



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 08:19 pm GMT

PDB ID : 7Z0L  
EMDB ID : EMD-14427  
Title : IL-27 signalling complex  
Authors : Jin, Y.; Gardner, S.; Bubeck, D.  
Deposited on : 2022-02-23  
Resolution : 4.00 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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
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) : 2.39

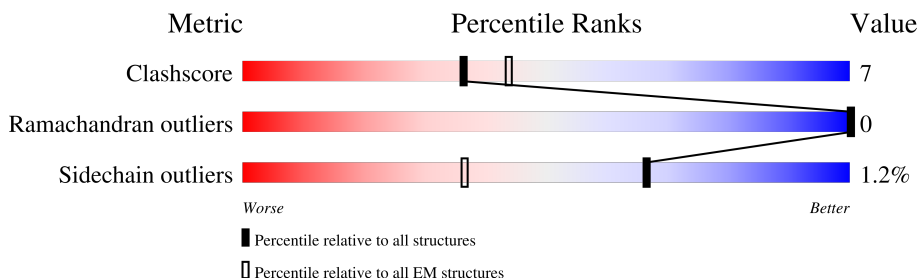
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	292	<div> <div>14%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	B	471	<div> <div>16%</div> <div>63%</div> <div>15%</div> <div>21%</div> </div>
3	C	230	<div> <div>.</div> <div>72%</div> <div>12%</div> <div>16%</div> </div>
4	E	2	<div> <div>50%</div> <div>50%</div> </div>
4	F	2	<div> <div>100%</div> </div>
4	G	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
4	H	2	<div> <div>50%</div> <div>50%</div> </div>
4	I	2	<div> <div>50%</div> <div>50%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13915 atoms, of which 6876 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 Interleukin-6 receptor subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	292	4557	1474	2244	372	454	13	0	0

- Molecule 2 is a protein called Interleukin-27 subunit beta, Interleukin-27 subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	370	5946	1901	2953	538	544	10	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP O35228
B	-2	VAL	-	expression tag	UNP O35228
B	-1	SER	-	expression tag	UNP O35228
B	0	ALA	-	expression tag	UNP O35228
B	1	ILE	-	expression tag	UNP O35228
B	2	VAL	-	expression tag	UNP O35228
B	3	LEU	-	expression tag	UNP O35228
B	4	TYR	-	expression tag	UNP O35228
B	5	VAL	-	expression tag	UNP O35228
B	6	LEU	-	expression tag	UNP O35228
B	7	LEU	-	expression tag	UNP O35228
B	8	ALA	-	expression tag	UNP O35228
B	9	ALA	-	expression tag	UNP O35228
B	10	ALA	-	expression tag	UNP O35228
B	11	ALA	-	expression tag	UNP O35228
B	12	HIS	-	expression tag	UNP O35228
B	13	SER	-	expression tag	UNP O35228
B	14	ALA	-	expression tag	UNP O35228
B	15	PHE	-	expression tag	UNP O35228
B	16	ALA	-	expression tag	UNP O35228
B	17	GLY	-	expression tag	UNP O35228

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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	SER	-	expression tag	UNP O35228
B	229	ARG	-	linker	UNP O35228
B	230	GLY	-	linker	UNP O35228
B	231	GLY	-	linker	UNP O35228
B	232	GLY	-	linker	UNP O35228
B	233	GLY	-	linker	UNP O35228
B	234	SER	-	linker	UNP O35228
B	235	GLY	-	linker	UNP O35228
B	236	GLY	-	linker	UNP O35228
B	237	GLY	-	linker	UNP O35228
B	238	GLY	-	linker	UNP O35228
B	239	SER	-	linker	UNP O35228
B	240	VAL	-	linker	UNP O35228
B	241	GLU	-	linker	UNP O35228
B	242	SER	-	linker	UNP O35228
B	243	GLY	-	linker	UNP O35228
B	244	GLU	-	linker	UNP O35228
B	245	ASN	-	linker	UNP O35228
B	246	LEU	-	linker	UNP O35228
B	247	TYR	-	linker	UNP O35228
B	248	PHE	-	linker	UNP O35228
B	249	GLN	-	linker	UNP O35228
B	457	ALA	-	expression tag	UNP Q8K3I6
B	458	ALA	-	expression tag	UNP Q8K3I6
B	459	ALA	-	expression tag	UNP Q8K3I6
B	460	HIS	-	expression tag	UNP Q8K3I6
B	461	HIS	-	expression tag	UNP Q8K3I6
B	462	HIS	-	expression tag	UNP Q8K3I6
B	463	HIS	-	expression tag	UNP Q8K3I6
B	464	HIS	-	expression tag	UNP Q8K3I6
B	465	HIS	-	expression tag	UNP Q8K3I6
B	466	HIS	-	expression tag	UNP Q8K3I6
B	467	HIS	-	expression tag	UNP Q8K3I6

- Molecule 3 is a protein called Interleukin-27 receptor subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	194	Total	C	H	N	O	S	0	0
			3081	1007	1516	258	291	9		

There are 33 discrepancies between the modelled and reference sequences:

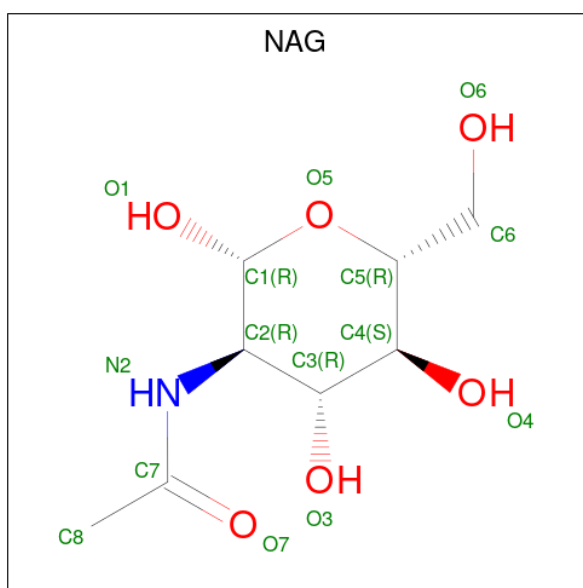
Chain	Residue	Modelled	Actual	Comment	Reference
C	6	MET	-	initiating methionine	UNP O70394
C	7	VAL	-	expression tag	UNP O70394
C	8	SER	-	expression tag	UNP O70394
C	9	ALA	-	expression tag	UNP O70394
C	10	ILE	-	expression tag	UNP O70394
C	11	VAL	-	expression tag	UNP O70394
C	12	LEU	-	expression tag	UNP O70394
C	13	TYR	-	expression tag	UNP O70394
C	14	VAL	-	expression tag	UNP O70394
C	15	LEU	-	expression tag	UNP O70394
C	16	LEU	-	expression tag	UNP O70394
C	17	ALA	-	expression tag	UNP O70394
C	18	ALA	-	expression tag	UNP O70394
C	19	ALA	-	expression tag	UNP O70394
C	20	ALA	-	expression tag	UNP O70394
C	21	HIS	-	expression tag	UNP O70394
C	22	SER	-	expression tag	UNP O70394
C	23	ALA	-	expression tag	UNP O70394
C	24	PHE	-	expression tag	UNP O70394
C	25	ALA	-	expression tag	UNP O70394
C	26	GLY	-	expression tag	UNP O70394
C	27	SER	-	expression tag	UNP O70394
C	225	ALA	-	expression tag	UNP O70394
C	226	ALA	-	expression tag	UNP O70394
C	227	ALA	-	expression tag	UNP O70394
C	228	HIS	-	expression tag	UNP O70394
C	229	HIS	-	expression tag	UNP O70394
C	230	HIS	-	expression tag	UNP O70394
C	231	HIS	-	expression tag	UNP O70394
C	232	HIS	-	expression tag	UNP O70394
C	233	HIS	-	expression tag	UNP O70394
C	234	HIS	-	expression tag	UNP O70394
C	235	HIS	-	expression tag	UNP O70394

- Molecule 4 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
4	E	2	Total	C	H	N	O	
			55	16	27	2	10	0
4	F	2	Total	C	H	N	O	
			55	16	27	2	10	0
4	G	2	Total	C	H	N	O	
			55	16	27	2	10	0
4	H	2	Total	C	H	N	O	
			55	16	27	2	10	0
4	I	2	Total	C	H	N	O	
			55	16	27	2	10	0

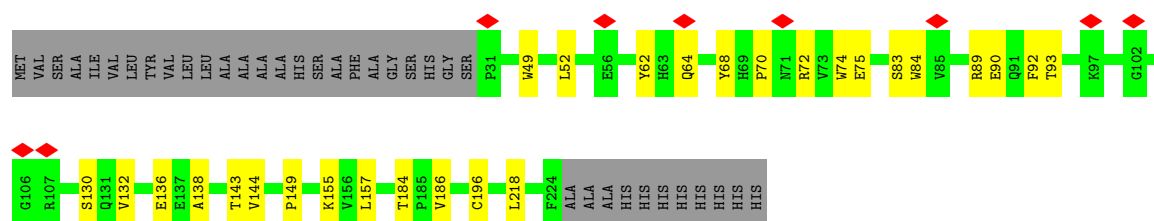
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	N	O
			28	8	14	1	5
5	A	1	Total	C	H	N	O
			28	8	14	1	5



Chain C: 



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

Chain E: 



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

Chain F: 



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

Chain G: 



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

Chain H: 



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

Chain I: 





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	208431	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction was performed following 3D reconstruction. Local CTF refinement was carried out during refinement	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.120	Depositor
Minimum map value	-0.741	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	222.59999, 222.59999, 222.59999	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.29	0/2373	0.54	0/3240
2	B	0.29	0/3072	0.60	0/4171
3	C	0.28	0/1619	0.57	0/2220
All	All	0.29	0/7064	0.58	0/9631

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	359	ARG	Sidechain
2	B	436	ARG	Sidechain

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2313	2244	2243	25	0
2	B	2993	2953	2947	57	0
3	C	1565	1516	1516	21	0
4	E	28	27	25	1	0
4	F	28	27	25	1	0
4	G	28	27	25	3	0
4	H	28	27	25	7	0
4	I	28	27	25	3	0
5	A	28	28	26	3	0
All	All	7039	6876	6857	103	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 (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASN:HD21	4:G:1:NAG:C1	1.91	0.84
3:C:64:GLN:NE2	3:C:70:PRO:O	2.28	0.66
2:B:160:SER:O	2:B:206:LEU:HB2	1.97	0.64
2:B:203:ALA:N	2:B:213:SER:OG	2.22	0.64
4:I:1:NAG:H3	4:I:1:NAG:H83	1.79	0.64
2:B:436:ARG:NE	2:B:440:ASP:OD2	2.31	0.64
2:B:204:GLN:NE2	2:B:208:ASP:OD1	2.29	0.60
3:C:84:TRP:CG	4:I:1:NAG:H5	2.37	0.59
2:B:96:PHE:HB2	2:B:312:PHE:HB2	1.82	0.59
2:B:203:ALA:O	2:B:213:SER:N	2.29	0.59
2:B:360:LEU:HD13	3:C:89:ARG:HG3	1.84	0.59
2:B:66:ARG:NH1	2:B:75:SER:OG	2.35	0.58
2:B:96:PHE:CD1	2:B:312:PHE:HB2	2.38	0.58
2:B:309:SER:HB2	4:H:1:NAG:H83	1.85	0.58
2:B:380:CYS:N	2:B:383:GLU:OE2	2.36	0.58
2:B:448:ARG:NH1	2:B:453:ALA:O	2.36	0.58
2:B:362:LEU:HD21	2:B:430:LEU:HD11	1.85	0.58
1:A:157:ASN:OD1	5:A:401:NAG:H83	2.04	0.57
2:B:275:LEU:O	2:B:279:VAL:HG23	2.05	0.57
3:C:68:TYR:CE2	3:C:93:THR:HG21	2.40	0.56
1:A:82:ILE:HD11	1:A:88:SER:HB3	1.87	0.55
3:C:89:ARG:HA	3:C:92:PHE:CE2	2.42	0.55
2:B:311:THR:CG2	4:H:2:NAG:H83	2.37	0.54
3:C:130:SER:HA	3:C:218:LEU:HD21	1.89	0.54
4:E:1:NAG:H61	4:E:2:NAG:N2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASN:N	1:A:199:GLU:O	2.41	0.53
2:B:435:SER:HB3	2:B:439:ARG:HH12	1.72	0.53
4:H:2:NAG:O7	4:H:2:NAG:O3	2.24	0.52
1:A:38:VAL:O	1:A:122:SER:HA	2.11	0.51
1:A:133:THR:HG21	4:G:1:NAG:HN2	1.75	0.51
2:B:162:LYS:HE2	2:B:206:LEU:O	2.11	0.51
2:B:370:ARG:NH1	2:B:390:GLU:OE2	2.42	0.51
2:B:339:GLY:CA	2:B:359:ARG:HE	2.25	0.50
2:B:65:TYR:CE2	2:B:90:ILE:HG23	2.46	0.50
2:B:308:VAL:O	2:B:310:LEU:HD12	2.12	0.50
2:B:367:ARG:HD3	3:C:68:TYR:CD2	2.45	0.50
1:A:155:GLU:HG2	5:A:401:NAG:H81	1.94	0.50
1:A:174:SER:HB2	1:A:180:CYS:SG	2.52	0.49
1:A:116:TYR:HA	2:B:417:TRP:CD1	2.47	0.49
2:B:145:VAL:HG21	2:B:165:LEU:HD11	1.94	0.49
2:B:163:TYR:CD2	2:B:181:ILE:O	2.67	0.48
2:B:275:LEU:HD21	2:B:362:LEU:HG	1.95	0.48
3:C:62:TYR:HA	3:C:74:TRP:O	2.13	0.48
2:B:332:ARG:O	2:B:335:PRO:HD2	2.13	0.48
2:B:309:SER:O	4:H:1:NAG:H5	2.12	0.48
2:B:359:ARG:HB3	2:B:359:ARG:CZ	2.44	0.48
3:C:155:LYS:HA	3:C:155:LYS:HE2	1.96	0.47
3:C:72:ARG:HD3	3:C:74:TRP:CZ2	2.48	0.47
2:B:356:TRP:CH2	3:C:89:ARG:HB3	2.49	0.47
2:B:363:ARG:HD2	2:B:367:ARG:NH2	2.29	0.47
1:A:48:CYS:HG	1:A:103:CYS:HG	1.64	0.46
1:A:158:TYR:CE2	1:A:198:ALA:HB2	2.51	0.46
2:B:101:TYR:HB2	2:B:120:PHE:CZ	2.51	0.46
4:I:2:NAG:H82	4:I:2:NAG:O3	2.16	0.46
3:C:149:PRO:HD2	3:C:157:LEU:CD1	2.46	0.45
2:B:398:LYS:HE2	3:C:74:TRP:CZ3	2.51	0.45
2:B:201:VAL:O	2:B:216:SER:N	2.39	0.45
3:C:52:LEU:H	3:C:52:LEU:HD12	1.82	0.45
4:H:1:NAG:C1	4:H:1:NAG:H82	2.47	0.45
2:B:65:TYR:CZ	2:B:90:ILE:HG23	2.52	0.45
1:A:30:TYR:HA	1:A:116:TYR:CD1	2.52	0.45
1:A:188:TYR:HB3	1:A:215:VAL:CG2	2.47	0.45
2:B:123:GLU:HA	2:B:126:ILE:CD1	2.47	0.44
2:B:363:ARG:HD2	2:B:367:ARG:CZ	2.46	0.44
2:B:311:THR:HG22	4:H:2:NAG:H83	1.98	0.44
3:C:62:TYR:CE1	3:C:75:GLU:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:ARG:NH2	2:B:394:GLU:OE2	2.42	0.44
2:B:429:SER:O	2:B:433:VAL:HG23	2.17	0.44
1:A:37:VAL:HA	1:A:121:LEU:O	2.18	0.44
1:A:44:PHE:CE2	1:A:120:MET:SD	3.11	0.44
2:B:62:ILE:O	2:B:106:THR:N	2.38	0.43
2:B:167:TYR:CE1	2:B:176:ARG:HB2	2.53	0.43
1:A:133:THR:CG2	4:G:1:NAG:HN2	2.31	0.43
1:A:172:CYS:SG	1:A:180:CYS:HB3	2.58	0.43
1:A:61:ASN:H	1:A:64:TYR:HD2	1.65	0.43
4:F:1:NAG:H61	4:F:2:NAG:C7	2.48	0.43
3:C:132:VAL:HG22	3:C:144:VAL:HG22	2.00	0.43
1:A:216:ASP:O	1:A:306:GLY:HA2	2.18	0.43
2:B:169:ARG:HG2	2:B:197:TYR:CE2	2.54	0.43
4:H:1:NAG:C1	4:H:1:NAG:C8	2.96	0.42
2:B:163:TYR:HE2	2:B:183:ALA:N	2.17	0.42
2:B:376:ALA:HB1	2:B:378:PHE:CZ	2.54	0.42
2:B:355:LEU:O	2:B:359:ARG:HG3	2.18	0.42
3:C:143:THR:HA	3:C:186:VAL:O	2.20	0.42
3:C:49:TRP:CZ2	3:C:83:SER:HA	2.55	0.42
2:B:96:PHE:CE2	2:B:159:PHE:CE2	3.07	0.42
2:B:205:ASP:OD2	2:B:209:TYR:HB2	2.19	0.42
1:A:64:TYR:CD1	1:A:106:LEU:O	2.73	0.42
1:A:277:SER:OG	1:A:279:ARG:NH2	2.50	0.42
2:B:187:THR:HB	3:C:184:THR:HG22	2.02	0.42
2:B:380:CYS:HB2	2:B:383:GLU:HG3	2.02	0.42
2:B:39:TYR:CE2	2:B:93:VAL:HG11	2.55	0.41
1:A:44:PHE:O	1:A:91:PHE:N	2.46	0.41
2:B:206:LEU:C	2:B:208:ASP:H	2.23	0.41
1:A:116:TYR:CZ	2:B:417:TRP:HB3	2.56	0.41
2:B:448:ARG:HD3	2:B:452:SER:OG	2.21	0.41
1:A:44:PHE:N	1:A:91:PHE:O	2.44	0.41
2:B:162:LYS:HD3	2:B:182:GLU:OE2	2.21	0.40
3:C:136:GLU:O	3:C:138:ALA:N	2.54	0.40
2:B:65:TYR:CD2	2:B:90:ILE:HG12	2.56	0.40
1:A:224:TYR:CD1	5:A:402:NAG:H2	2.57	0.40
2:B:124:ARG:HA	2:B:209:TYR:HB3	2.04	0.40
3:C:68:TYR:CZ	3:C:93:THR:HG21	2.56	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	290/292 (99%)	280 (97%)	10 (3%)	0	100	100
2	B	358/471 (76%)	336 (94%)	22 (6%)	0	100	100
3	C	192/230 (84%)	178 (93%)	14 (7%)	0	100	100
All	All	840/993 (85%)	794 (94%)	46 (6%)	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	267/267 (100%)	264 (99%)	3 (1%)	70	80
2	B	329/399 (82%)	325 (99%)	4 (1%)	67	78
3	C	178/202 (88%)	176 (99%)	2 (1%)	70	80
All	All	774/868 (89%)	765 (99%)	9 (1%)	66	78

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	TYR
1	A	164	TRP
1	A	224	TYR
2	B	87	ARG
2	B	163	TYR

*Continued on next page...*

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Mol	Chain	Res	Type
2	B	185	THR
2	B	359	ARG
3	C	90	GLU
3	C	196	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

10 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	$\# Z  > 2$
4	NAG	E	1	1,4	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
4	NAG	E	2	4	14,14,15	0.45	0	17,19,21	0.44	0
4	NAG	F	1	1,4	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	G	1	1,4	14,14,15	0.37	0	17,19,21	1.39	1 (5%)
4	NAG	G	2	4	14,14,15	0.17	0	17,19,21	0.45	0
4	NAG	H	1	2,4	14,14,15	0.31	0	17,19,21	1.33	2 (11%)
4	NAG	H	2	4	14,14,15	0.47	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	I	1	3,4	14,14,15	0.16	0	17,19,21	1.17	2 (11%)
4	NAG	I	2	4	14,14,15	0.38	0	17,19,21	0.64	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
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	3,4	-	5/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	4.79	118.69	112.19
4	H	1	NAG	C2-N2-C7	3.56	127.97	122.90
4	I	1	NAG	C2-N2-C7	3.24	127.52	122.90
4	H	1	NAG	C1-C2-N2	2.81	115.30	110.49
4	I	1	NAG	C4-C3-C2	-2.23	107.75	111.02
4	E	1	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2

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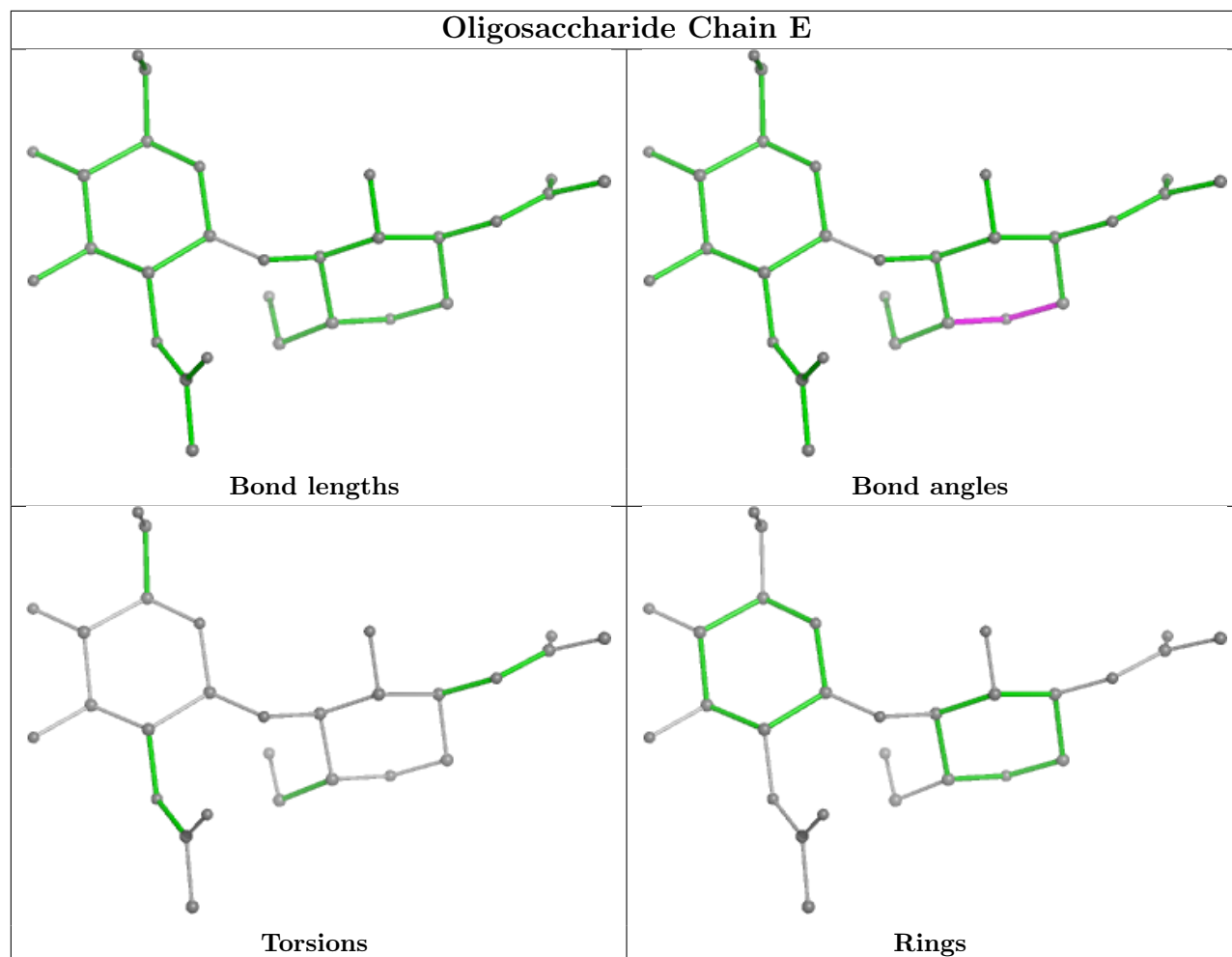
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C1-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	G	1	NAG	C1-C2-N2-C7
4	H	1	NAG	C1-C2-N2-C7
4	I	1	NAG	C3-C2-N2-C7
4	H	2	NAG	C3-C2-N2-C7

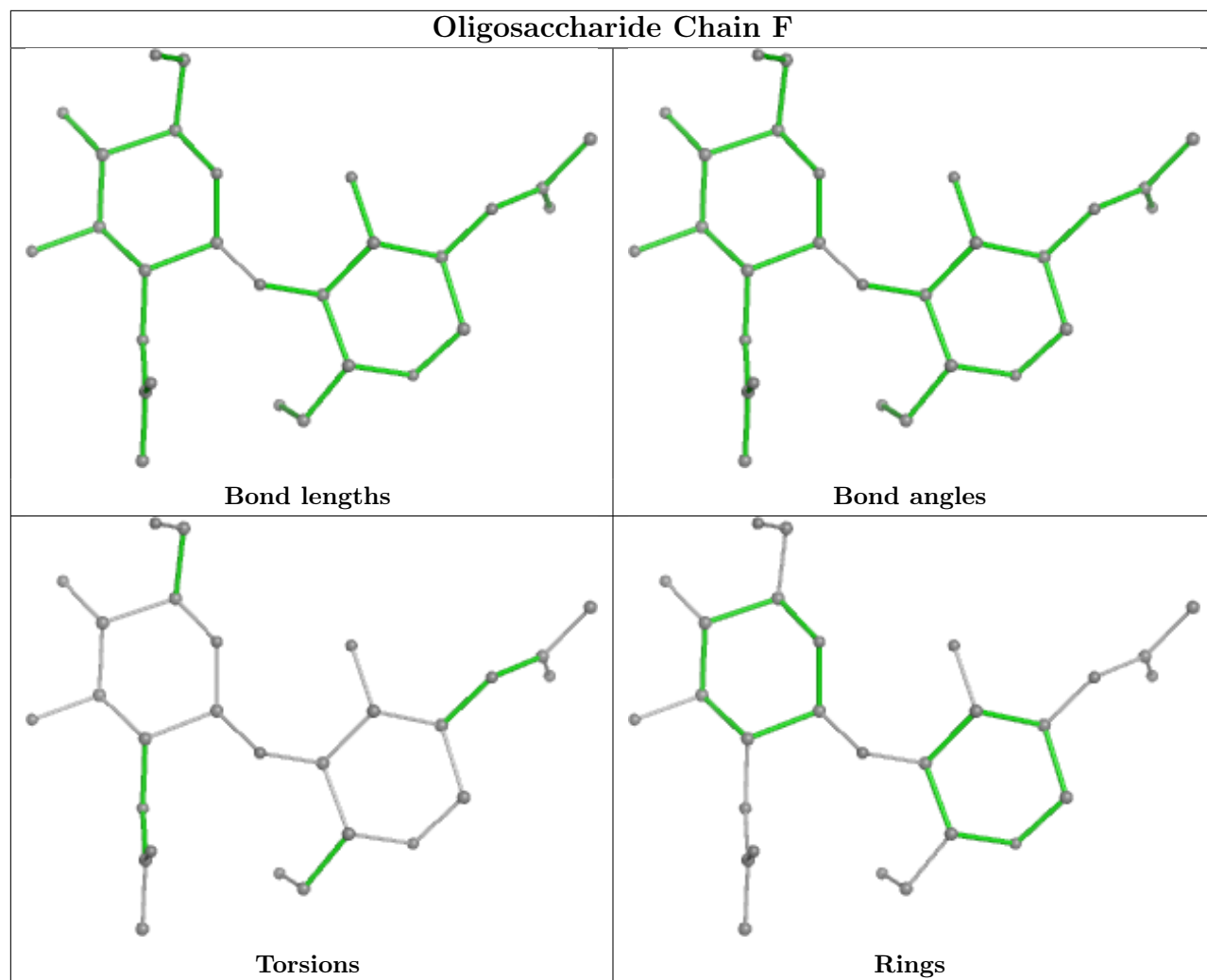
There are no ring outliers.

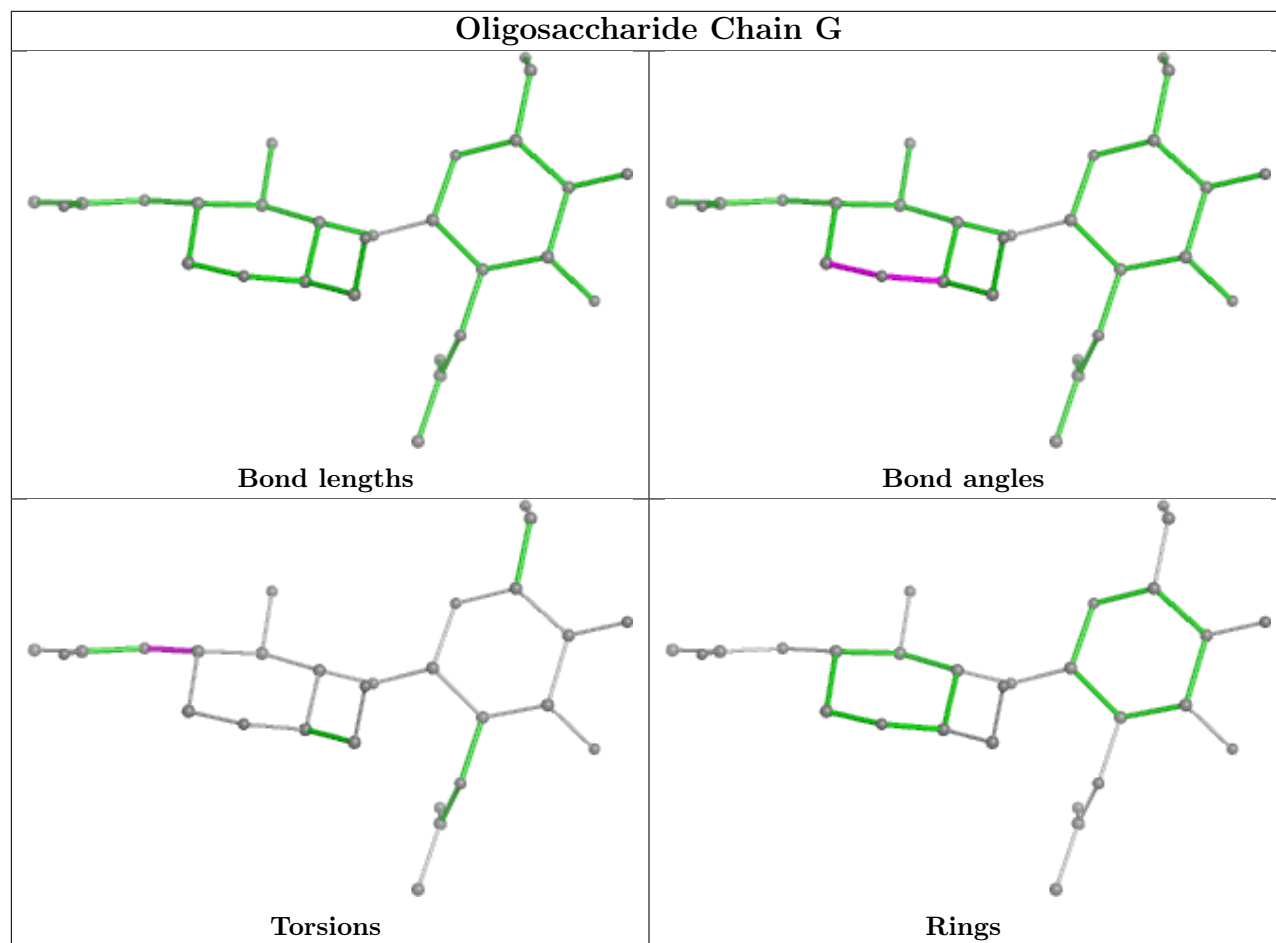
9 monomers are involved in 15 short contacts:

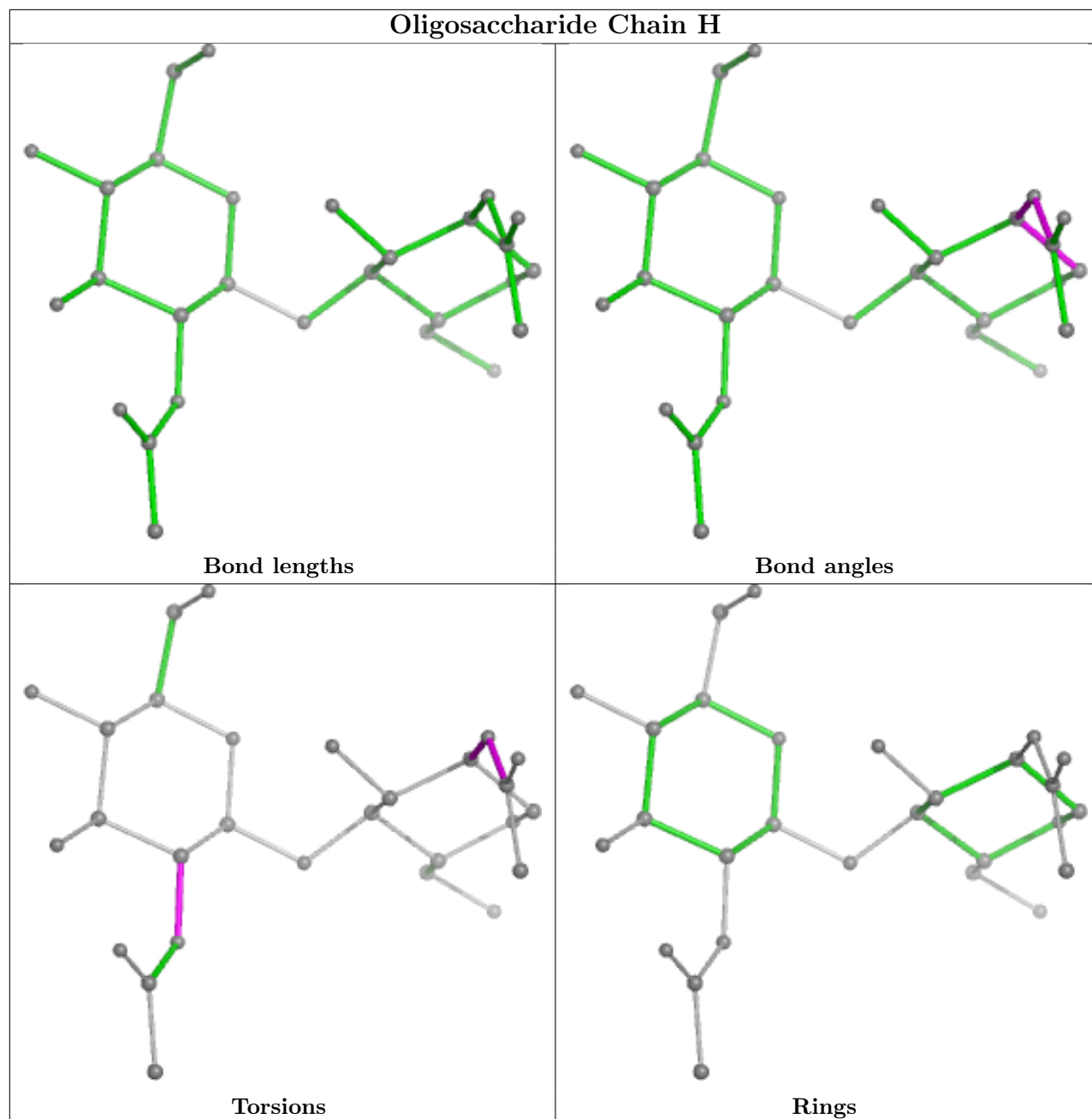
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0
4	I	1	NAG	2	0
4	H	2	NAG	3	0
4	E	2	NAG	1	0
4	G	1	NAG	3	0
4	H	1	NAG	4	0
4	F	2	NAG	1	0
4	F	1	NAG	1	0
4	I	2	NAG	1	0

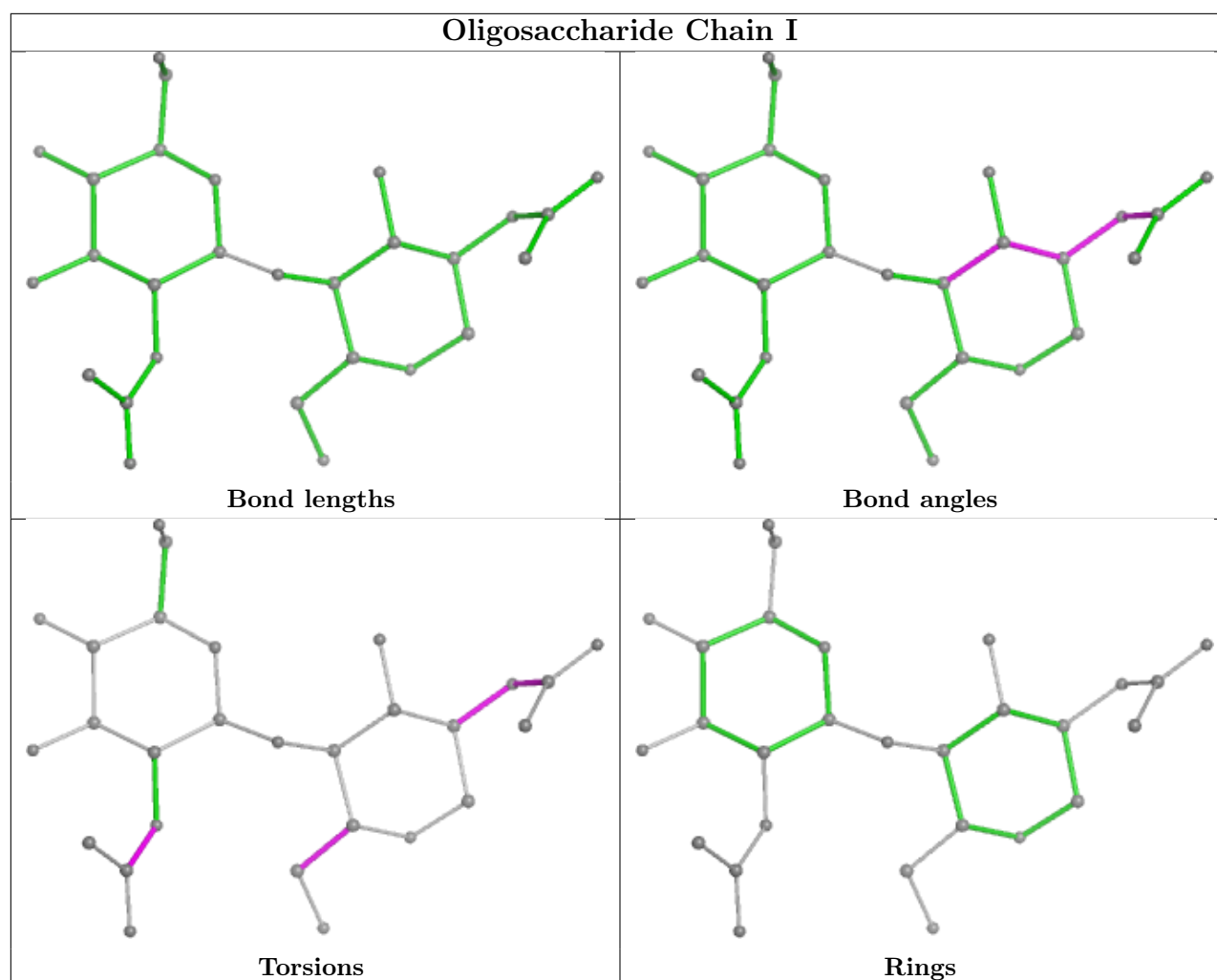
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
5	NAG	A	401	1	14,14,15	0.64	0	17,19,21	1.38	1 (5%)
5	NAG	A	402	1	14,14,15	0.58	0	17,19,21	0.87	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	401	1	-	3/6/23/26	0/1/1/1
5	NAG	A	402	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	NAG	C1-O5-C5	5.19	119.22	112.19
5	A	402	NAG	C1-O5-C5	3.23	116.57	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2
5	A	401	NAG	O5-C5-C6-O6
5	A	402	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	NAG	2	0
5	A	402	NAG	1	0

## 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.

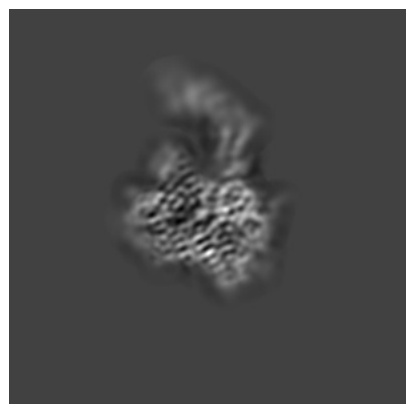
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14427. These allow visual inspection of the internal detail of the map and identification of artifacts.

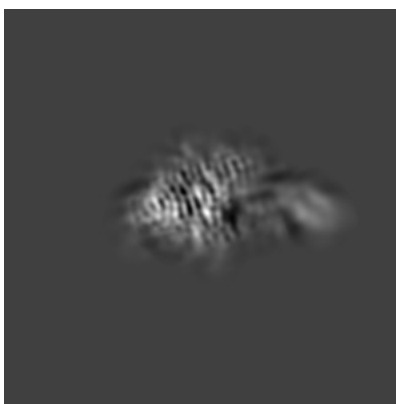
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

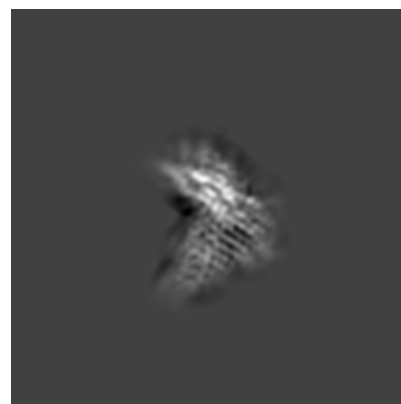
#### 6.1.1 Primary map



X

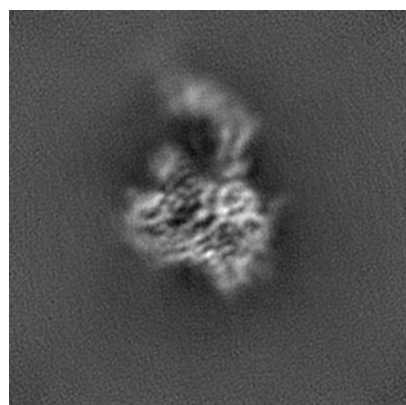


Y

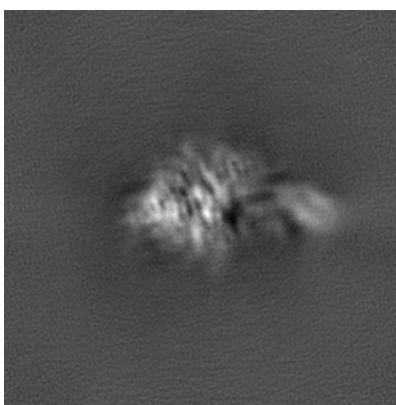


Z

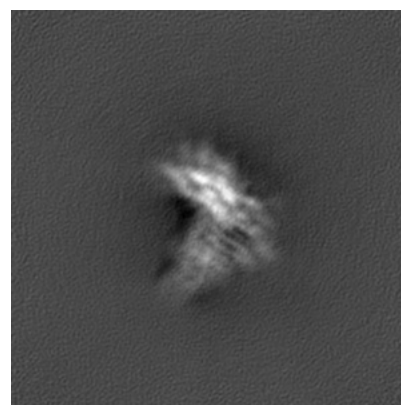
#### 6.1.2 Raw map



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: 105

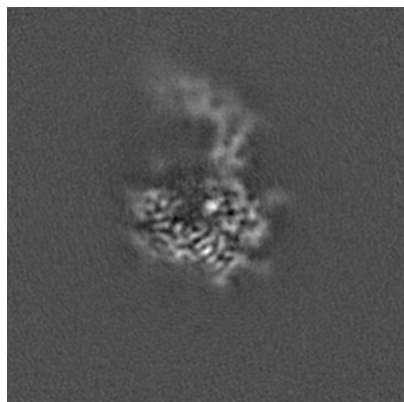


Y Index: 105

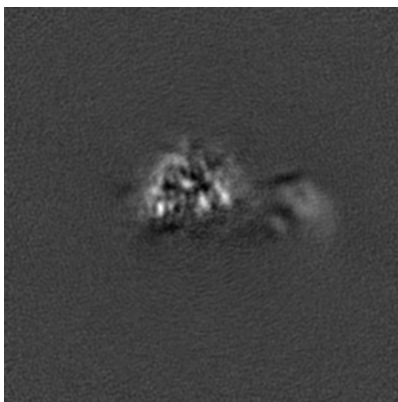


Z Index: 105

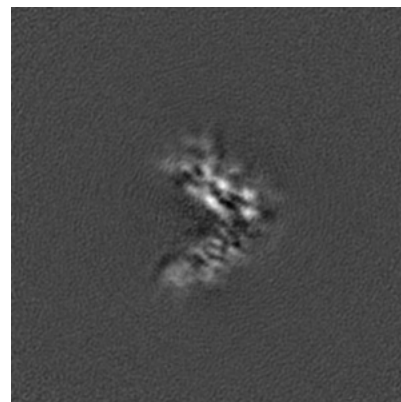
### 6.2.2 Raw map



X Index: 105



Y Index: 105



Z Index: 105

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: 103

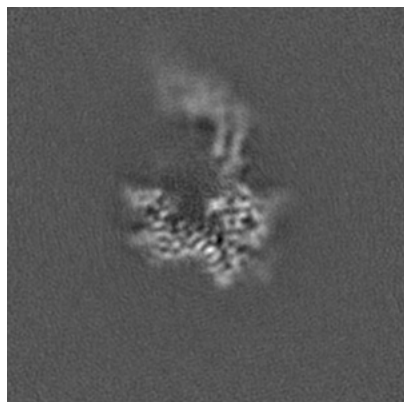


Y Index: 111

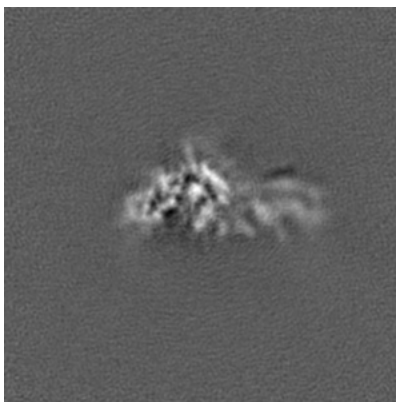


Z Index: 100

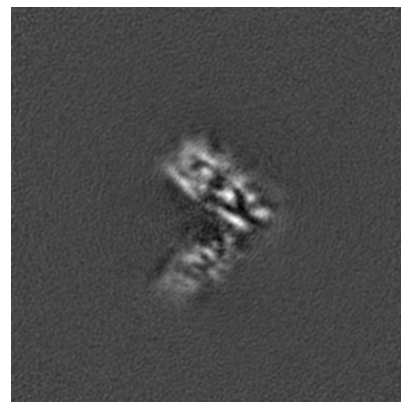
### 6.3.2 Raw map



X Index: 102



Y Index: 111

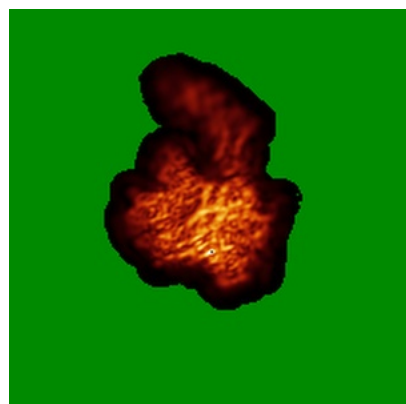


Z Index: 100

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

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

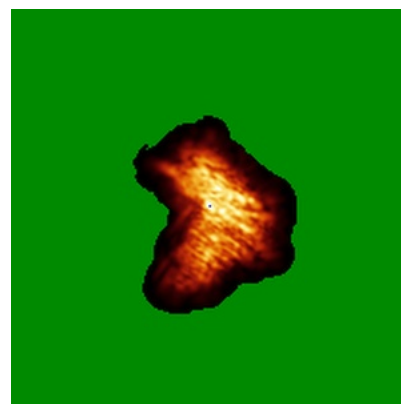
### 6.4.1 Primary map



X

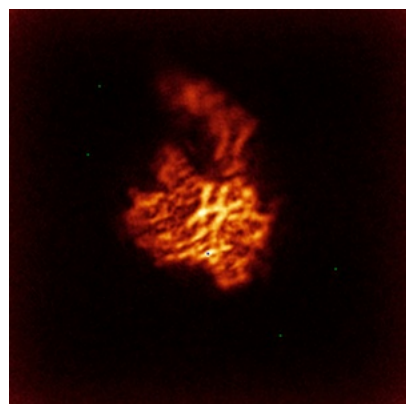


Y

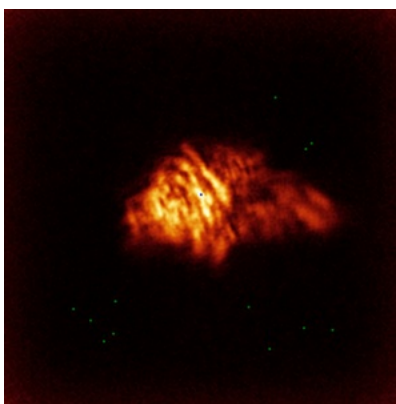


Z

### 6.4.2 Raw map



X



Y

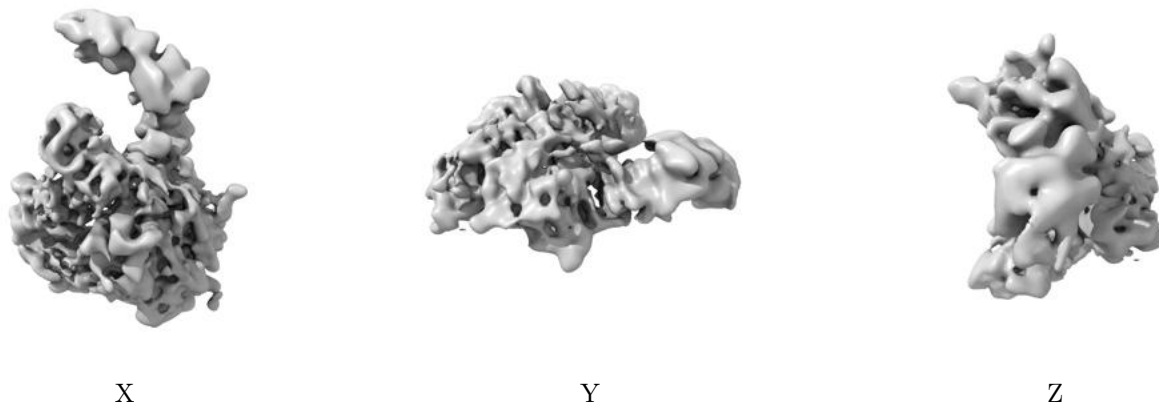


Z

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.

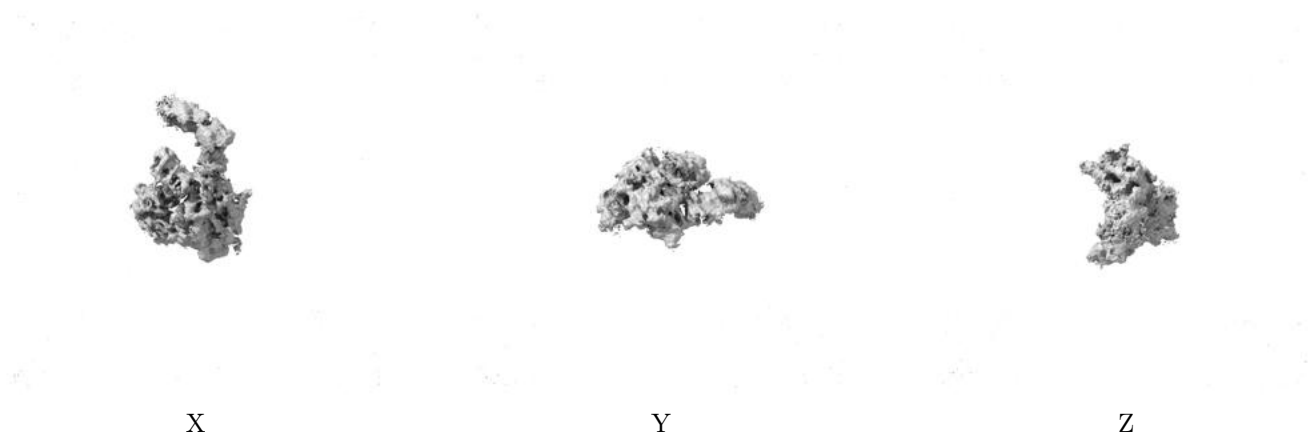
## 6.5 Orthogonal surface views [i](#)

### 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.

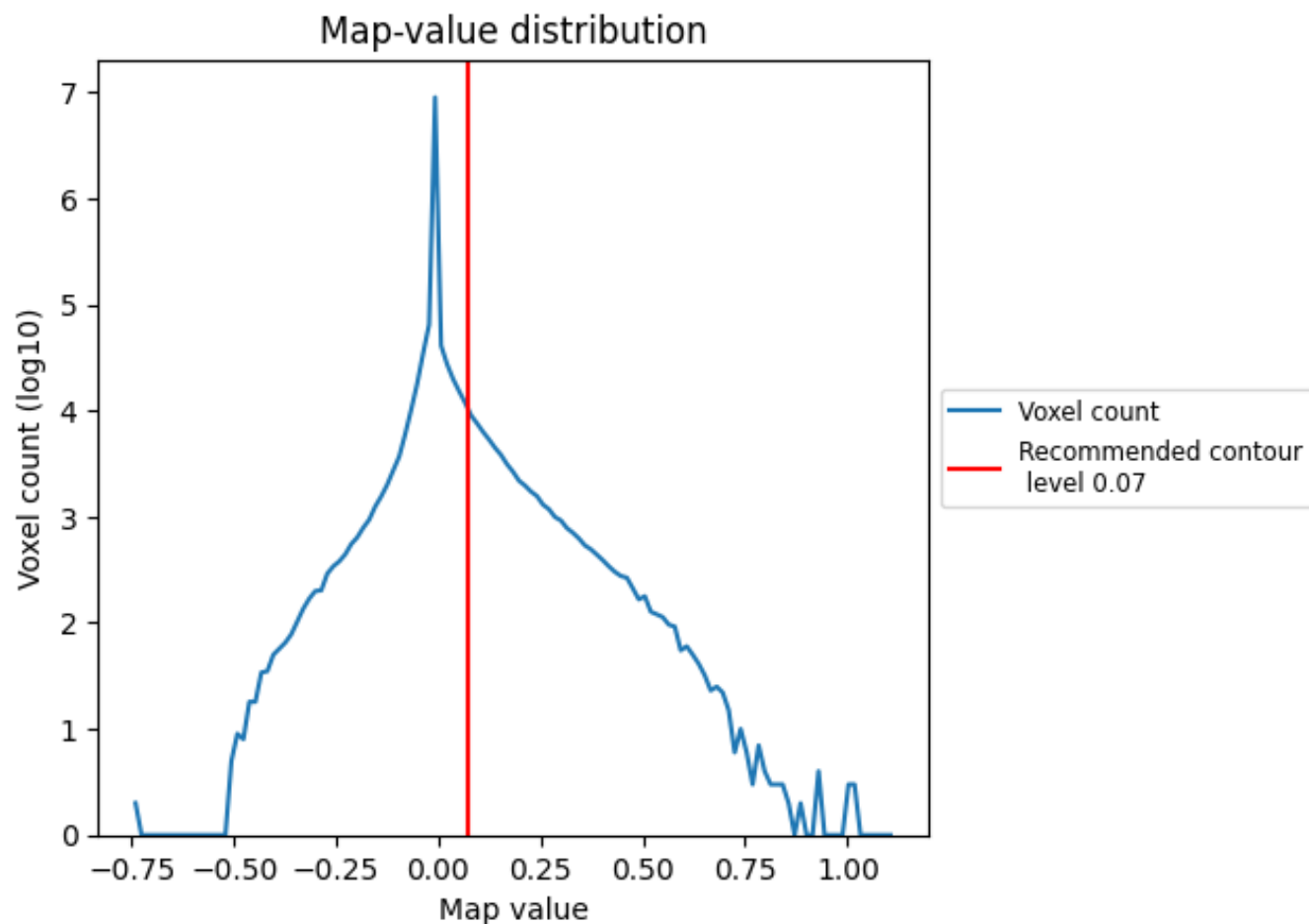
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

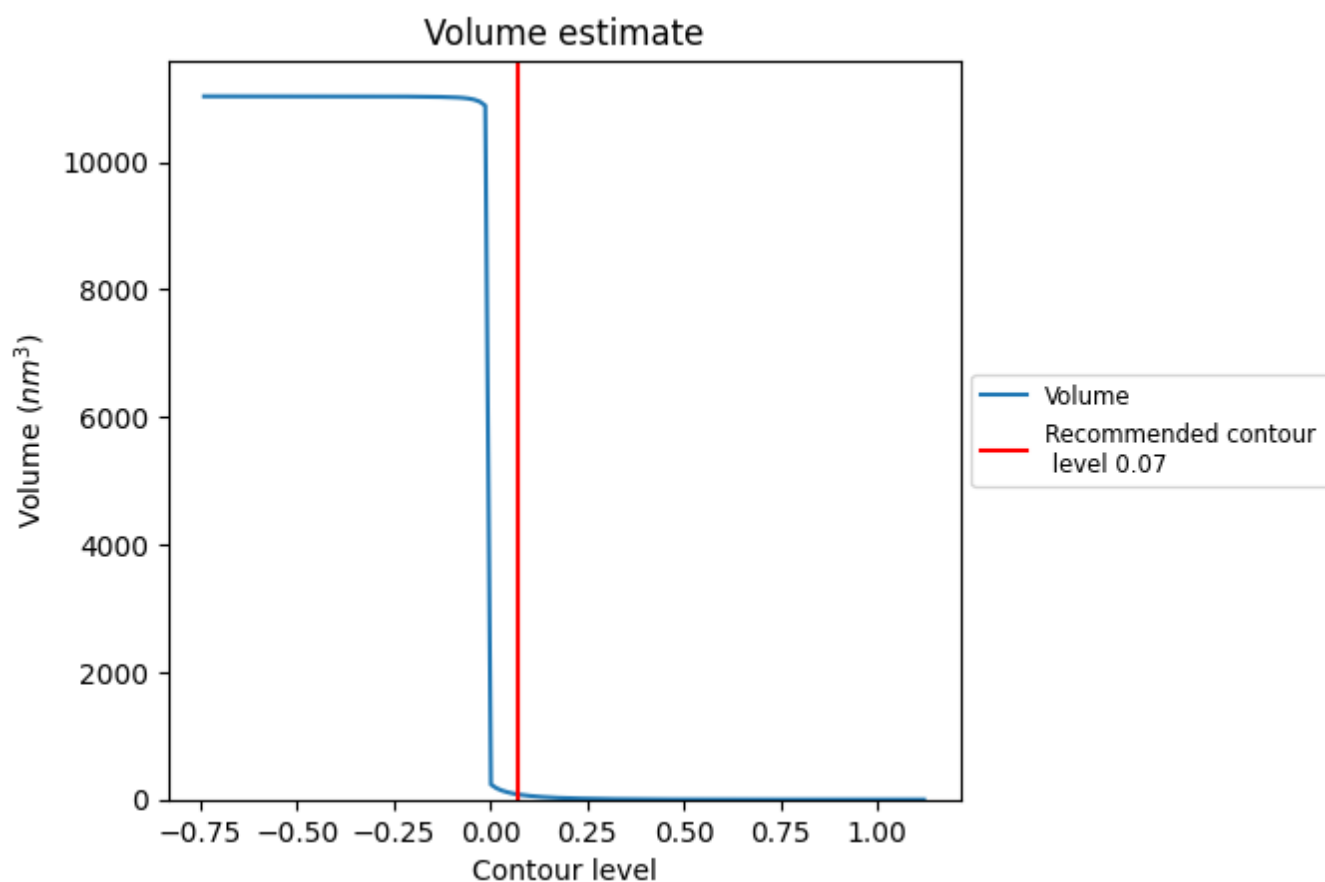
This section contains the results of statistical analysis of the map.

### 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.

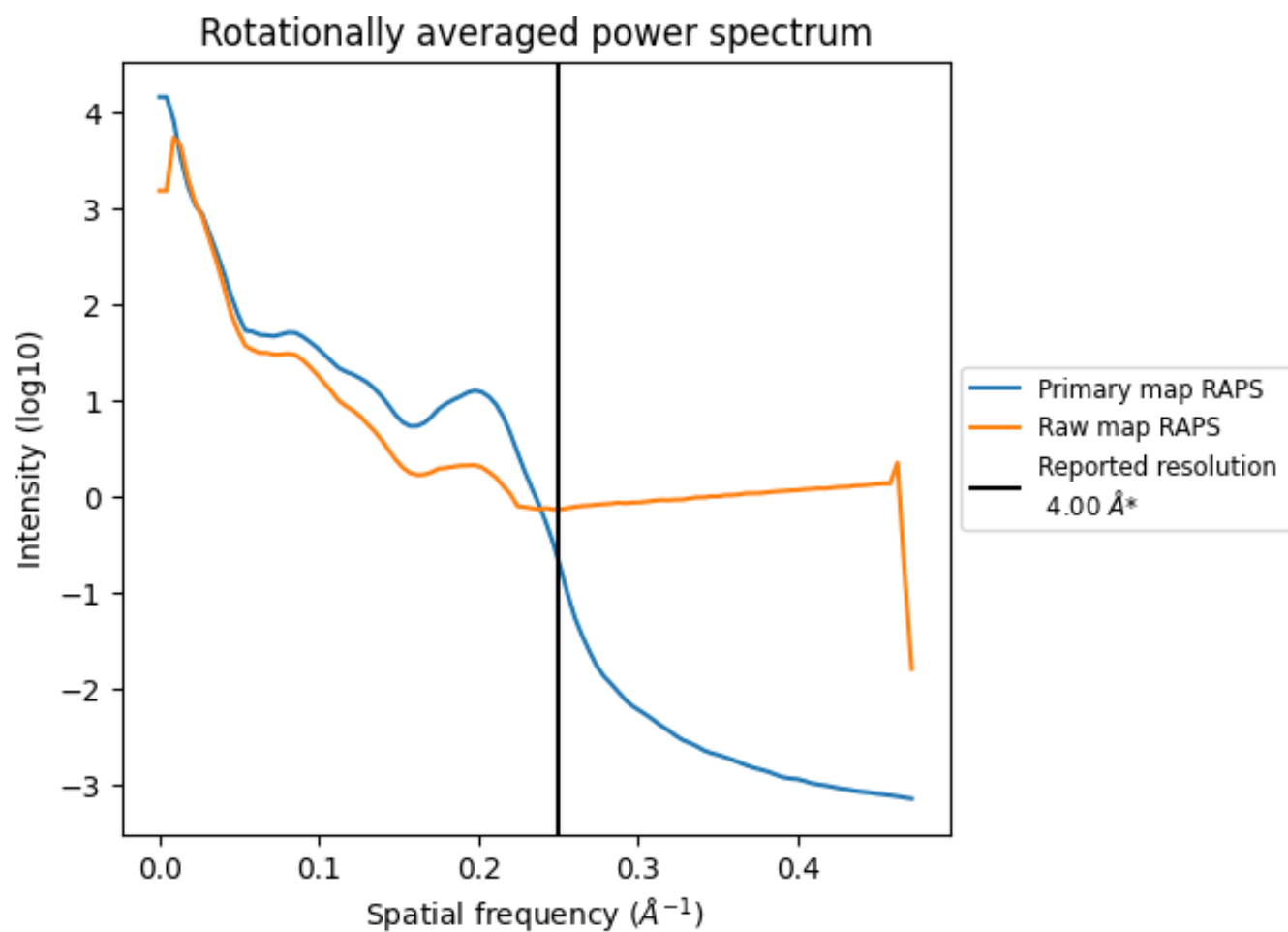
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm<sup>3</sup>; this corresponds to an approximate mass of 74 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 ⓘ

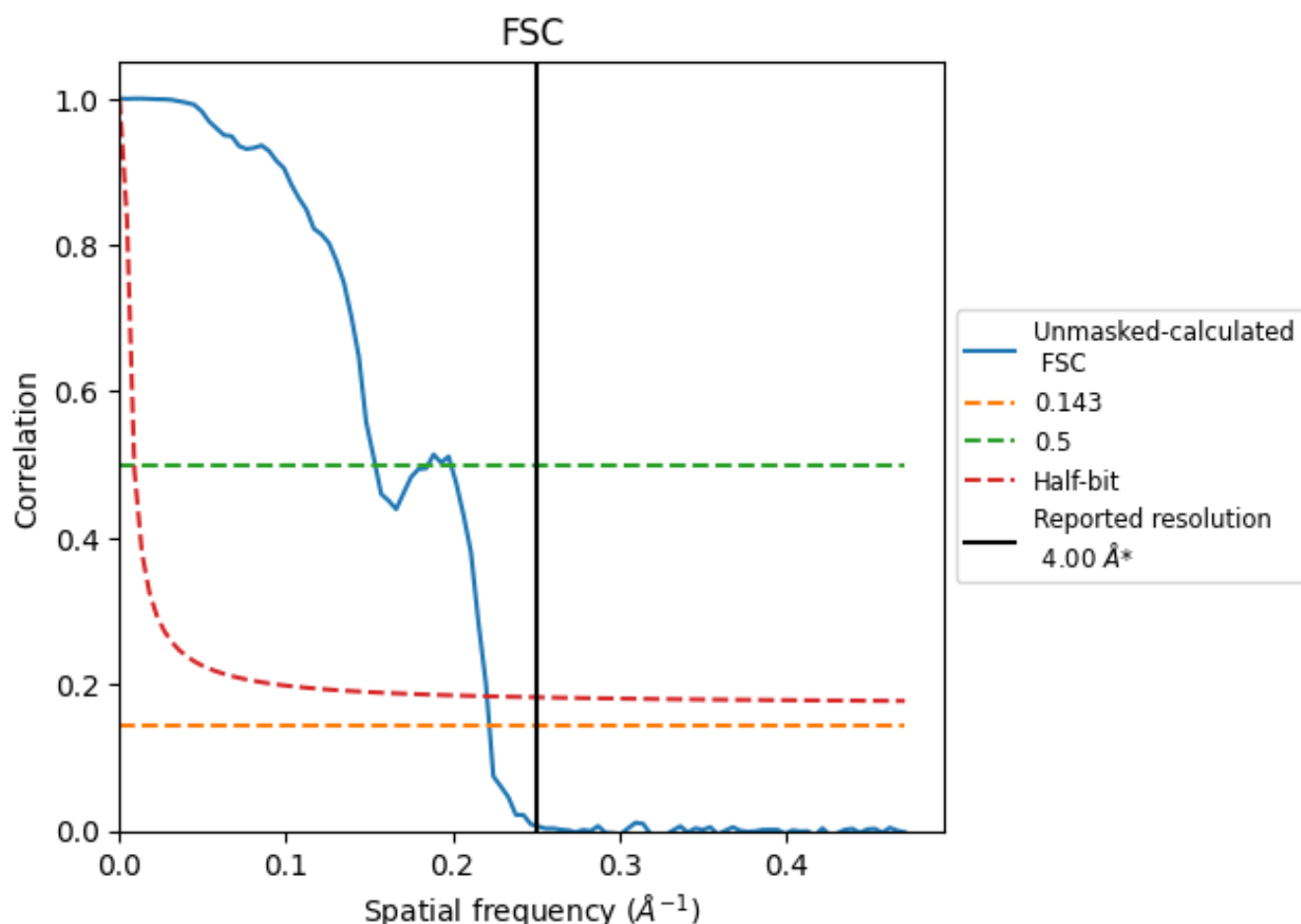


\*Reported resolution corresponds to spatial frequency of  $0.250 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

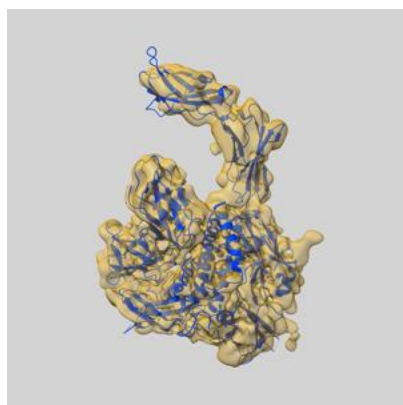
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	6.51	4.53

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 4.0 by more than 10 %

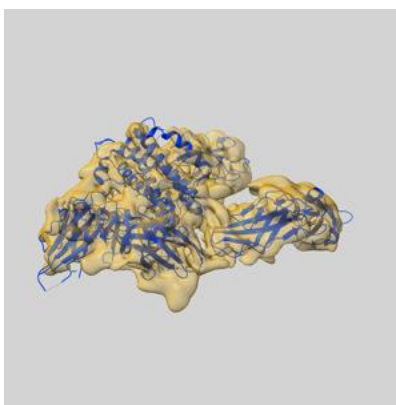
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14427 and PDB model 7Z0L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

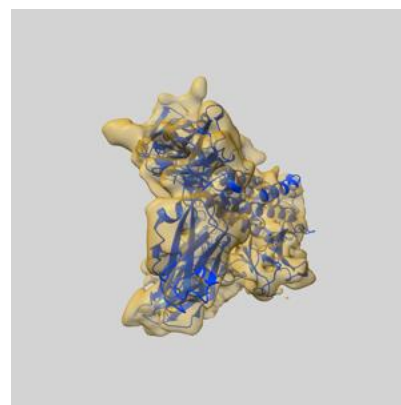
### 9.1 Map-model overlay [i](#)



X



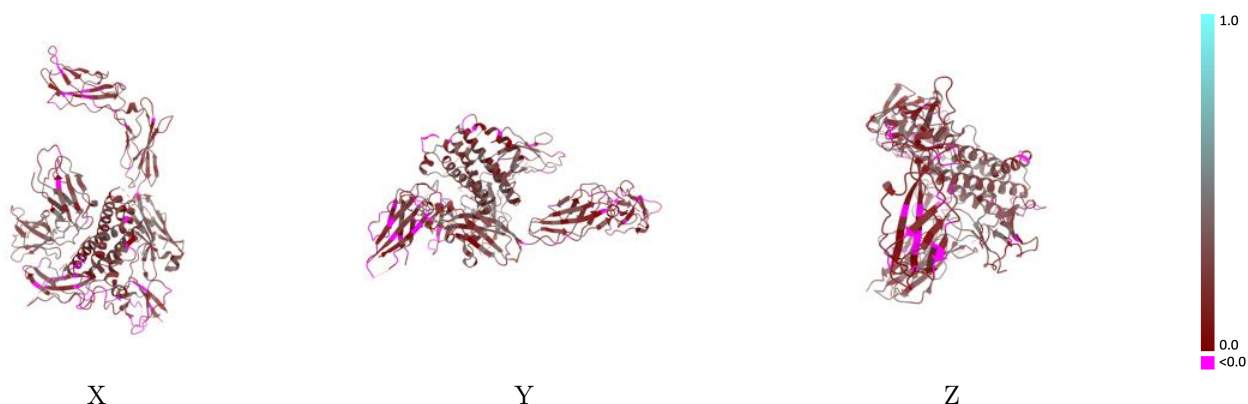
Y



Z

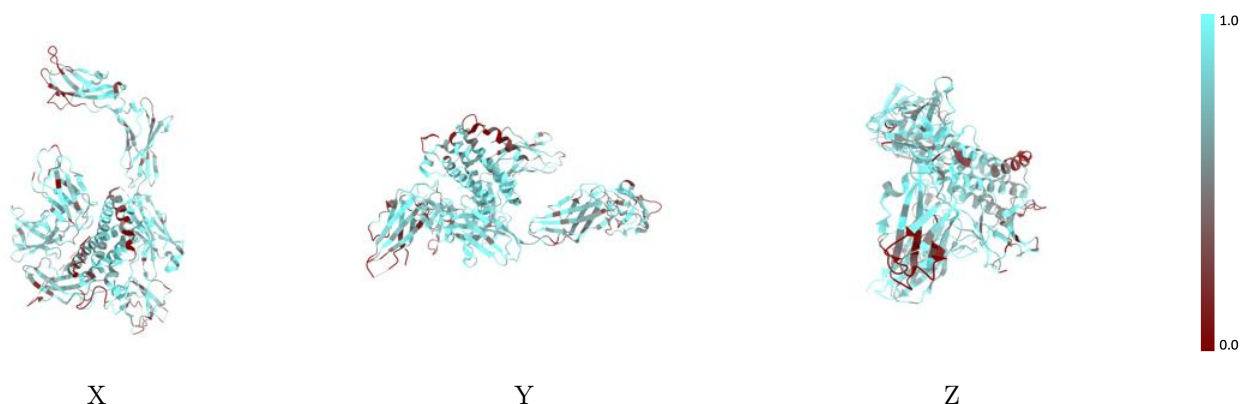
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



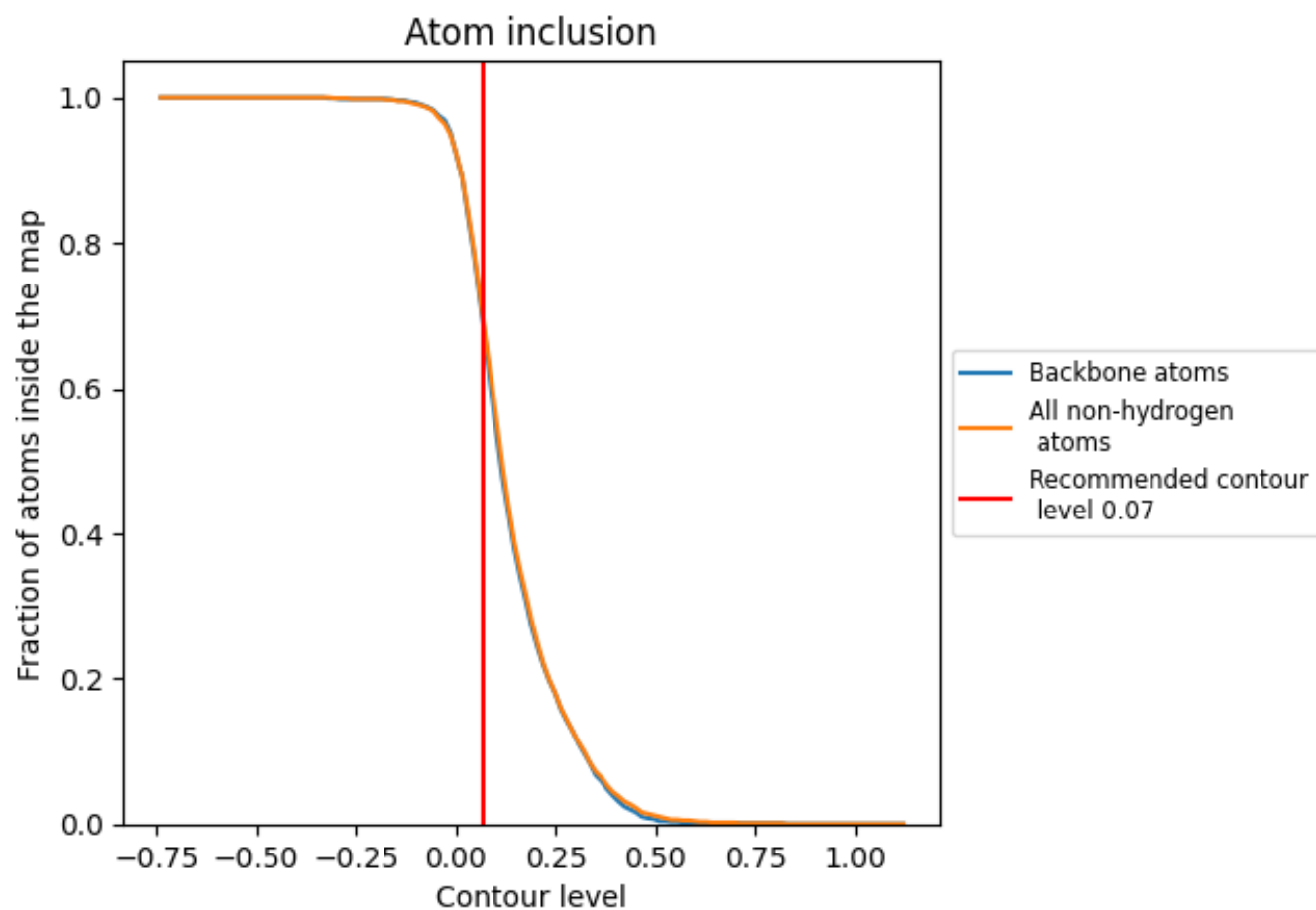
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 68% of all backbone atoms, 68% 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> 0.6850	<div></div> 0.2120
A	<div></div> 0.6990	<div></div> 0.1890
B	<div></div> 0.6630	<div></div> 0.1850
C	<div></div> 0.7680	<div></div> 0.2880
E	<div></div> 1.0000	<div></div> 0.3000
F	<div></div> 0.8570	<div></div> 0.3230
G	<div></div> 0.4640	<div></div> 0.2620
H	<div></div> 0.8210	<div></div> 0.3340
I	<div></div> 0.7500	<div></div> 0.2730

1.0

0.0

<0.0