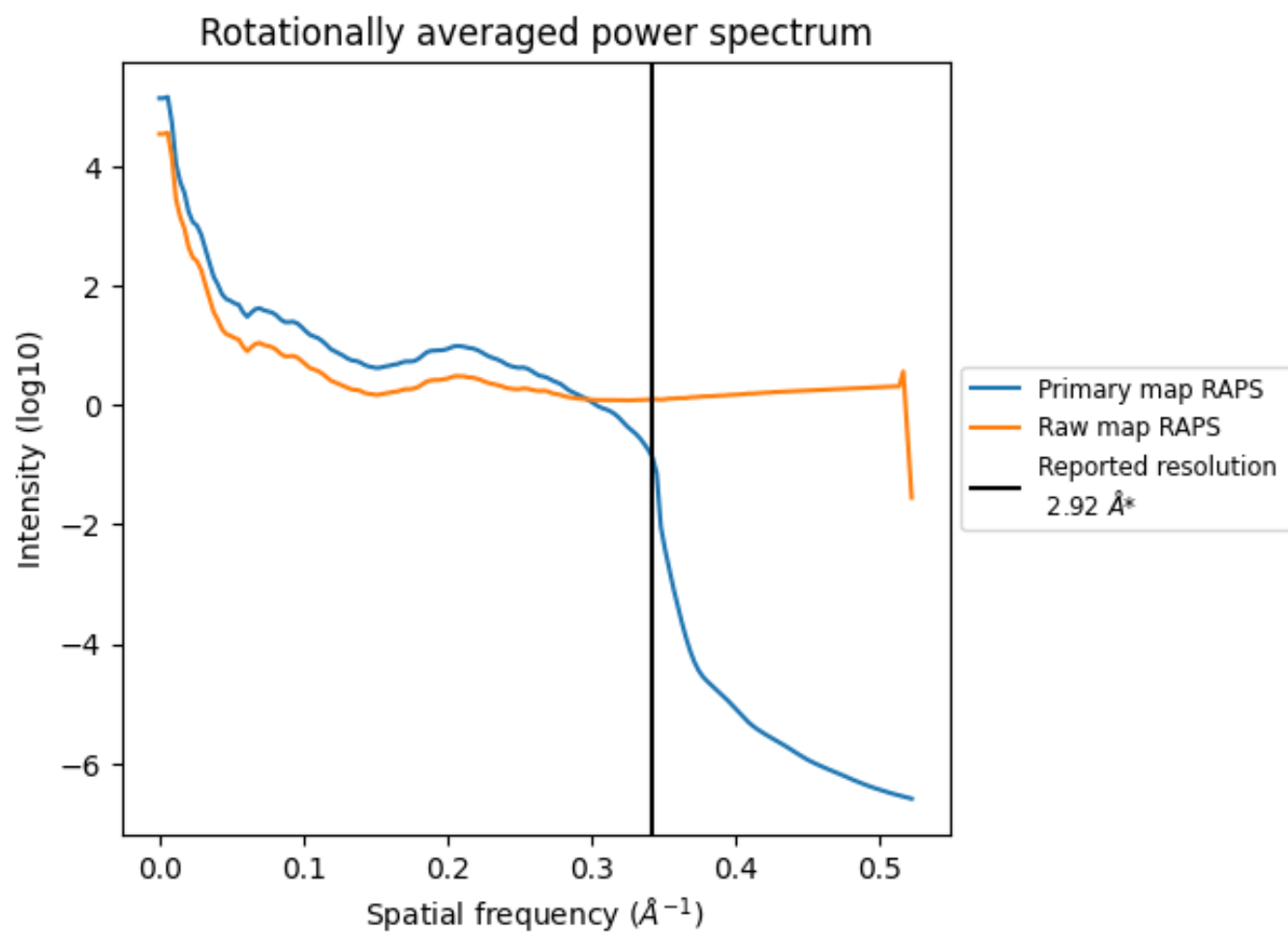
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm<sup>3</sup>; this corresponds to an approximate mass of 122 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 ⓘ

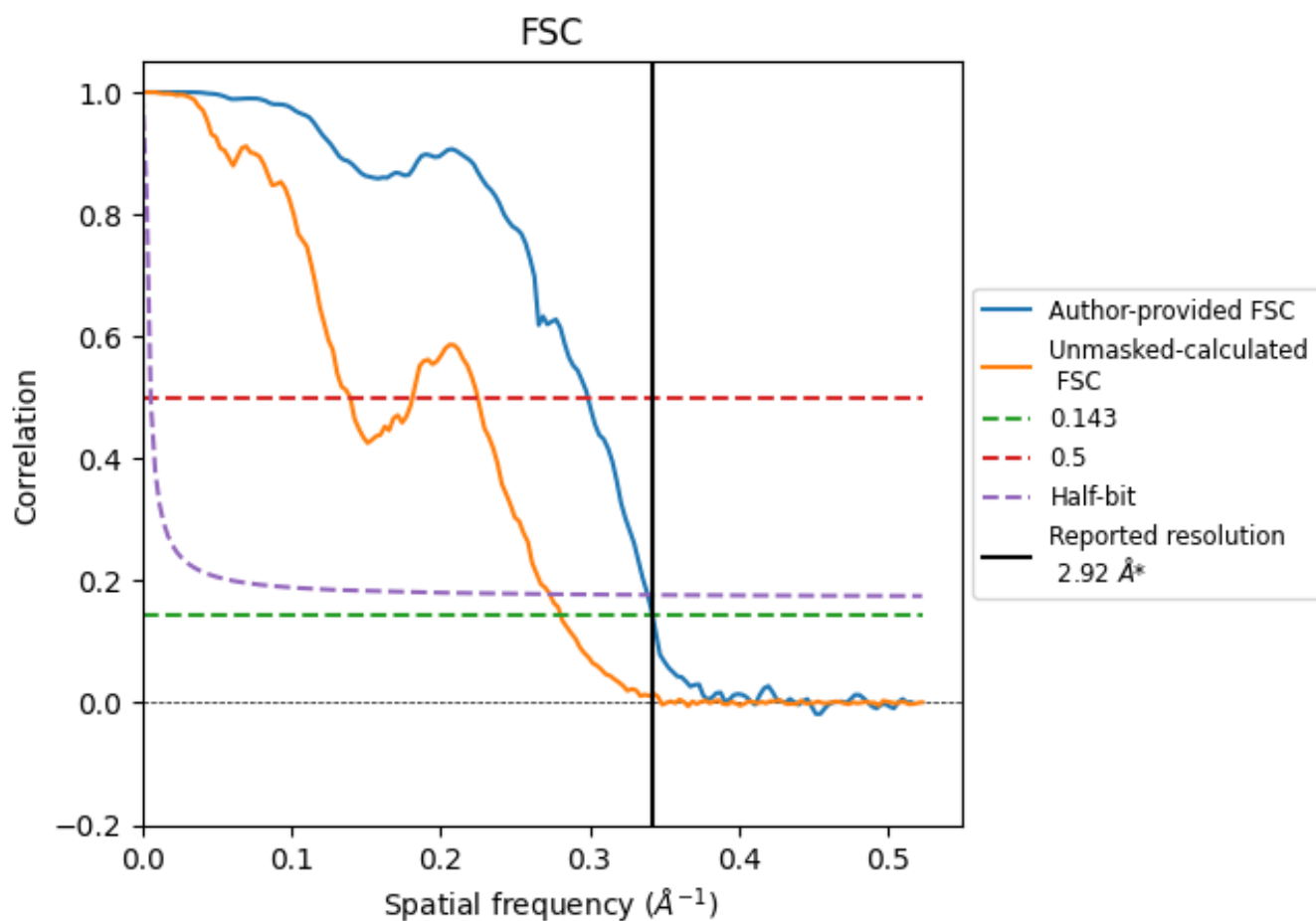


\*Reported resolution corresponds to spatial frequency of 0.342 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

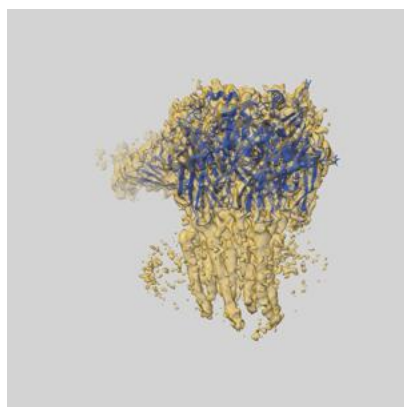
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.35	2.95
Unmasked-calculated*	3.56	7.17	3.66

\*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 3.56 differs from the reported value 2.92 by more than 10 %

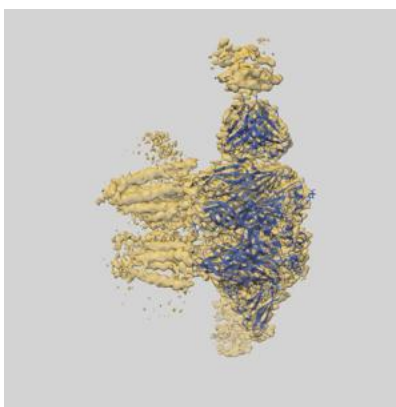
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70874 and PDB model 9OUO. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

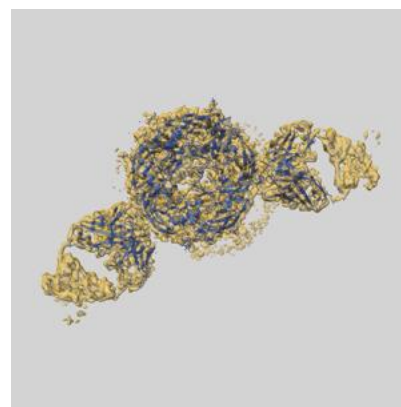
### 9.1 Map-model overlay [i](#)



X



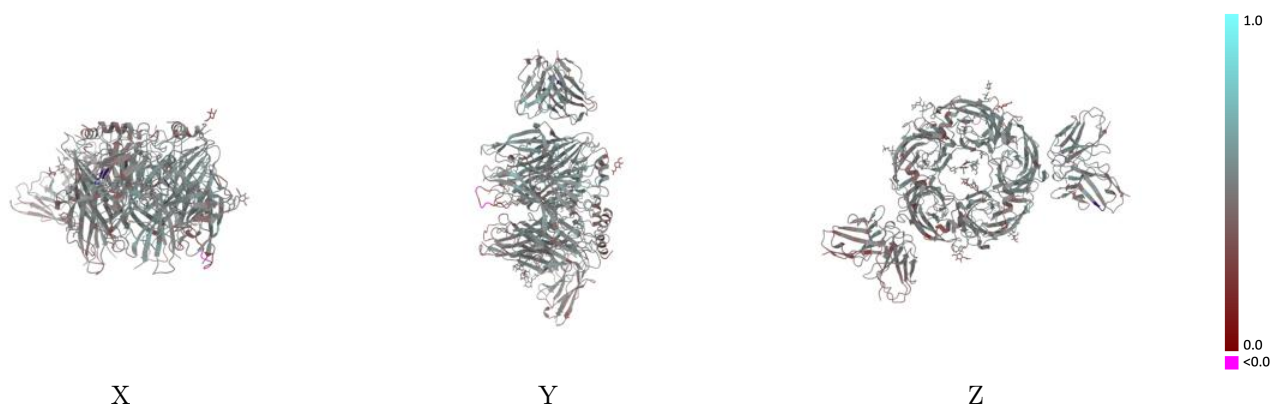
Y



Z

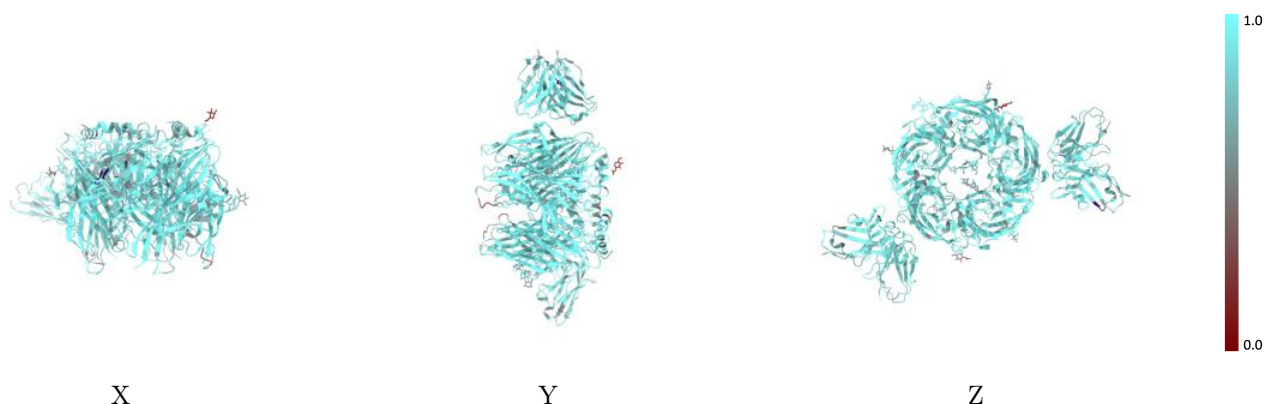
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



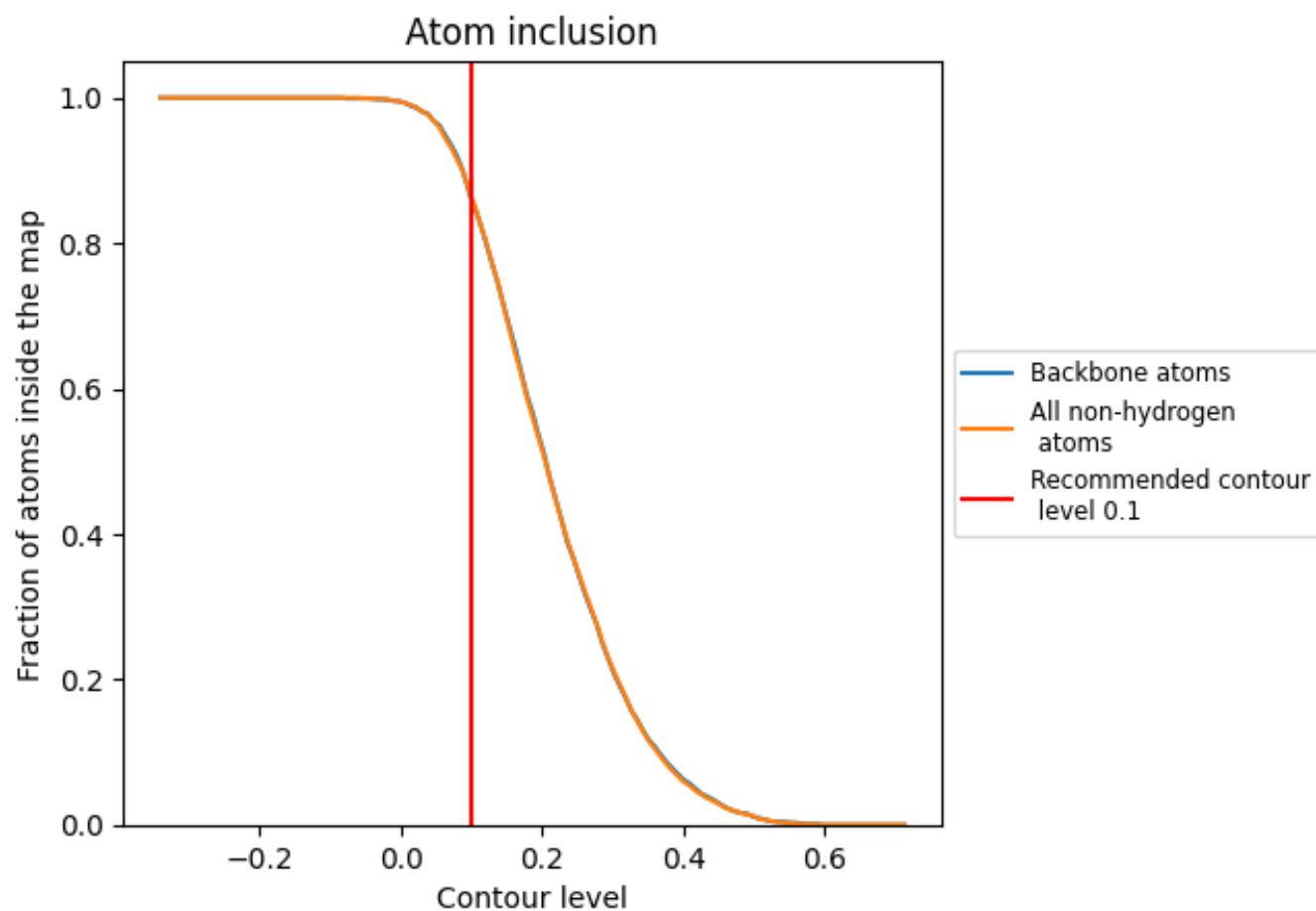
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.4760
A	 0.8660	 0.4670
B	 0.8800	 0.4780
C	 0.9020	 0.5120
D	 0.8880	 0.4780
E	 0.8930	 0.4790
F	 0.7500	 0.4640
G	 0.8070	 0.4490
H	 0.8360	 0.4370
I	 0.6410	 0.3550
J	 0.8350	 0.4810
K	 0.8450	 0.4980
L	 0.8390	 0.4310
M	 0.6070	 0.3690
N	 0.8210	 0.4250
O	 0.8930	 0.4650
P	 0.6670	 0.4460

