



## Full wwPDB EM Validation Report ⓘ

Sep 29, 2024 – 02:45 AM EDT

PDB ID : 8D6A  
EMDB ID : EMD-27221  
Title : Cryo-EM structure of human LIF signaling complex: model containing the interaction core region  
Authors : Zhou, Y.; Franklin, M.C.  
Deposited on : 2022-06-06  
Resolution : 3.54 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 : 2022.3.0, CSD as543be (2022)  
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

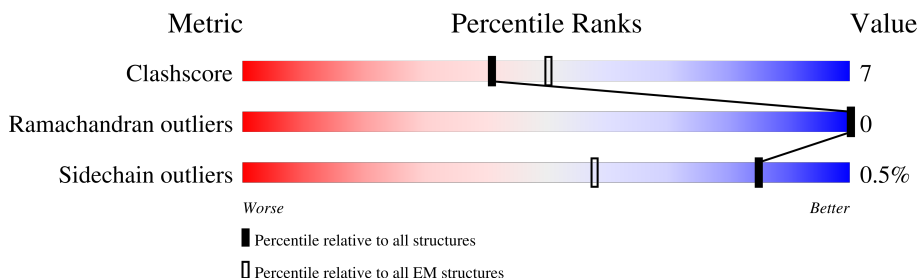
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.54 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	D	179	 82% 12% 6%
2	A	625	 50% 13% 37%
3	B	817	 41% 8% 51%
4	C	2	 50% 100%
4	E	2	 100%
4	F	2	 100%
4	G	2	 100%
4	H	2	 100%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7912 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Leukemia inhibitory factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	169	Total	C	N	O	S	0	0
			1310	834	233	236	7		

- Molecule 2 is a protein called Interleukin-6 receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	392	Total	C	N	O	S	0	0
			3167	2025	528	601	13		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	620	GLU	-	expression tag	UNP P40189
A	621	GLN	-	expression tag	UNP P40189
A	622	LYS	-	expression tag	UNP P40189
A	623	LEU	-	expression tag	UNP P40189
A	624	ILE	-	expression tag	UNP P40189
A	625	SER	-	expression tag	UNP P40189
A	626	GLU	-	expression tag	UNP P40189
A	627	GLU	-	expression tag	UNP P40189
A	628	ASP	-	expression tag	UNP P40189
A	629	LEU	-	expression tag	UNP P40189
A	630	GLY	-	expression tag	UNP P40189
A	631	GLY	-	expression tag	UNP P40189
A	632	GLU	-	expression tag	UNP P40189
A	633	GLN	-	expression tag	UNP P40189
A	634	LYS	-	expression tag	UNP P40189
A	635	LEU	-	expression tag	UNP P40189
A	636	ILE	-	expression tag	UNP P40189
A	637	SER	-	expression tag	UNP P40189
A	638	GLU	-	expression tag	UNP P40189
A	639	GLU	-	expression tag	UNP P40189
A	640	ASP	-	expression tag	UNP P40189

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Chain	Residue	Modelled	Actual	Comment	Reference
A	641	LEU	-	expression tag	UNP P40189
A	642	HIS	-	expression tag	UNP P40189
A	643	HIS	-	expression tag	UNP P40189
A	644	HIS	-	expression tag	UNP P40189
A	645	HIS	-	expression tag	UNP P40189
A	646	HIS	-	expression tag	UNP P40189
A	647	HIS	-	expression tag	UNP P40189

- Molecule 3 is a protein called Leukemia inhibitory factor receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	402	Total	C	N	O	S	0	0
			3225	2064	545	604	12		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	834	GLU	-	expression tag	UNP P42702
B	835	GLN	-	expression tag	UNP P42702
B	836	LYS	-	expression tag	UNP P42702
B	837	LEU	-	expression tag	UNP P42702
B	838	ILE	-	expression tag	UNP P42702
B	839	SER	-	expression tag	UNP P42702
B	840	GLU	-	expression tag	UNP P42702
B	841	GLU	-	expression tag	UNP P42702
B	842	ASP	-	expression tag	UNP P42702
B	843	LEU	-	expression tag	UNP P42702
B	844	GLY	-	expression tag	UNP P42702
B	845	GLY	-	expression tag	UNP P42702
B	846	GLU	-	expression tag	UNP P42702
B	847	GLN	-	expression tag	UNP P42702
B	848	LYS	-	expression tag	UNP P42702
B	849	LEU	-	expression tag	UNP P42702
B	850	ILE	-	expression tag	UNP P42702
B	851	SER	-	expression tag	UNP P42702
B	852	GLU	-	expression tag	UNP P42702
B	853	GLU	-	expression tag	UNP P42702
B	854	ASP	-	expression tag	UNP P42702
B	855	LEU	-	expression tag	UNP P42702
B	856	HIS	-	expression tag	UNP P42702
B	857	HIS	-	expression tag	UNP P42702
B	858	HIS	-	expression tag	UNP P42702

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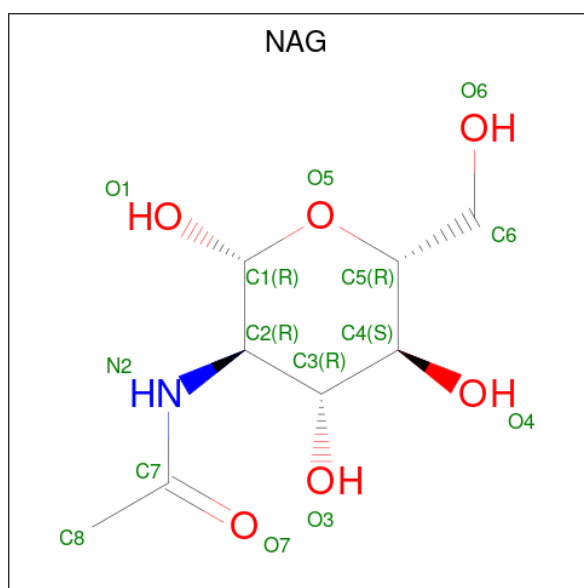
Chain	Residue	Modelled	Actual	Comment	Reference
B	859	HIS	-	expression tag	UNP P42702
B	860	HIS	-	expression tag	UNP P42702
B	861	HIS	-	expression tag	UNP P42702

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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







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

Chain G:  100%

MAG1  
MAG2

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

Chain H:  100%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	171328	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.716	Depositor
Minimum map value	-0.226	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	D	0.24	0/1336	0.38	0/1809
2	A	0.23	0/3256	0.45	0/4442
3	B	0.24	0/3309	0.45	0/4511
All	All	0.24	0/7901	0.44	0/10762

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1310	0	1332	13	0
2	A	3167	0	3101	51	0
3	B	3225	0	3185	43	0
4	C	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	70	0	65	0	0
All	All	7912	0	7808	105	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 (105) 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)
3:B:341:CYS:HB3	3:B:351:CYS:HA	1.66	0.78
2:A:160:LEU:HB3	2:A:172:CYS:HB3	1.69	0.74
3:B:466:CYS:HA	3:B:511:CYS:HA	1.70	0.72
3:B:318:THR:HG22	3:B:319:GLU:H	1.59	0.68
3:B:281:LEU:HD12	3:B:284:HIS:HA	1.75	0.67
3:B:441:VAL:HB	3:B:528:HIS:HB2	1.76	0.66
2:A:426:PRO:HB3	2:A:506:SER:HB3	1.78	0.64
2:A:157:ASN:HD21	2:A:176:ARG:HH21	1.47	0.62
3:B:442:LYS:HD3	3:B:443:ASP:H	1.63	0.62
3:B:372:VAL:HG23	3:B:379:TYR:HB3	1.82	0.62
2:A:327:SER:HB2	2:A:358:GLU:HB3	1.82	0.61
1:D:37:ARG:HH12	2:A:168:LYS:HB3	1.67	0.60
2:A:199:GLU:HG3	2:A:208:THR:HG22	1.84	0.60
3:B:496:LEU:HD21	3:B:499:LEU:HD12	1.83	0.60
2:A:335:LYS:HB3	2:A:348:GLN:HB2	1.83	0.59
3:B:136:PRO:HG3	3:B:224:ILE:HG12	1.84	0.59
2:A:182:CYS:SG	2:A:183:THR:N	2.75	0.59
3:B:177:LEU:HD12	3:B:181:SER:HA	1.84	0.59
2:A:395:ARG:HE	2:A:418:ALA:HB2	1.68	0.59
2:A:442:GLU:HG3	2:A:479:ARG:HB3	1.85	0.59
2:A:133:SER:O	2:A:145:GLU:N	2.28	0.58
1:D:174:GLY:HA2	1:D:180:LYS:HE3	1.84	0.58
2:A:231:ILE:HD11	2:A:241:LYS:HD3	1.86	0.57
2:A:292:PHE:N	2:A:321:THR:OG1	2.36	0.57
3:B:487:VAL:HG22	3:B:488:GLU:H	1.70	0.56
3:B:358:VAL:HG12	3:B:360:ALA:H	1.70	0.56
3:B:332:PRO:O	3:B:357:ARG:NH2	2.39	0.55
2:A:162:SER:HB3	2:A:194:ILE:HD11	1.89	0.54
3:B:352:SER:HB3	3:B:394:GLN:HG3	1.88	0.54
2:A:446:PRO:HB2	2:A:450:VAL:HG21	1.88	0.54
2:A:238:SER:HB3	2:A:289:LEU:H	1.73	0.54
2:A:454:ILE:O	2:A:497:THR:OG1	2.26	0.54
2:A:172:CYS:SG	2:A:183:THR:N	2.70	0.53
2:A:151:GLU:O	2:A:152:THR:HG22	2.08	0.53
2:A:255:LEU:HD12	2:A:301:CYS:HB2	1.90	0.53
3:B:282:ILE:HG21	3:B:301:ILE:HD12	1.91	0.53
2:A:263:THR:HG22	2:A:266:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:398:ALA:HB3	2:A:414:LEU:HB3	1.92	0.52
3:B:226:ASN:HB3	3:B:229:PHE:HB2	1.92	0.52
3:B:469:GLU:HB3	3:B:479:GLN:HE22	1.75	0.52
1:D:48:ILE:HA	1:D:51:GLN:HE21	1.75	0.51
3:B:434:HIS:CD2	3:B:435:THR:H	2.29	0.51
2:A:259:ILE:HB	2:A:272:ILE:HD12	1.94	0.50
2:A:324:ASP:N	2:A:324:ASP:OD1	2.44	0.50
2:A:345:ARG:NH2	2:A:419:CYS:SG	2.85	0.50
3:B:282:ILE:HG23	3:B:283:GLY:H	1.76	0.50
3:B:343:THR:OG1	3:B:345:ASP:O	2.30	0.49
1:D:115:SER:HB3	1:D:187:LEU:HD21	1.94	0.49
2:A:134:CYS:HA	2:A:144:CYS:HA	1.93	0.49
2:A:345:ARG:HH12	2:A:419:CYS:HA	1.77	0.49
3:B:496:LEU:HG	3:B:497:ASP:H	1.77	0.49
2:A:327:SER:OG	2:A:328:LYS:N	2.46	0.48
1:D:109:VAL:HG13	1:D:148:LEU:HD12	1.94	0.48
1:D:64:ILE:HA	1:D:67:TYR:CE1	2.48	0.48
3:B:170:VAL:HG12	3:B:224:ILE:HG22	1.94	0.48
2:A:246:ASN:ND2	2:A:257:TYR:OH	2.46	0.48
2:A:249:ILE:HG23	2:A:255:LEU:HD21	1.96	0.47
2:A:180:THR:HG23	2:A:181:SER:H	1.79	0.47
2:A:125:PRO:O	2:A:150:ARG:NH2	2.34	0.47
3:B:499:LEU:HD23	3:B:500:ASN:N	2.29	0.47
3:B:247:ILE:HD12	3:B:248:PRO:HD2	1.97	0.46
1:D:75:PRO:HA	1:D:78:LEU:HG	1.97	0.45
3:B:159:ASP:N	3:B:159:ASP:OD1	2.47	0.45
2:A:427:VAL:HG23	2:A:498:PRO:HG3	1.97	0.45
2:A:327:SER:HB3	2:A:354:LEU:HD21	1.98	0.44
2:A:454:ILE:HG12	2:A:472:GLN:HA	1.99	0.44
3:B:318:THR:HG22	3:B:319:GLU:N	2.31	0.44
2:A:262:ARG:HD2	2:A:266:ALA:HB3	2.00	0.44
3:B:473:SER:O	3:B:473:SER:OG	2.30	0.44
3:B:454:HIS:HA	3:B:491:SER:HA	2.00	0.44
3:B:465:LEU:HG	3:B:481:ASN:ND2	2.32	0.44
2:A:257:TYR:HB3	2:A:299:ILE:HD11	2.00	0.44
3:B:447:THR:HG22	3:B:448:ALA:H	1.83	0.44
3:B:443:ASP:OD2	3:B:530:THR:OG1	2.34	0.43
2:A:372:ARG:HD3	2:A:373:TRP:N	2.33	0.43
3:B:320:ASP:N	3:B:320:ASP:OD1	2.51	0.43
2:A:246:ASN:HB2	2:A:250:LYS:HD3	2.00	0.43
2:A:372:ARG:HD2	2:A:395:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:436:ASP:N	2:A:436:ASP:OD1	2.49	0.43
3:B:177:LEU:H	3:B:177:LEU:HD23	1.83	0.43
2:A:417:PRO:HB3	2:A:503:GLY:HA3	2.00	0.43
2:A:435:LYS:HD2	2:A:435:LYS:HA	1.82	0.43
3:B:282:ILE:HD12	3:B:314:VAL:HG22	2.01	0.42
3:B:301:ILE:HG12	3:B:304:ILE:HG22	2.01	0.42
2:A:460:LEU:HB2	2:A:491:CYS:SG	2.60	0.42
3:B:491:SER:OG	3:B:492:TYR:N	2.53	0.42
2:A:455:LEU:HD23	2:A:455:LEU:H	1.83	0.42
1:D:37:ARG:HH11	2:A:163:GLU:HG3	1.85	0.42
2:A:399:THR:HG23	2:A:411:ALA:HB1	2.02	0.41
1:D:97:THR:HG23	1:D:100:ALA:H	1.85	0.41
1:D:195:ILE:HD12	1:D:195:ILE:HA	1.90	0.41
3:B:336:PRO:HG3	3:B:410:LEU:HD22	2.02	0.41
2:A:450:VAL:HG11	2:A:453:TYR:CZ	2.56	0.41
3:B:268:THR:HG22	3:B:300:LYS:HG3	2.02	0.41
3:B:469:GLU:HG3	3:B:508:ARG:HB3	2.03	0.41
1:D:102:LEU:HD22	1:D:151:VAL:HG23	2.03	0.41
3:B:208:ASP:N	3:B:208:ASP:OD1	2.54	0.41
3:B:468:ILE:HG12	3:B:509:ILE:HG22	2.01	0.41
1:D:96:GLY:O	1:D:101:LYS:NZ	2.54	0.40
1:D:109:VAL:HG23	1:D:144:LEU:HD22	2.02	0.40
2:A:332:PHE:HB3	2:A:351:TRP:HB3	2.03	0.40
3:B:136:PRO:HB2	3:B:236:SER:HB3	2.03	0.40
2:A:291:PRO:HG2	2:A:360:ASN:ND2	2.35	0.40
2:A:177:ASP:OD2	2:A:178:THR:N	2.54	0.40
3:B:462:ILE:HD12	3:B:462:ILE:HA	1.98	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	167/179 (93%)	161 (96%)	6 (4%)	0	100	100
2	A	390/625 (62%)	353 (90%)	37 (10%)	0	100	100
3	B	400/817 (49%)	366 (92%)	34 (8%)	0	100	100
All	All	957/1621 (59%)	880 (92%)	77 (8%)	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	D	144/153 (94%)	143 (99%)	1 (1%)	81	90
2	A	357/566 (63%)	356 (100%)	1 (0%)	91	96
3	B	371/746 (50%)	369 (100%)	2 (0%)	86	93
All	All	872/1465 (60%)	868 (100%)	4 (0%)	85	93

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

Mol	Chain	Res	Type
1	D	40	CYS
2	A	372	ARG
3	B	167	ARG
3	B	440	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	47	GLN
1	D	51	GLN
1	D	54	GLN
1	D	123	GLN
1	D	150	ASN
1	D	193	GLN

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Mol	Chain	Res	Type
2	A	342	GLN
2	A	360	ASN
2	A	485	ASN
3	B	338	GLN
3	B	434	HIS
3	B	479	GLN

### 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 ⓘ

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	C	1	2,4	14,14,15	0.41	0	17,19,21	0.38	0
4	NAG	C	2	4	14,14,15	0.28	0	17,19,21	0.55	0
4	NAG	E	1	3,4	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	E	2	4	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	F	1	3,4	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	F	2	4	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	G	1	3,4	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	H	1	3,4	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	H	2	4	14,14,15	0.25	0	17,19,21	0.44	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	C	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	4/6/23/26	0/1/1/1
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	NAG	F	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	NAG	G	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	3,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	F	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C1-C2-N2-C7

*Continued on next page...*

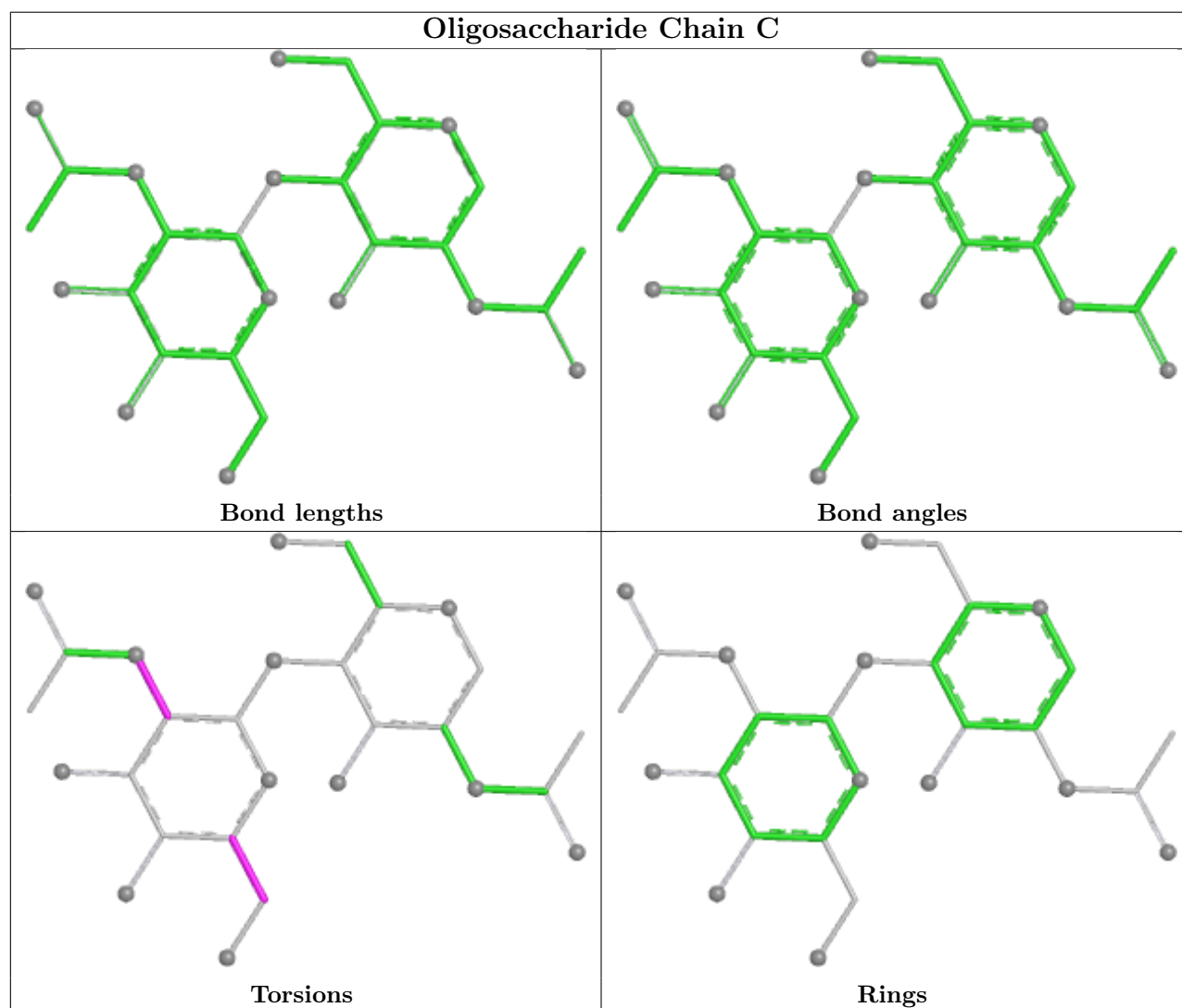
*Continued from previous page...*

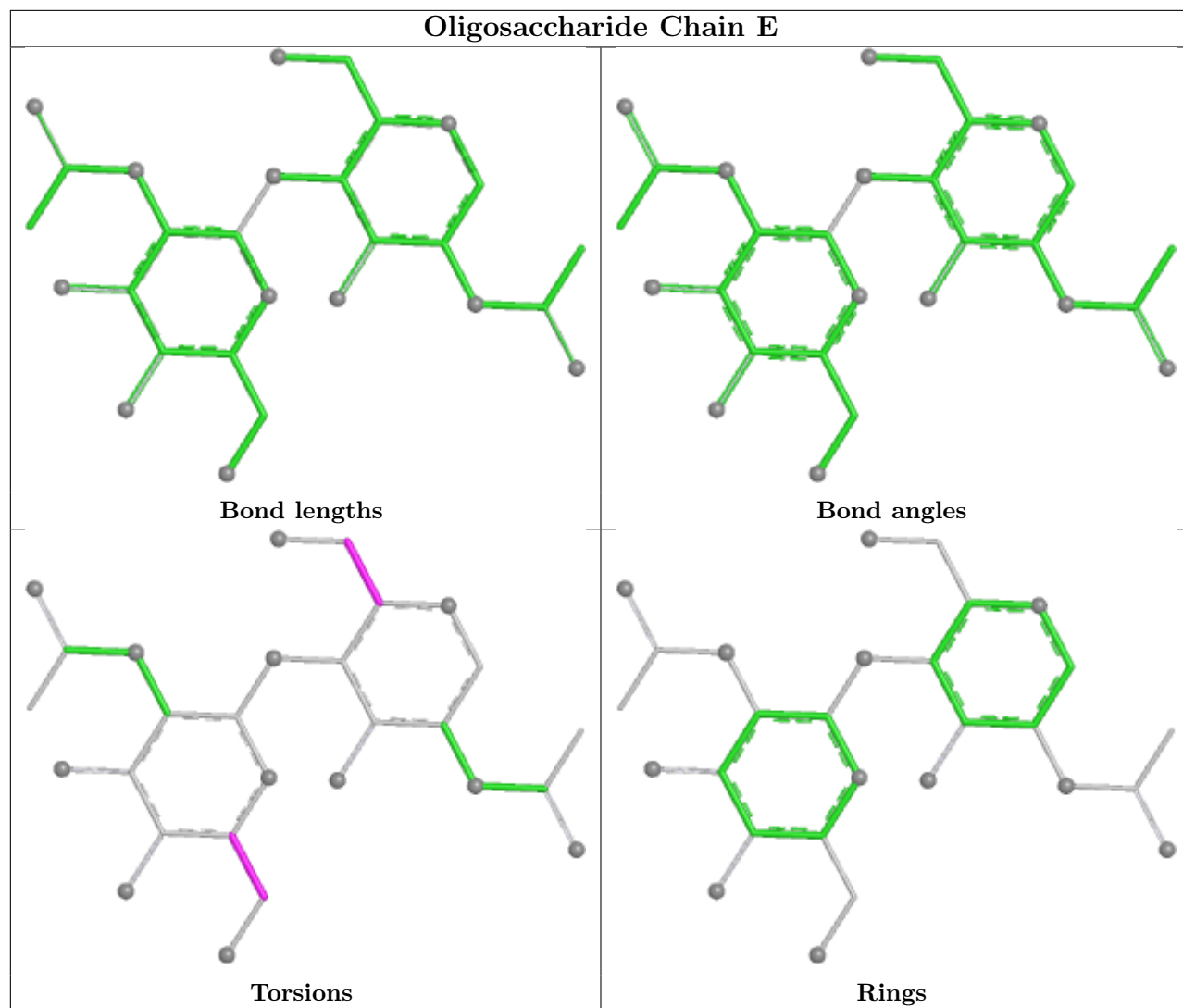
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C1-C2-N2-C7
4	C	2	NAG	C3-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7

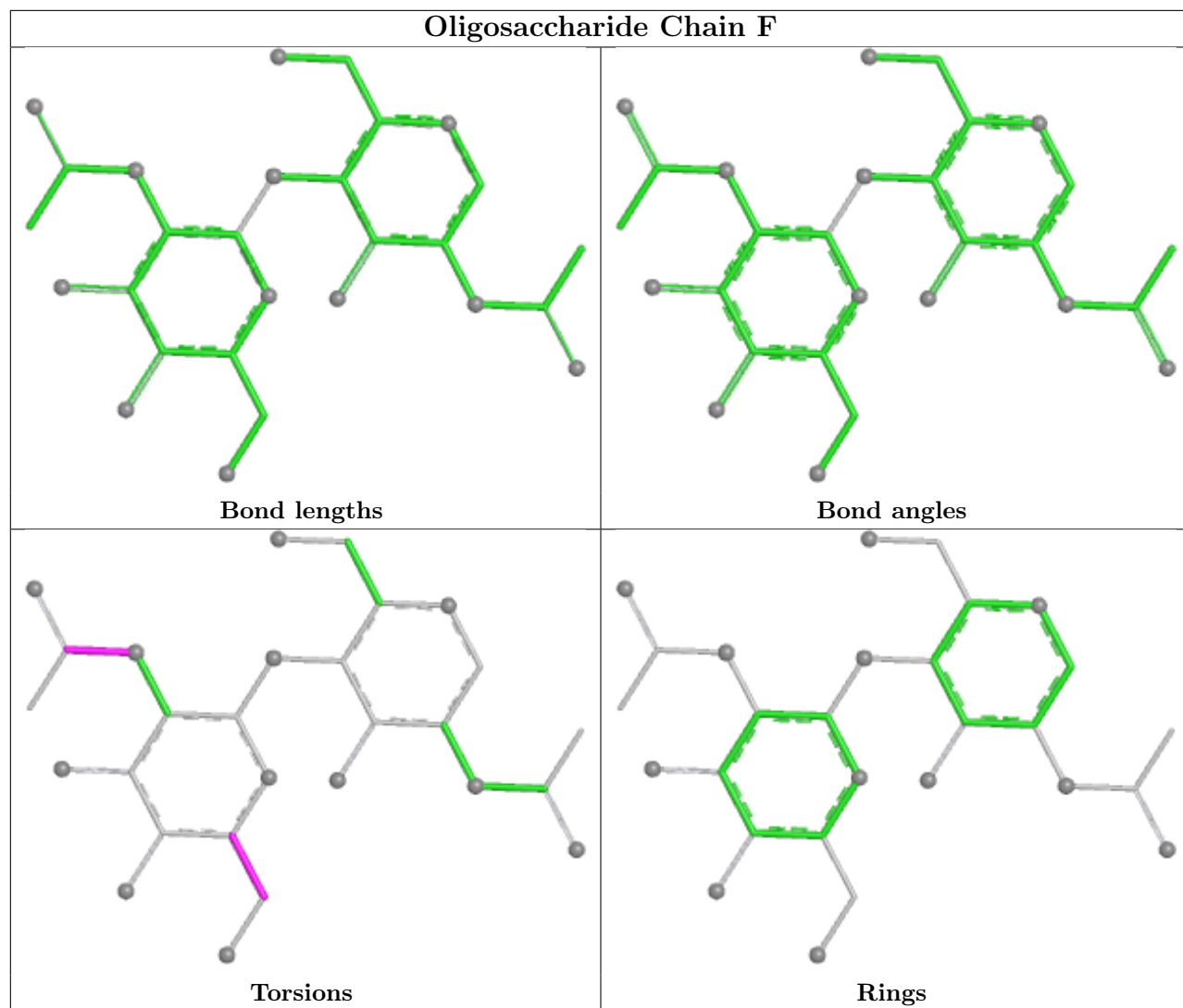
There are no ring outliers.

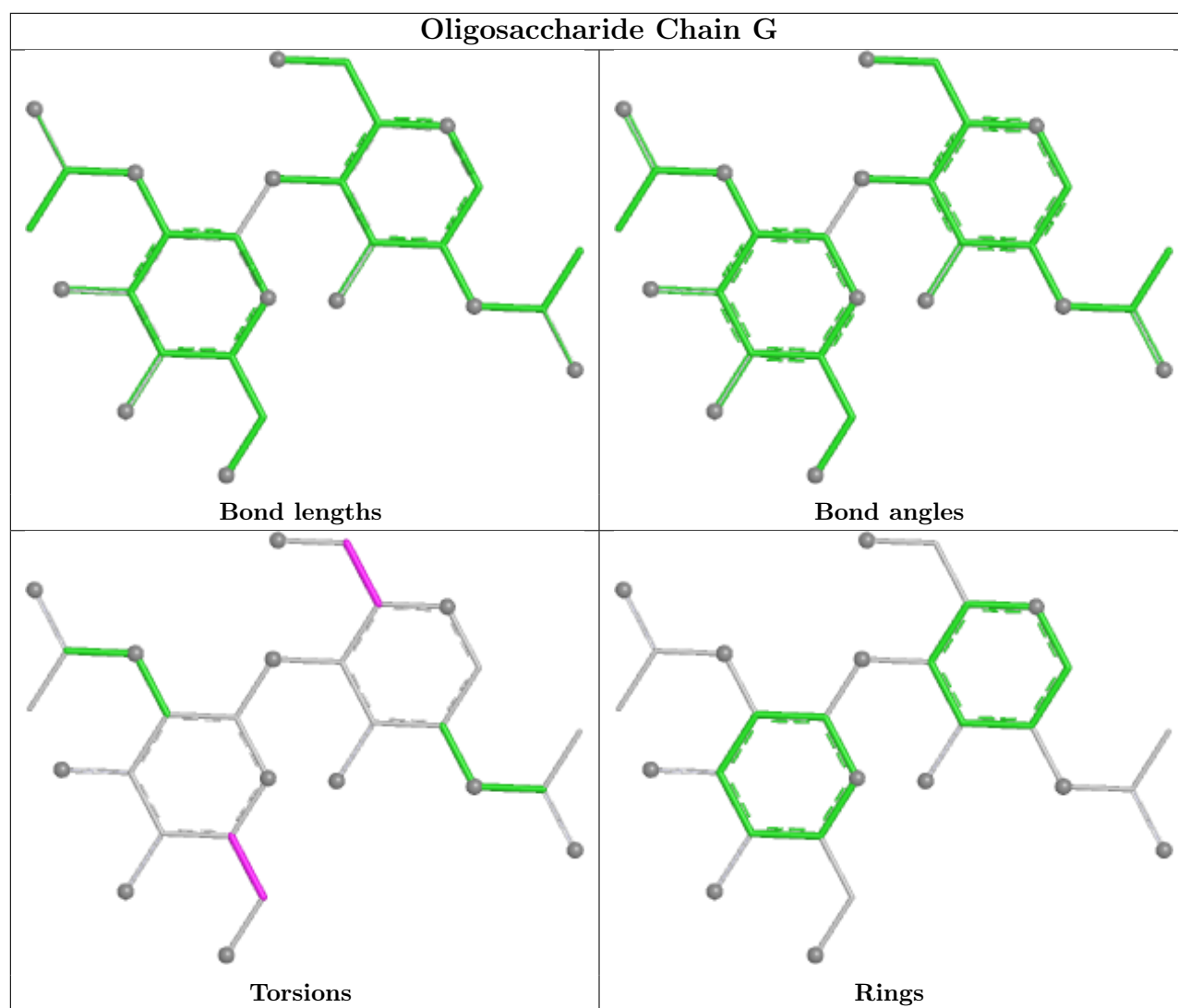
No monomer is involved in short contacts.

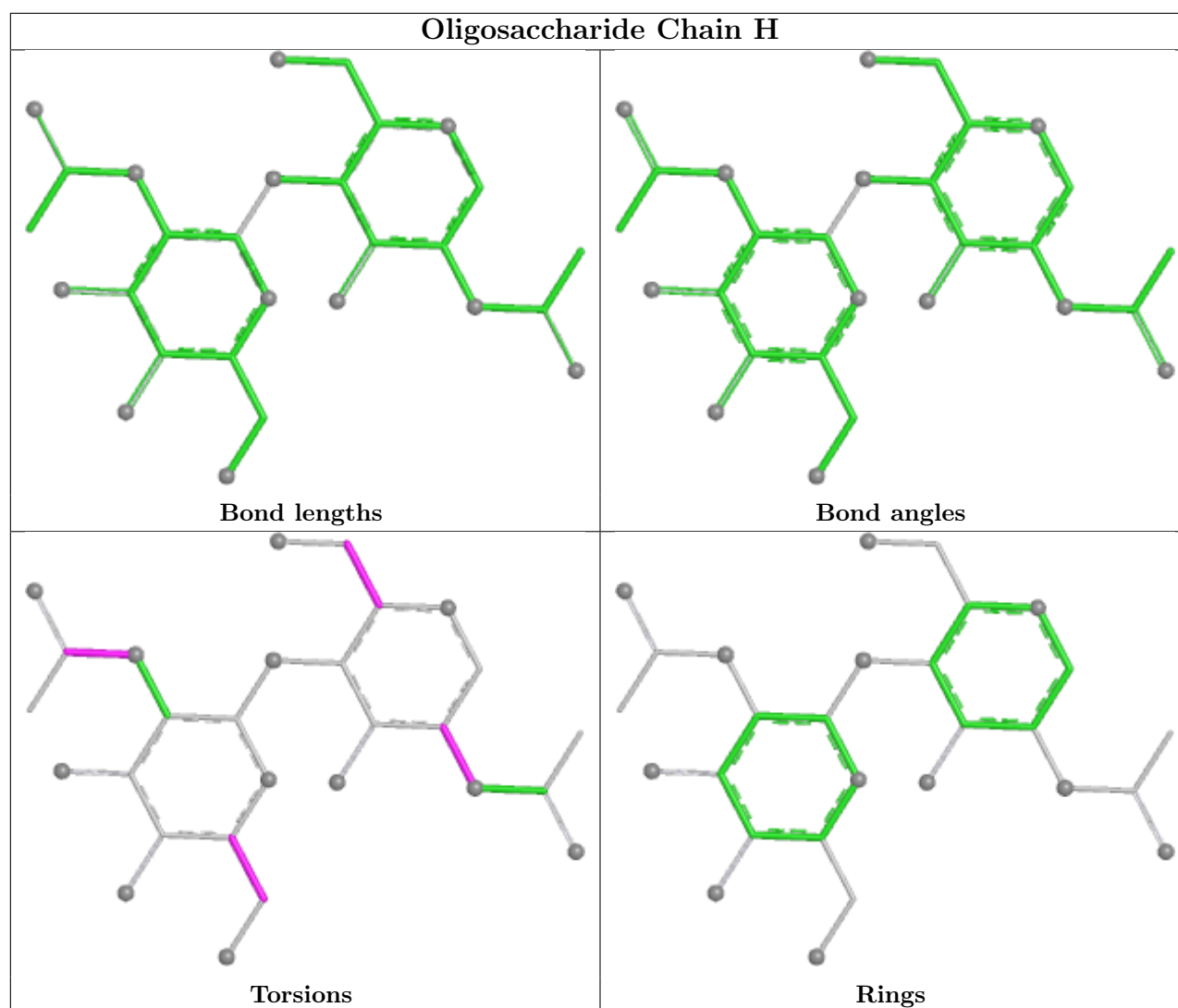
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

5 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	705	2	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	A	701	2	14,14,15	0.40	0	17,19,21	0.42	0
5	NAG	A	703	2	14,14,15	0.27	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	702	2	14,14,15	0.37	0	17,19,21	0.42	0
5	NAG	A	704	2	14,14,15	0.37	0	17,19,21	0.37	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
5	NAG	A	705	2	-	1/6/23/26	0/1/1/1
5	NAG	A	701	2	-	2/6/23/26	0/1/1/1
5	NAG	A	703	2	-	4/6/23/26	0/1/1/1
5	NAG	A	702	2	-	3/6/23/26	0/1/1/1
5	NAG	A	704	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	NAG	O5-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	A	703	NAG	O5-C5-C6-O6
5	A	702	NAG	O5-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
5	A	705	NAG	O5-C5-C6-O6
5	A	703	NAG	C4-C5-C6-O6
5	A	703	NAG	C1-C2-N2-C7
5	A	703	NAG	C3-C2-N2-C7
5	A	702	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



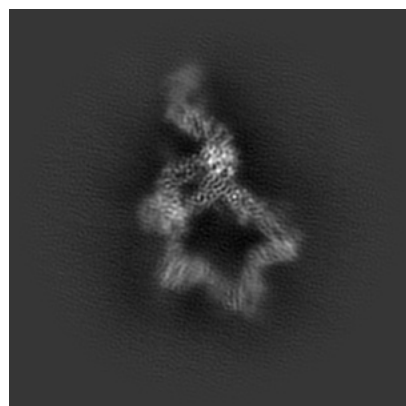
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27221. These allow visual inspection of the internal detail of the map and identification of artifacts.

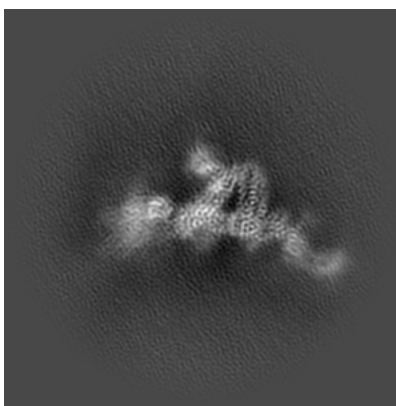
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

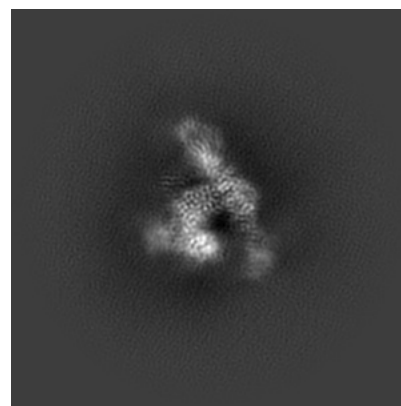
#### 6.1.1 Primary map



X

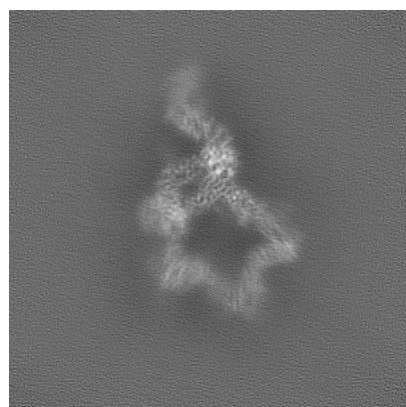


Y

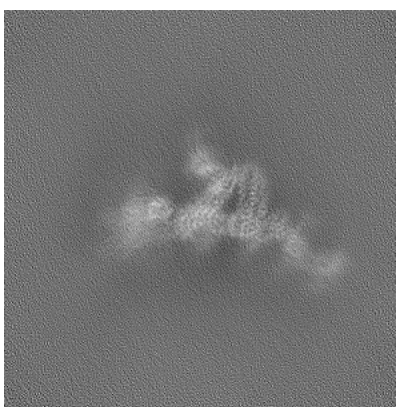


Z

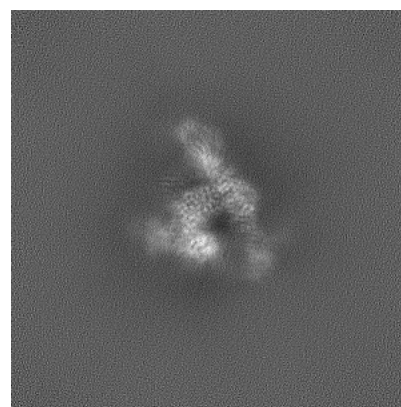
#### 6.1.2 Raw map



X



Y

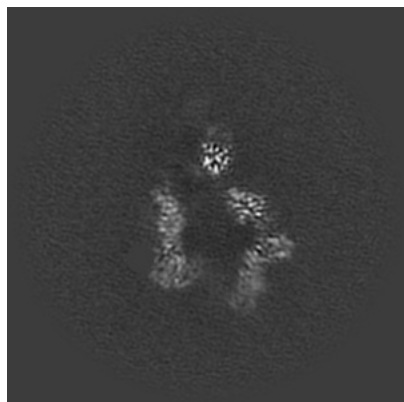


Z

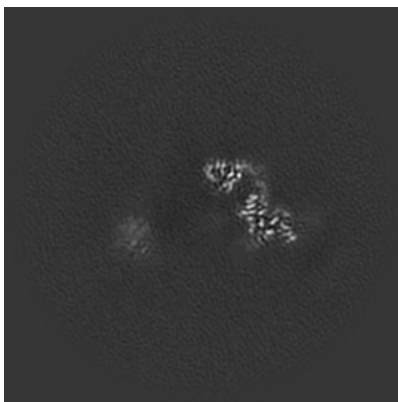
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

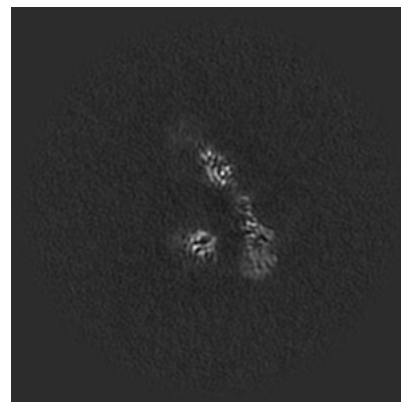
### 6.2.1 Primary map



X Index: 200

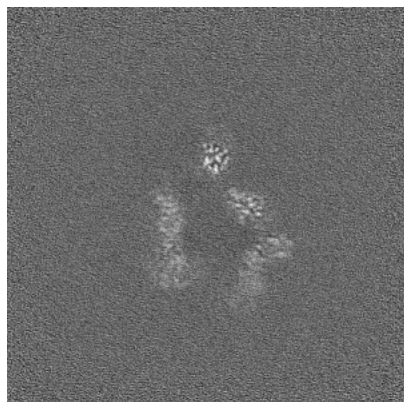


Y Index: 200

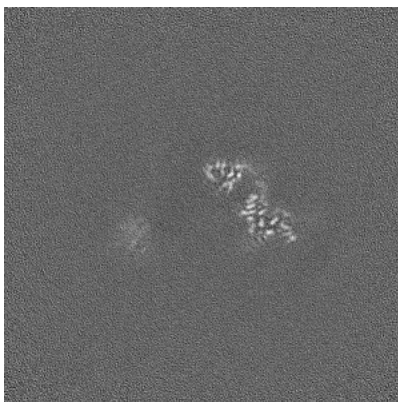


Z Index: 200

### 6.2.2 Raw map



X Index: 200



Y Index: 200

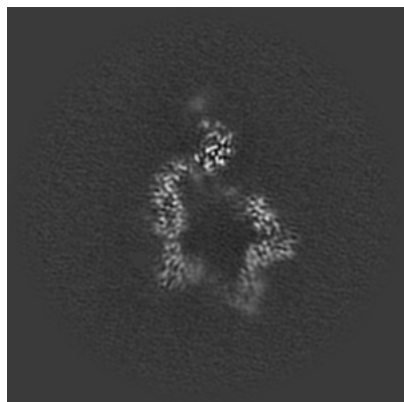


Z Index: 200

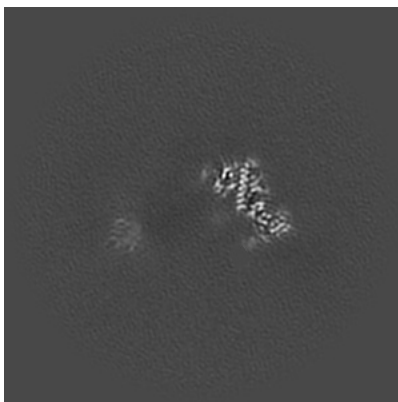
The images above show central slices of the map in three orthogonal directions.

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

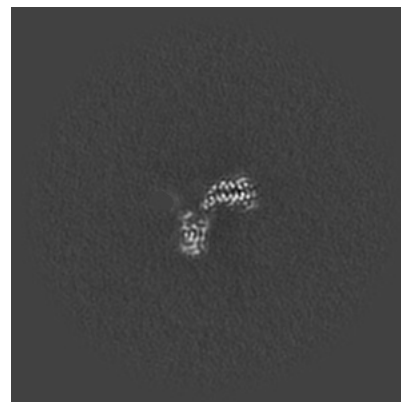
### 6.3.1 Primary map



X Index: 193

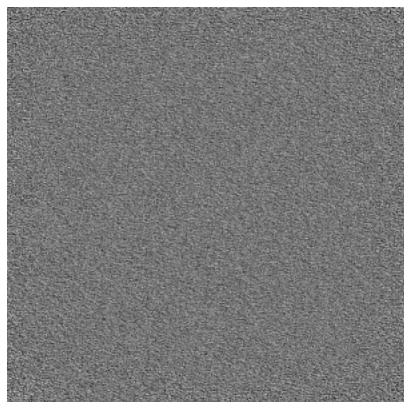


Y Index: 209

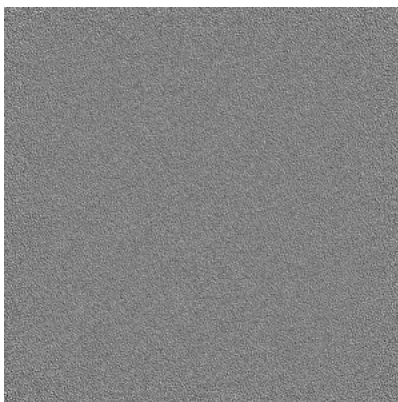


Z Index: 238

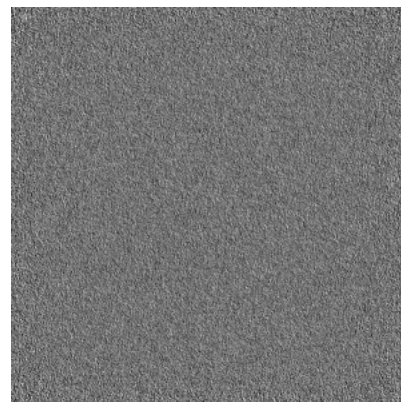
### 6.3.2 Raw map



X Index: 0



Y Index: 0



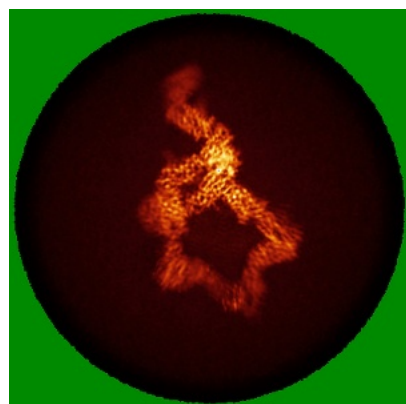
Z Index: 0

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

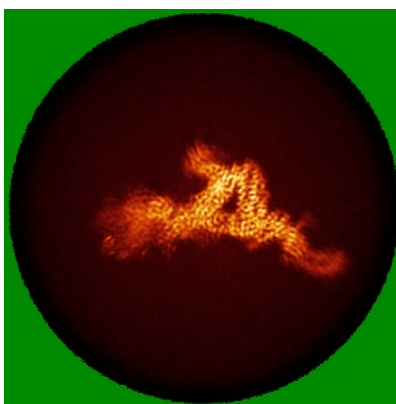


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

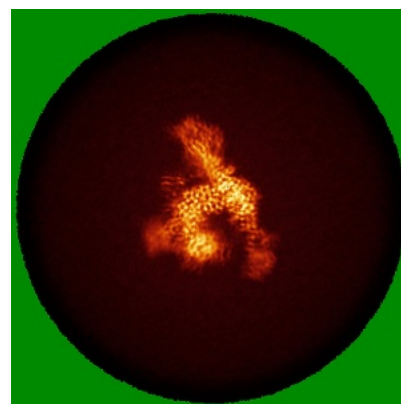
### 6.4.1 Primary map



X

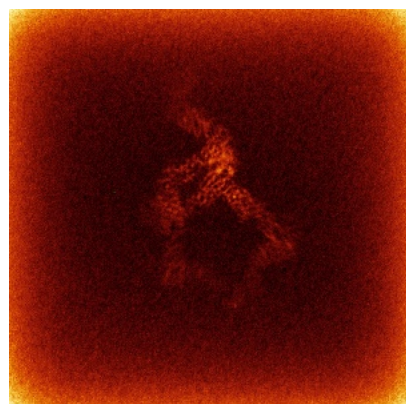


Y

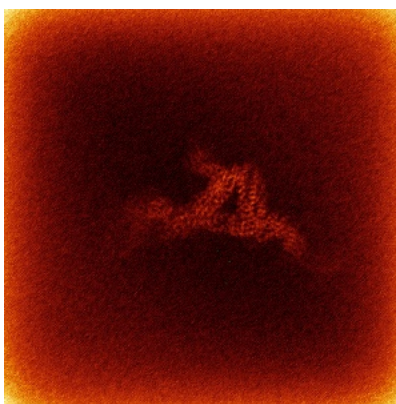


Z

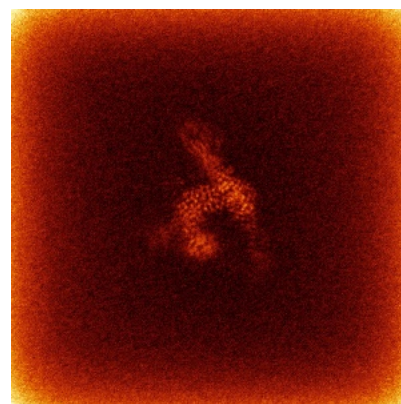
### 6.4.2 Raw map



X



Y

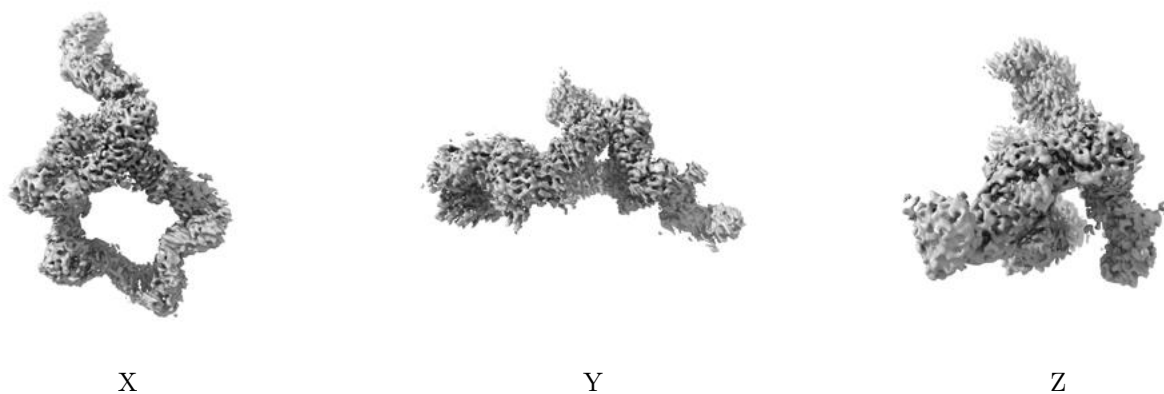


Z

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.

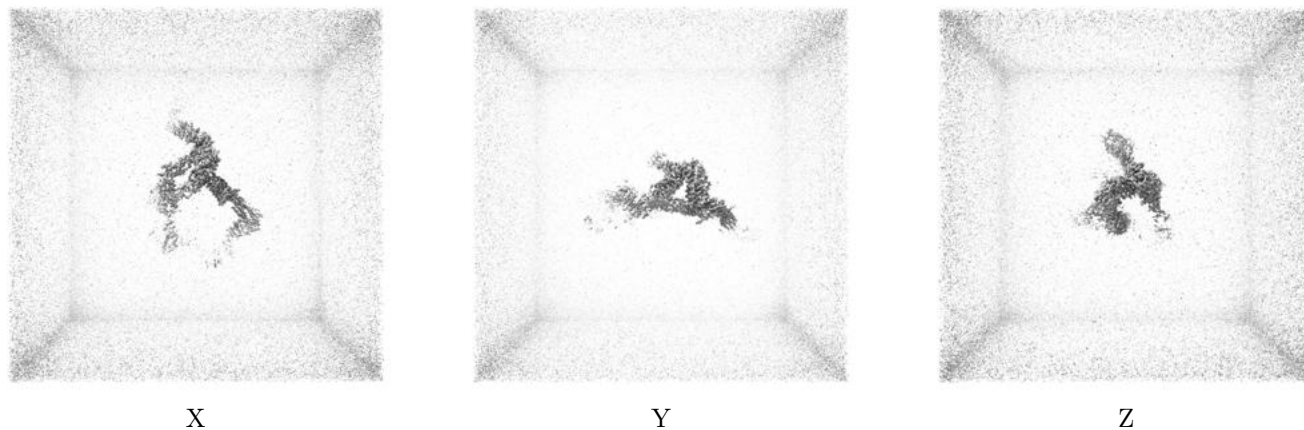
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

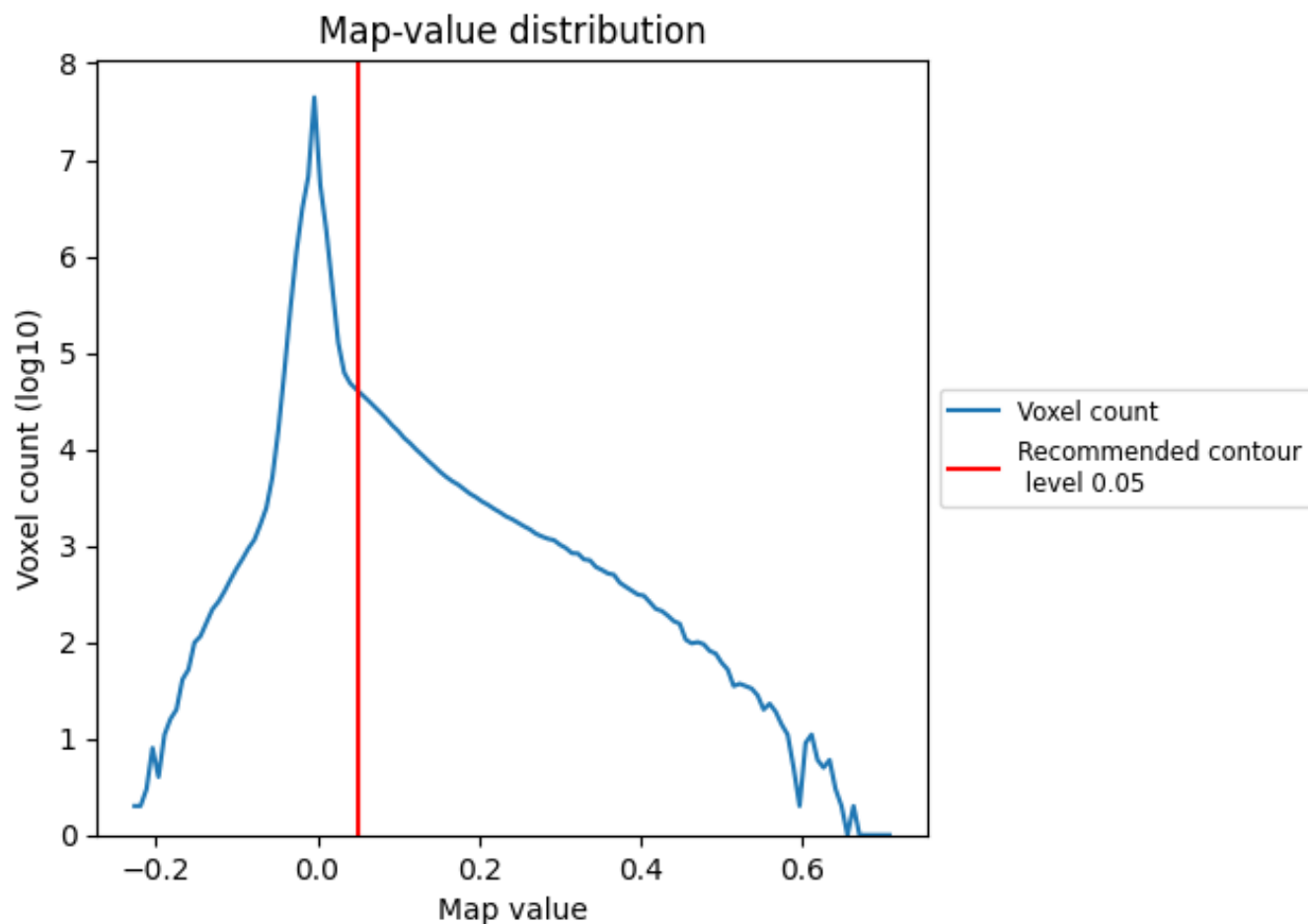
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

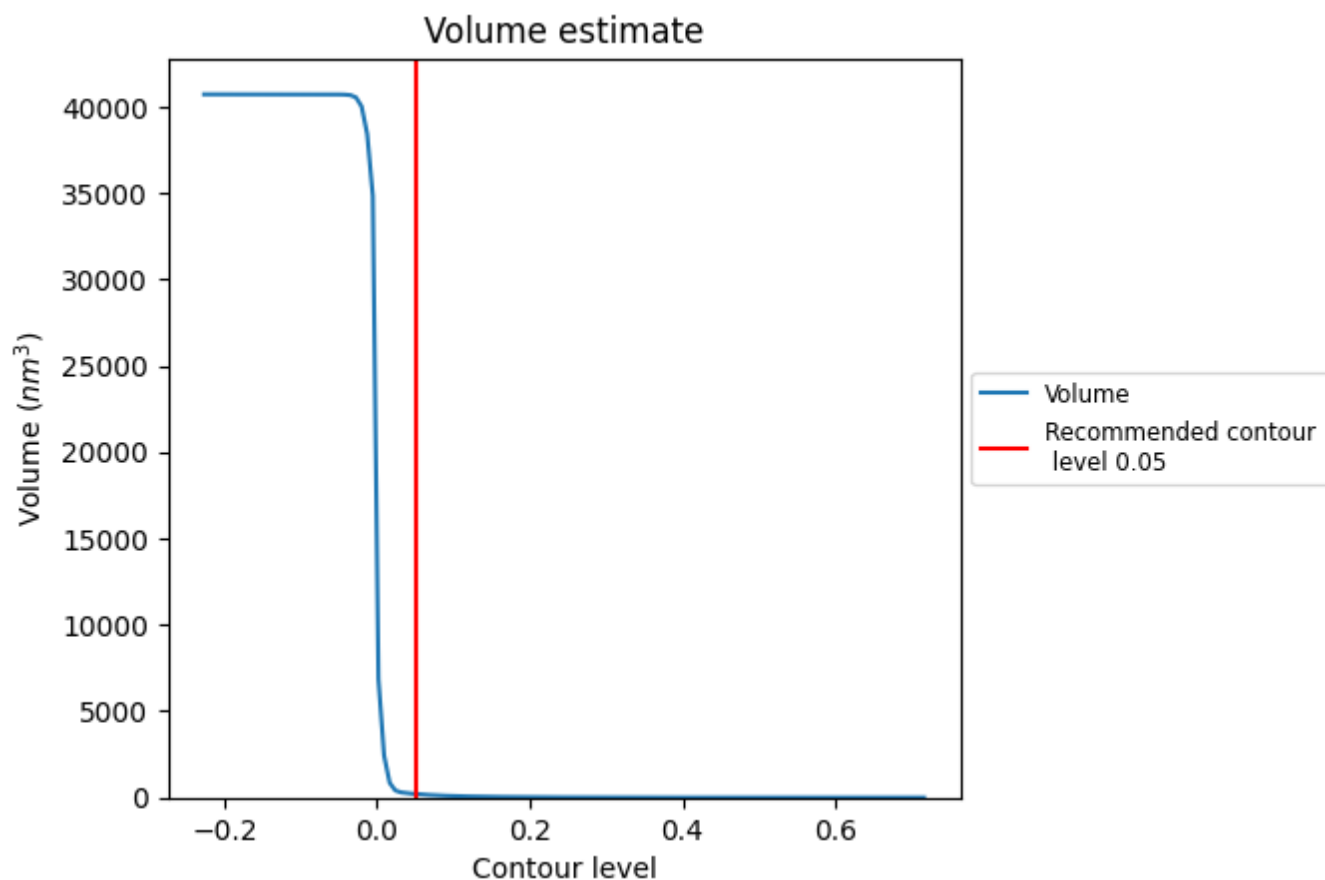
This section contains the results of statistical analysis of the map.

### 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.

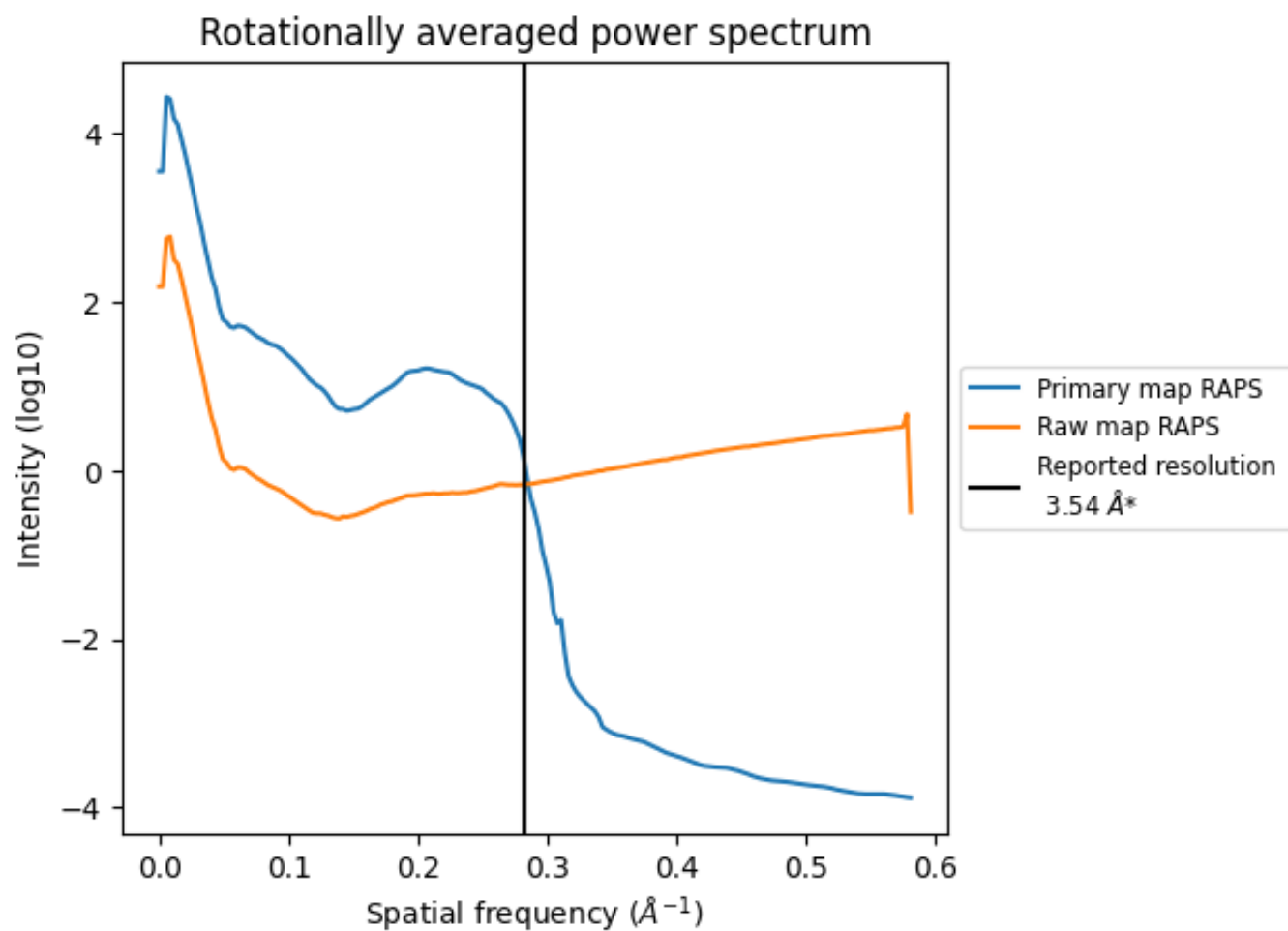
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209  $\text{nm}^3$ ; this corresponds to an approximate mass of 189 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 ⓘ



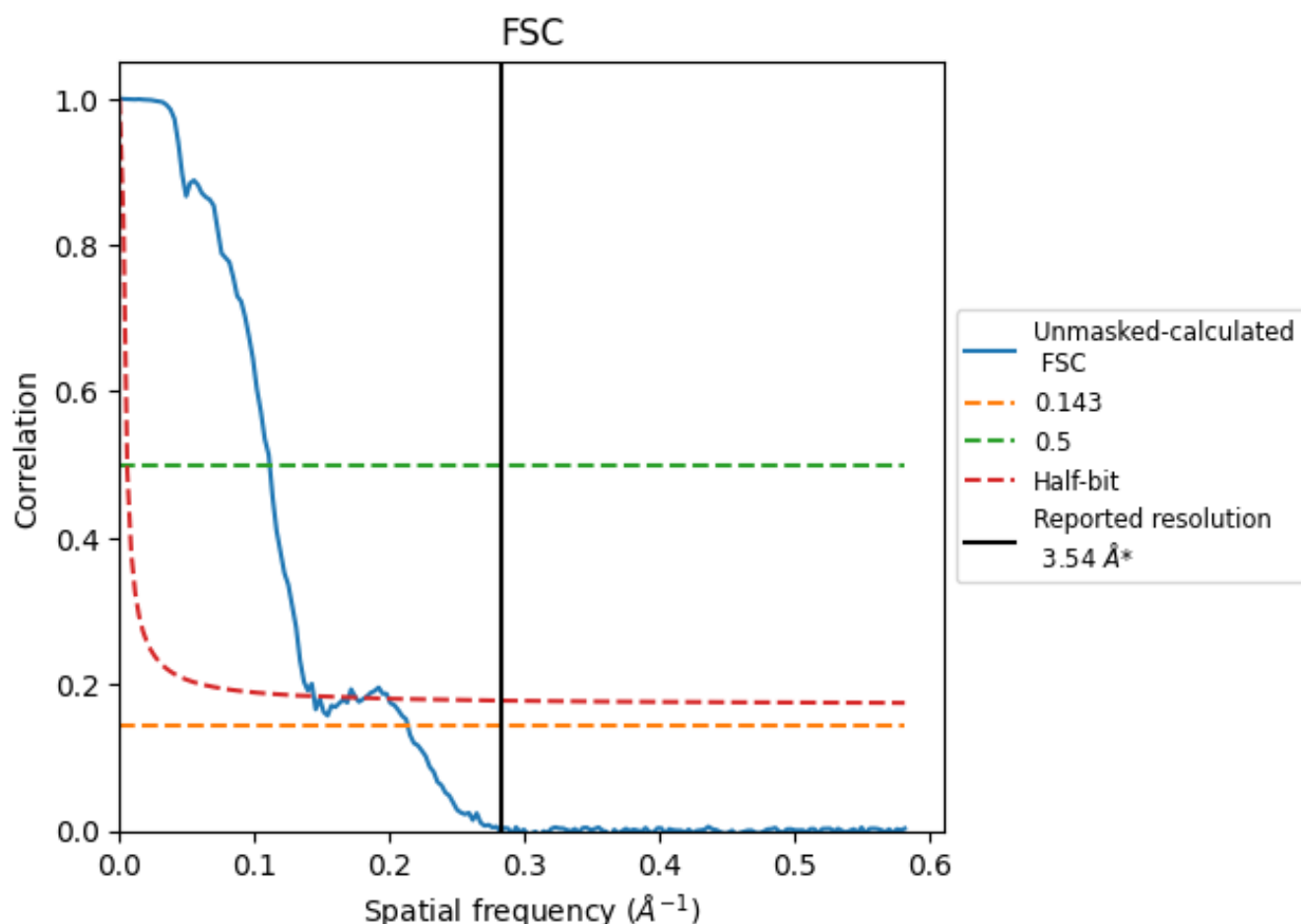
\*Reported resolution corresponds to spatial frequency of 0.282 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

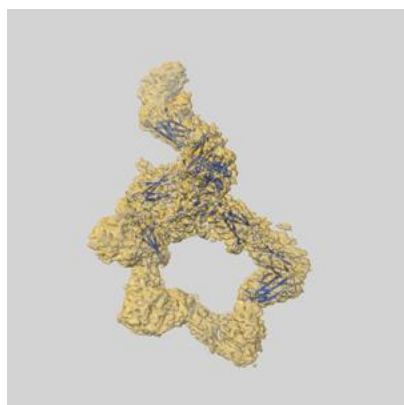
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.68	9.00	6.95

\*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 4.68 differs from the reported value 3.54 by more than 10 %

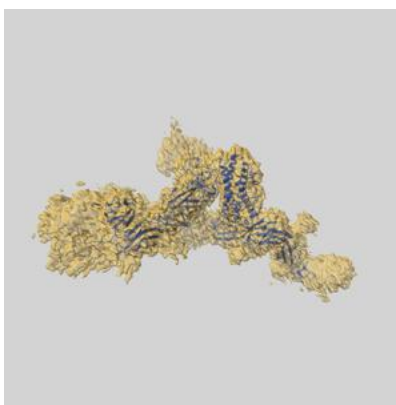
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27221 and PDB model 8D6A. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

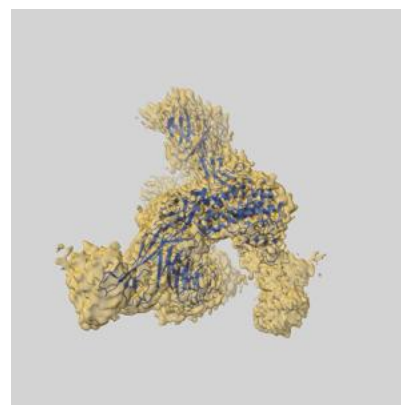
### 9.1 Map-model overlay [i](#)



X



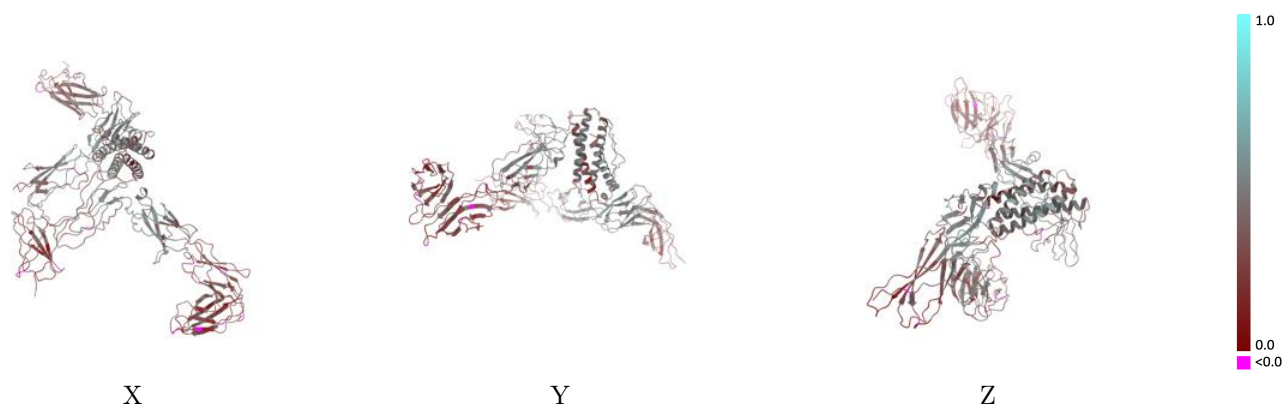
Y



Z

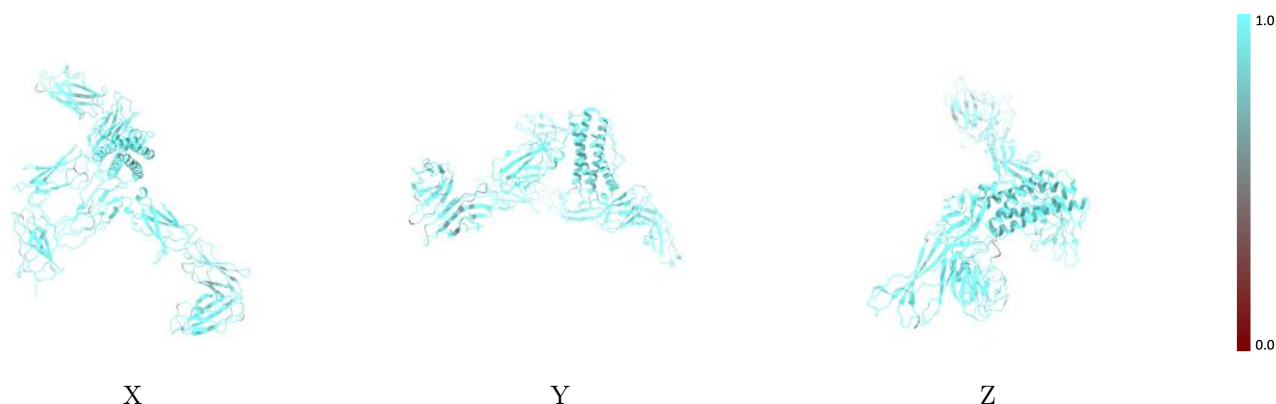
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



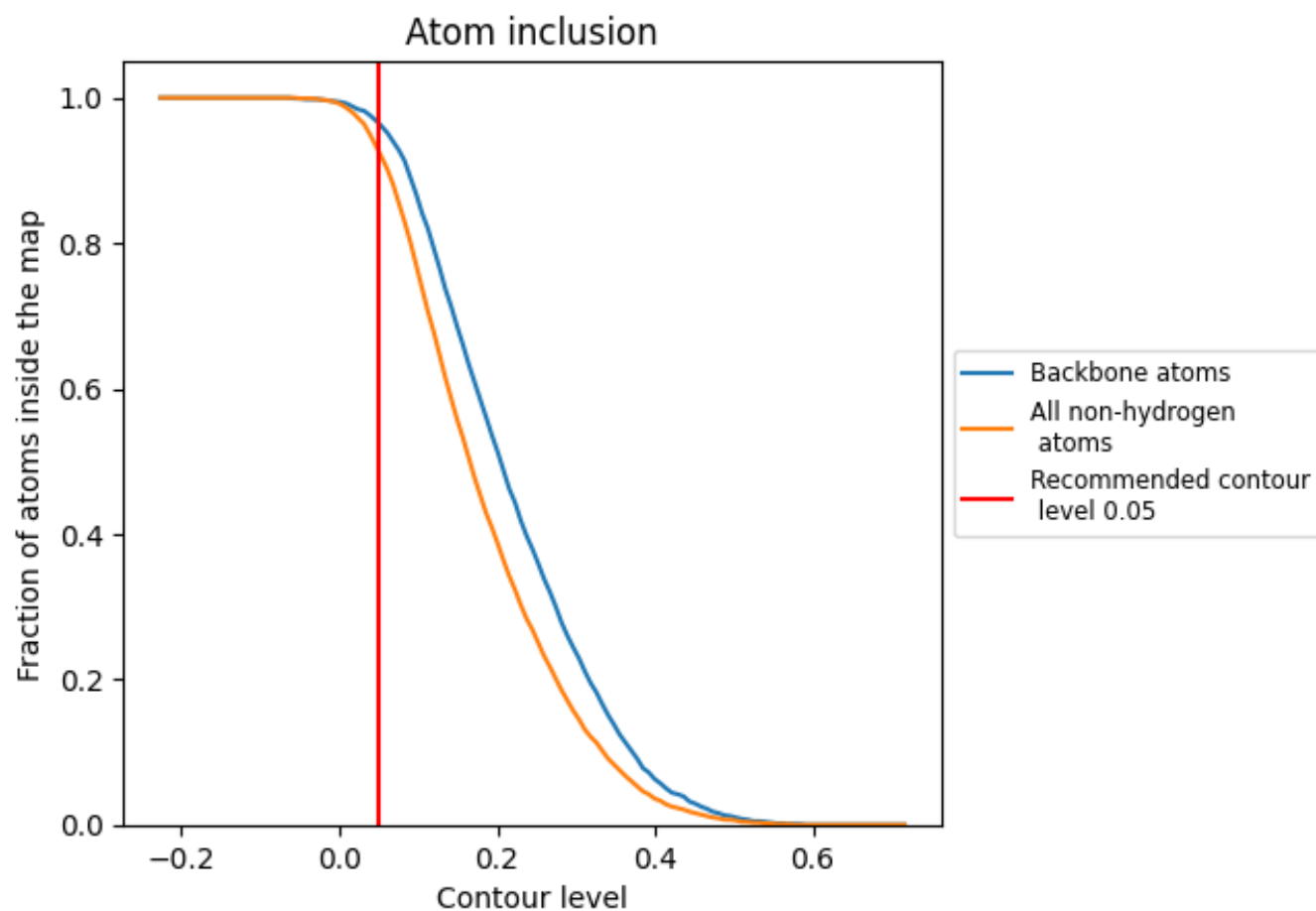
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9260	<div></div> 0.3570
A	<div></div> 0.9120	<div></div> 0.3400
B	<div></div> 0.9340	<div></div> 0.3530
C	<div></div> 0.5000	<div></div> 0.1840
D	<div></div> 0.9530	<div></div> 0.4220
E	<div></div> 0.8930	<div></div> 0.2120
F	<div></div> 0.8210	<div></div> 0.2420
G	<div></div> 1.0000	<div></div> 0.3280
H	<div></div> 0.9290	<div></div> 0.3020

1.0

0.0

<0.0