



Full wwPDB EM Validation Report ⓘ

Oct 31, 2022 – 03:49 pm GMT

PDB ID : 8AE3
EMDB ID : EMD-15380
Title : Cryo-EM structure of full-length human immunoglobulin M - F(ab')₂ conformation 4
Authors : Chen, Q.; Rosenthal, P.; Tolar, P.
Deposited on : 2022-07-12
Resolution : 6.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

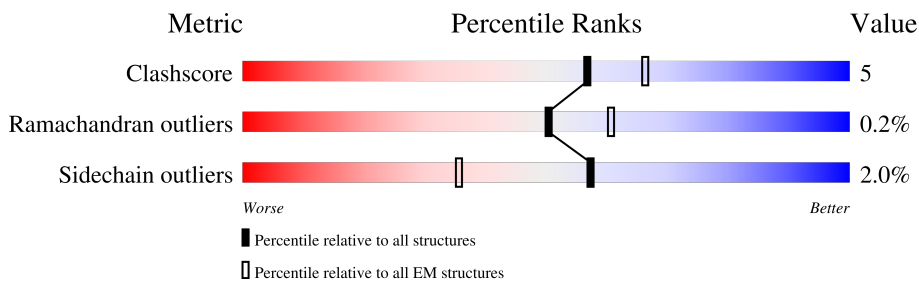
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 Å.

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




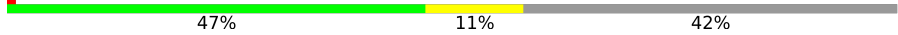





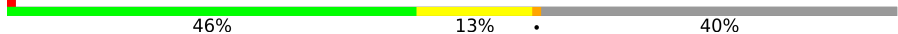



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	117	
1	B	117	
2	L	215	
2	S	215	
3	H	226	
3	Q	226	
4	C	383	
4	D	383	

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Mol	Chain	Length	Quality of chain
4	E	383	 51% 7% 42%
4	F	383	 47% 11% 42%
4	G	383	 51% 7% 42%
4	K	383	 52% 8% 40%
4	N	383	 49% 11% 39%
4	O	383	 50% 9% 41%
4	R	383	 54% 6% 40%
4	T	383	 46% 13% 40%
5	J	136	 64% 14% 22%
6	I	2	 50% 50%
6	M	2	 100% 50% 50%
6	P	2	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 26999 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 IgM C2-domain from mouse.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	106	Total	C	N	O	S	0	0
			826	528	137	157	4		
1	B	97	Total	C	N	O	S	0	0
			765	490	125	146	4		

- Molecule 2 is a protein called IgM Fab, light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	215	Total	C	N	O	S	0	0
			1643	1023	279	336	5		
2	S	215	Total	C	N	O	S	0	0
			1643	1023	279	336	5		

- Molecule 3 is a protein called IgM Fab, heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	225	Total	C	N	O	S	0	0
			1721	1095	283	337	6		
3	Q	225	Total	C	N	O	S	0	0
			1721	1095	283	337	6		

- Molecule 4 is a protein called Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	232	Total	C	N	O	S	0	0
			1798	1132	304	353	9		
4	O	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
4	C	225	Total	C	N	O	S	0	0
			1748	1103	297	340	8		
4	D	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
4	F	221	Total	C	N	O	S	0	0
			1723	1087	292	336	8		
4	G	224	Total	C	N	O	S	0	0
			1742	1100	296	338	8		
4	R	230	Total	C	N	O	S	0	0
			1785	1124	301	351	9		
4	K	230	Total	C	N	O	S	0	0
			1786	1124	302	351	9		
4	T	228	Total	C	N	O	S	0	0
			1773	1116	299	349	9		

- Molecule 5 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

- Molecule 6 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
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	M	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

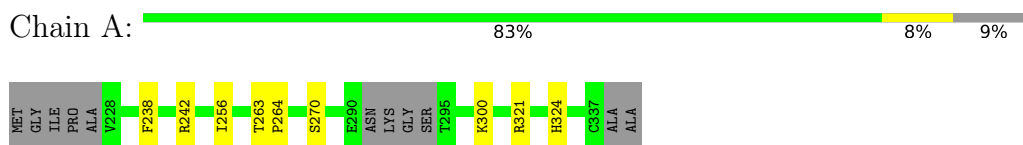


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	N	1	Total 14	C 8	N 1	O 5	0
7	O	1	Total 14	C 8	N 1	O 5	0
7	C	1	Total 14	C 8	N 1	O 5	0
7	D	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	F	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	R	1	Total 14	C 8	N 1	O 5	0
7	K	1	Total 14	C 8	N 1	O 5	0
7	T	1	Total 14	C 8	N 1	O 5	0

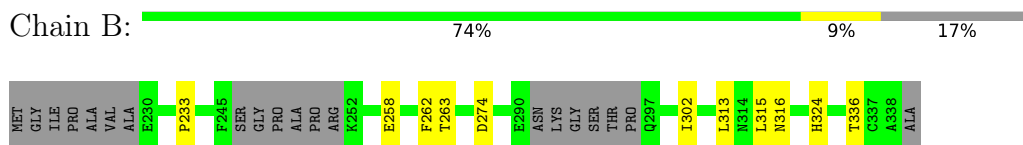
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

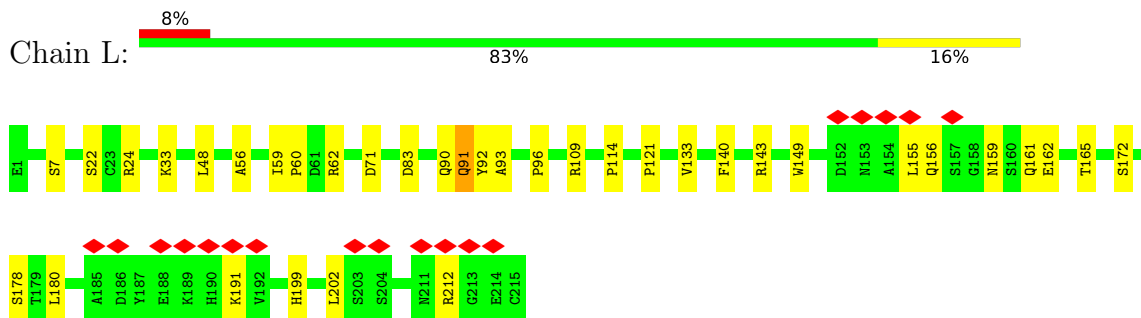
- Molecule 1: IgM C2-domain from mouse



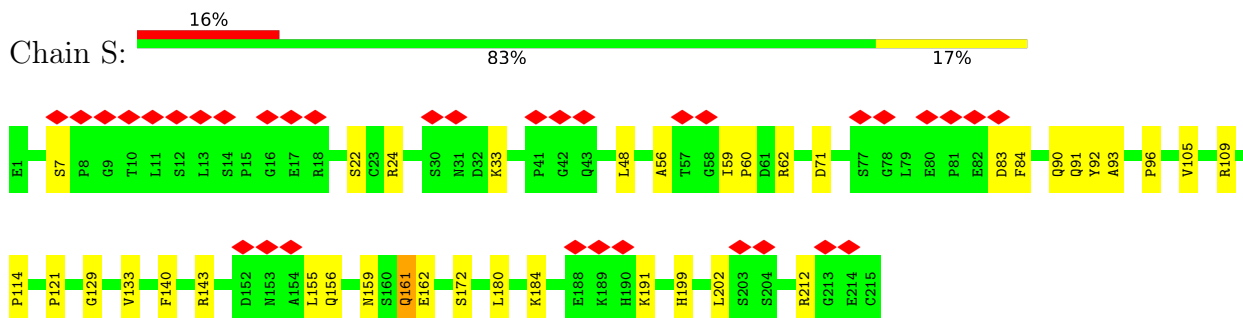
- Molecule 1: IgM C2-domain from mouse



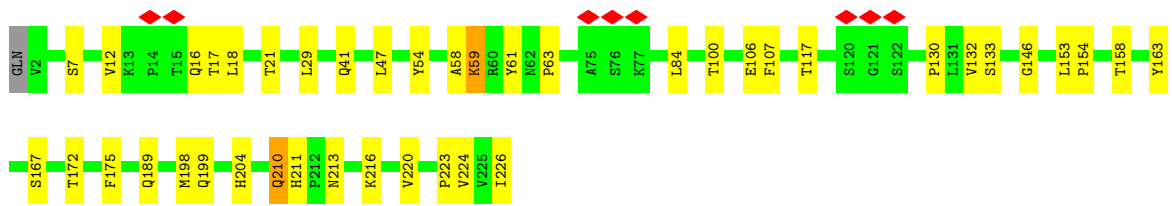
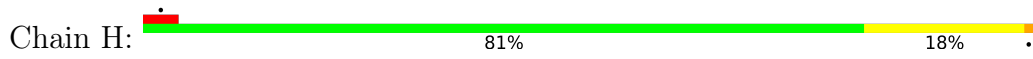
- Molecule 2: IgM Fab, light chain



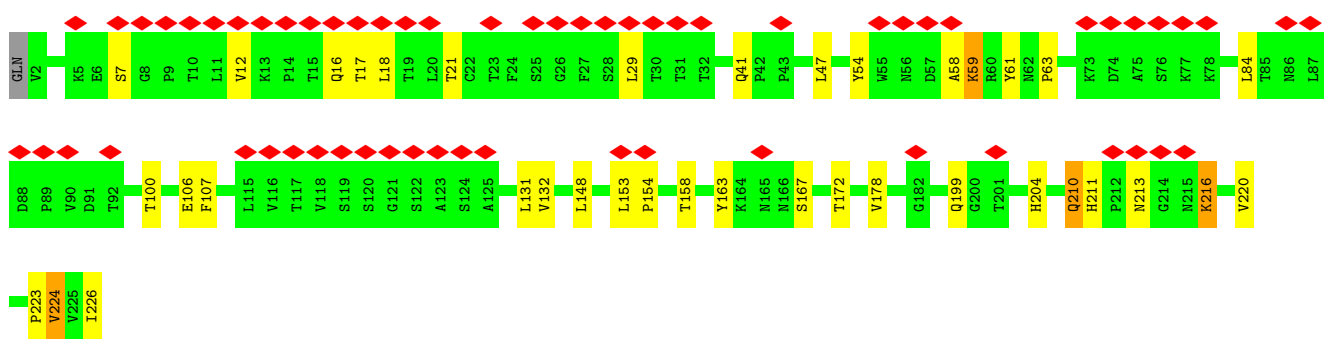
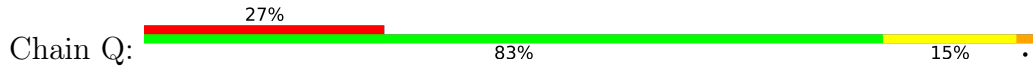
- Molecule 2: IgM Fab, light chain



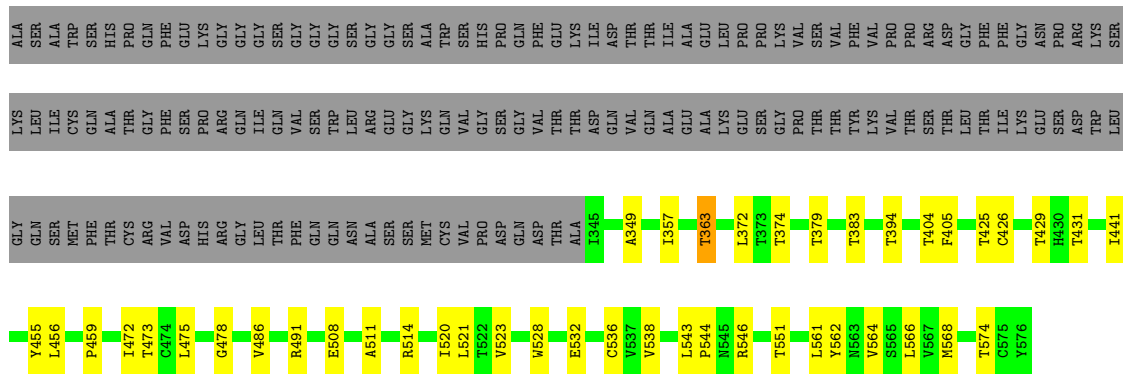
- Molecule 3: IgM Fab, heavy chain



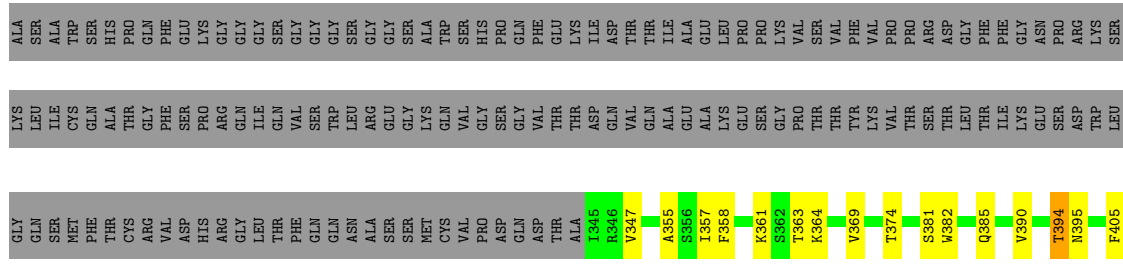
• Molecule 3: IgM Fab, heavy chain



• Molecule 4: Immunoglobulin heavy constant mu

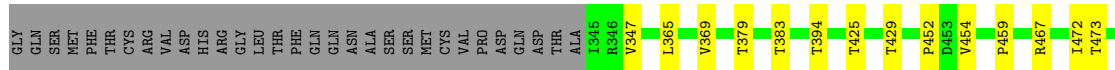
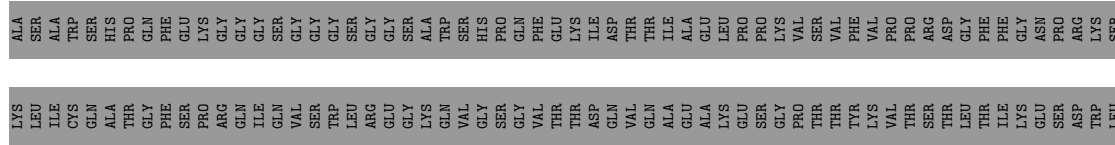


• Molecule 4: Immunoglobulin heavy constant mu

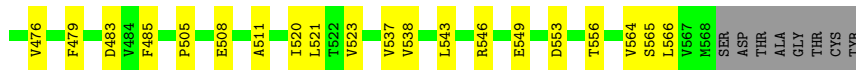
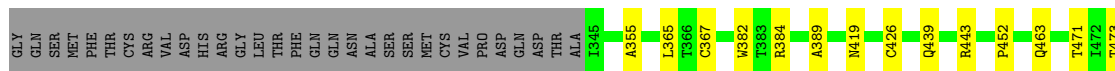
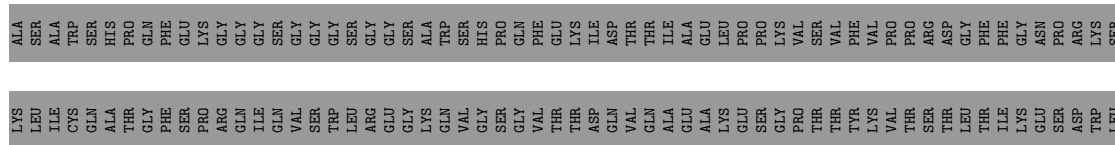




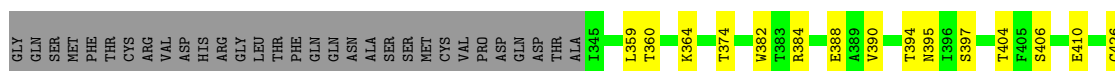
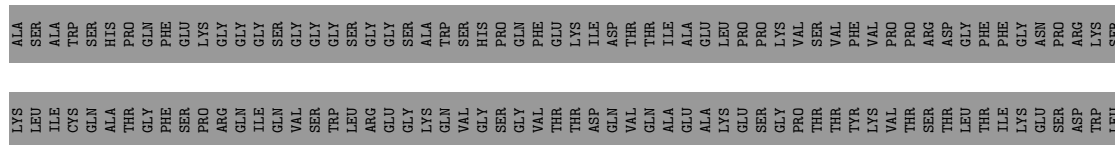
● Molecule 4: Immunoglobulin heavy constant mu



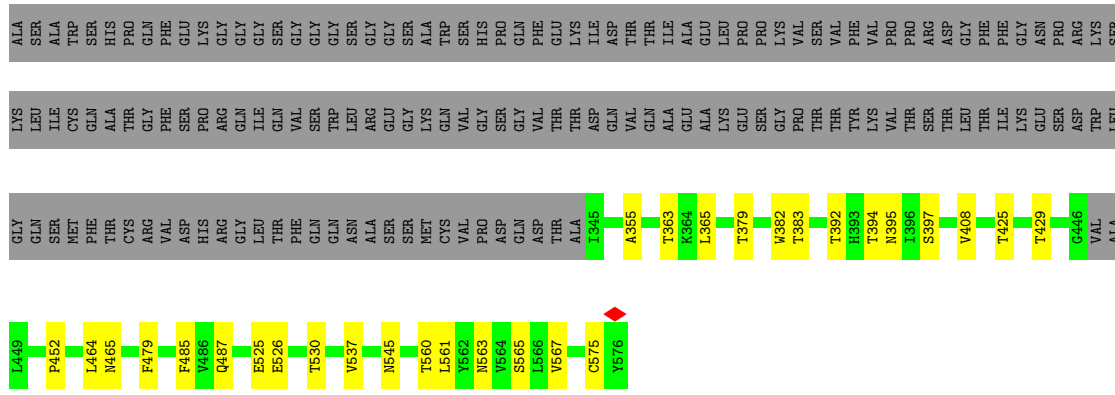
● Molecule 4: Immunoglobulin heavy constant mu



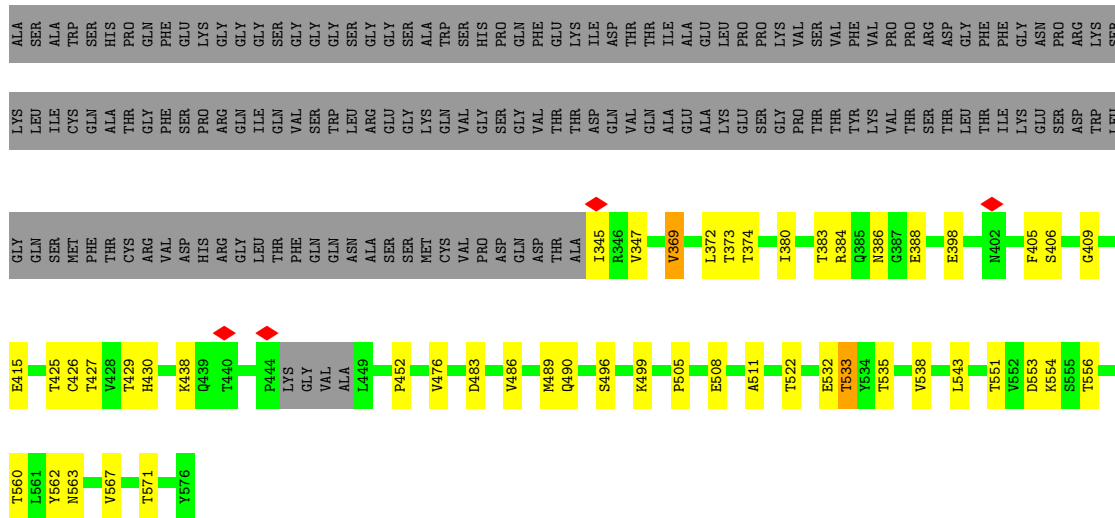
● Molecule 4: Immunoglobulin heavy constant mu



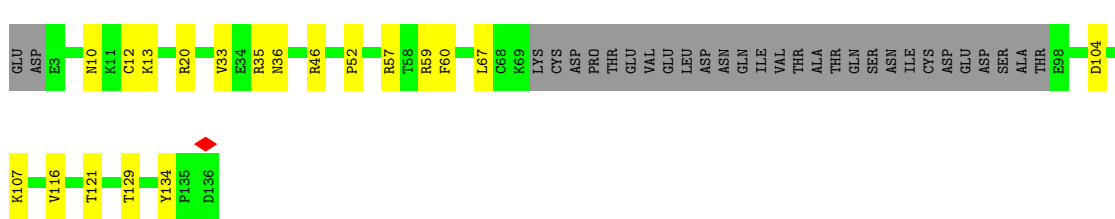
● Molecule 4: Immunoglobulin heavy constant mu



● Molecule 4: Immunoglobulin heavy constant mu



● Molecule 5: Immunoglobulin J chain



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26368	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 ($e^-/\text{\AA}^2$)	34.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	128440	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	7.367	Depositor
Minimum map value	-1.393	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.181	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	654.0, 654.0, 654.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.18, 2.18, 2.18	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	0.24	0/845	0.46	0/1154
1	B	0.23	0/780	0.45	0/1061
2	L	0.24	0/1677	0.47	0/2275
2	S	0.24	0/1677	0.47	0/2275
3	H	0.24	0/1763	0.48	0/2407
3	Q	0.24	0/1763	0.48	0/2407
4	C	0.23	0/1793	0.48	0/2455
4	D	0.23	0/1788	0.48	0/2449
4	E	0.23	0/1788	0.48	0/2449
4	F	0.23	0/1767	0.48	0/2420
4	G	0.23	0/1787	0.47	0/2447
4	K	0.23	0/1831	0.47	0/2506
4	N	0.23	0/1844	0.49	0/2526
4	O	0.23	0/1809	0.48	0/2478
4	R	0.23	0/1830	0.48	0/2507
4	T	0.23	0/1818	0.48	0/2490
5	J	0.23	0/864	0.53	0/1173
All	All	0.23	0/27424	0.48	0/37479

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	A	826	0	829	5	0
1	B	765	0	765	6	0
2	L	1643	0	1595	19	0
2	S	1643	0	1595	19	0
3	H	1721	0	1703	21	0
3	Q	1721	0	1703	20	0
4	C	1748	0	1712	15	0
4	D	1743	0	1707	19	0
4	E	1743	0	1707	14	0
4	F	1723	0	1681	24	0
4	G	1742	0	1707	18	0
4	K	1786	0	1736	19	0
4	N	1798	0	1752	26	0
4	O	1764	0	1723	20	0
4	R	1785	0	1734	15	0
4	T	1773	0	1721	28	0
5	J	851	0	842	14	0
6	I	28	0	25	0	0
6	M	28	0	25	0	0
6	P	28	0	25	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
7	E	14	0	13	0	0
7	F	14	0	13	1	0
7	G	14	0	13	0	0
7	K	14	0	13	1	0
7	N	14	0	13	0	0
7	O	14	0	13	1	0
7	R	14	0	13	0	0
7	T	14	0	13	1	0
All	All	26999	0	26417	270	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 5.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:563:ASN:HB3	4:T:563:ASN:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:114:PRO:HB3	2:S:140:PHE:HB3	1.71	0.72
4:G:563:ASN:HB3	4:R:563:ASN:HB3	1.72	0.72
2:L:114:PRO:HB3	2:L:140:PHE:HB3	1.70	0.72
4:F:416:ASP:HB3	4:G:414:CYS:HB3	1.75	0.69
4:F:558:LYS:HG2	4:F:560:THR:H	1.57	0.69
4:E:452:PRO:HB3	4:E:479:PHE:HB3	1.77	0.66
4:G:384:ARG:HD2	4:G:388:GLU:HB3	1.76	0.66
4:E:382:TRP:HB2	4:E:390:VAL:HG21	1.78	0.66
4:O:385:GLN:HE21	4:O:423:ARG:H	1.44	0.66
4:N:568:MET:HB2	4:O:568:MET:HG2	1.79	0.65
1:B:258:GLU:HG2	1:B:302:ILE:HG22	1.78	0.64
4:T:563:ASN:OD1	5:J:36:ASN:ND2	2.30	0.64
4:G:364:LYS:HD2	4:G:410:GLU:HB3	1.77	0.63
4:F:374:THR:HA	4:F:405:PHE:HB2	1.81	0.62
4:T:559:PRO:HG3	5:J:35:ARG:HE	1.64	0.62
4:D:452:PRO:HB3	4:D:479:PHE:HB3	1.82	0.61
4:D:473:THR:HG22	4:D:520:ILE:HG22	1.82	0.61
3:H:12:VAL:HG11	3:H:18:LEU:HD23	1.83	0.60
4:G:473:THR:HB	4:G:520:ILE:HG22	1.83	0.60
4:F:384:ARG:HE	4:F:390:VAL:HG12	1.66	0.60
4:F:527:GLU:HB3	4:F:532:GLU:HG3	1.83	0.59
4:N:459:PRO:HD3	4:N:472:ILE:HG12	1.83	0.58
3:Q:12:VAL:HG11	3:Q:18:LEU:HD23	1.84	0.58
4:T:476:VAL:HG11	4:T:538:VAL:HG21	1.84	0.58
2:L:156:GLN:HB3	2:L:159:ASN:HD21	1.68	0.58
4:K:565:SER:HB2	7:K:601:NAG:H81	1.84	0.58
4:F:452:PRO:HD2	4:F:543:LEU:HD21	1.86	0.58
2:L:149:TRP:HE1	2:L:178:SER:HG	1.51	0.57
4:F:382:TRP:HB2	4:F:390:VAL:HG21	1.85	0.57
4:N:478:GLY:HA2	4:N:514:ARG:HB3	1.85	0.57
4:E:459:PRO:HD3	4:E:472:ILE:HG12	1.86	0.57
4:T:373:THR:OG1	4:T:430:HIS:NE2	2.37	0.57
4:C:454:VAL:O	4:C:550:ARG:NH1	2.34	0.57
4:N:473:THR:HG22	4:N:520:ILE:HG22	1.85	0.57
4:D:355:ALA:HA	4:D:485:PHE:HB2	1.87	0.57
4:N:551:THR:OG1	5:J:46:ARG:NH2	2.37	0.57
4:F:347:VAL:HB	4:F:439:GLN:HG3	1.88	0.56
4:T:483:ASP:H	4:T:505:PRO:HG2	1.70	0.56
4:T:559:PRO:HA	5:J:33:VAL:HB	1.87	0.56
4:C:503:SER:HB3	4:C:518:HIS:H	1.70	0.56
1:A:270:SER:HB2	1:A:321:ARG:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:487:GLN:HG3	4:K:537:VAL:HG13	1.87	0.56
4:O:489:MET:HA	4:O:494:PRO:HA	1.88	0.56
4:E:473:THR:HB	4:E:520:ILE:HG22	1.87	0.56
4:R:384:ARG:NH1	4:R:388:GLU:OE2	2.39	0.55
4:N:574:THR:OG1	4:K:465:ASN:ND2	2.39	0.55
4:R:473:THR:HG22	4:R:520:ILE:HG22	1.88	0.55
3:H:41:GLN:HB2	3:H:47:LEU:HD23	1.89	0.54
3:H:130:PRO:HA	3:H:220:VAL:HG12	1.89	0.54
4:C:452:PRO:HB3	4:C:479:PHE:HB3	1.89	0.54
3:H:133:SER:HB3	3:H:223:PRO:HG3	1.87	0.54
4:R:568:MET:SD	4:R:568:MET:N	2.80	0.54
1:A:242:ARG:HB3	1:B:336:THR:HG23	1.89	0.54
4:C:467:ARG:NH1	4:C:525:GLU:OE2	2.40	0.54
2:S:156:GLN:HB3	2:S:159:ASN:HD21	1.73	0.54
3:Q:41:GLN:HB2	3:Q:47:LEU:HD23	1.90	0.54
2:L:109:ARG:HD2	2:L:172:SER:HB2	1.91	0.53
4:T:427:THR:HB	4:T:438:LYS:HG2	1.90	0.53
4:O:374:THR:HG22	4:O:405:PHE:HB2	1.90	0.53
4:F:489:MET:HA	4:F:494:PRO:HA	1.90	0.53
4:F:489:MET:SD	4:G:545:ASN:ND2	2.82	0.53
4:G:485:PHE:HB3	4:G:539:ALA:HB3	1.90	0.53
3:H:132:VAL:HG23	3:H:223:PRO:HB3	1.91	0.52
2:S:121:PRO:HD3	2:S:133:VAL:HG22	1.90	0.52
4:F:508:GLU:HB2	4:F:511:ALA:HB3	1.91	0.52
2:S:109:ARG:HD2	2:S:172:SER:HB2	1.91	0.52
4:K:567:VAL:HB	4:T:567:VAL:HG12	1.92	0.52
4:T:380:ILE:HG21	4:T:409:GLY:HA3	1.92	0.52
4:N:491:ARG:HH21	4:N:532:GLU:H	1.56	0.52
3:Q:131:LEU:HD21	3:Q:148:LEU:HD12	1.91	0.52
2:S:48:LEU:HA	2:S:59:ILE:HG12	1.92	0.52
4:C:489:MET:HA	4:C:494:PRO:HA	1.92	0.52
4:F:562:TYR:HA	4:G:562:TYR:HB2	1.92	0.52
4:T:489:MET:O	4:T:535:THR:OG1	2.28	0.51
4:T:486:VAL:HG22	4:T:538:VAL:HG23	1.91	0.51
2:L:48:LEU:HA	2:L:59:ILE:HG12	1.92	0.51
2:L:133:VAL:HB	2:L:180:LEU:HB3	1.91	0.51
3:H:153:LEU:HD22	3:H:154:PRO:HA	1.93	0.51
4:O:357:ILE:HG23	4:O:363:THR:HB	1.92	0.51
4:E:359:LEU:HG	4:E:360:THR:HG23	1.92	0.51
4:O:358:PHE:O	4:O:361:LYS:NZ	2.42	0.51
4:R:487:GLN:HE22	4:K:545:ASN:HD21	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:490:GLN:NE2	4:C:532:GLU:OE1	2.43	0.50
4:E:384:ARG:NH1	4:E:388:GLU:OE1	2.44	0.50
4:G:380:ILE:O	4:G:393:HIS:NE2	2.44	0.50
4:C:478:GLY:O	4:C:514:ARG:NH1	2.44	0.50
4:F:357:ILE:HG12	4:F:363:THR:HB	1.93	0.50
3:H:198:MET:HB3	3:H:226:ILE:HG12	1.92	0.50
2:S:7:SER:O	2:S:22:SER:OG	2.29	0.50
2:S:191:LYS:NZ	2:S:212:ARG:O	2.41	0.50
4:O:476:VAL:HG11	4:O:538:VAL:HG21	1.94	0.50
4:O:347:VAL:HG22	4:O:369:VAL:HG13	1.93	0.50
4:K:397:SER:HB2	4:K:408:VAL:HG12	1.92	0.50
2:L:7:SER:O	2:L:22:SER:OG	2.30	0.50
1:A:264:PRO:HB3	3:Q:226:ILE:HB	1.94	0.50
2:L:33:LYS:HB2	2:L:93:ALA:HB2	1.94	0.50
2:S:24:ARG:NH1	2:S:71:ASP:OD1	2.45	0.49
2:L:24:ARG:NH1	2:L:71:ASP:OD1	2.46	0.49
4:K:452:PRO:HB3	4:K:479:PHE:HB3	1.94	0.49
2:S:96:PRO:HG3	3:Q:63:PRO:HD3	1.95	0.49
2:L:96:PRO:HG3	3:H:63:PRO:HD3	1.95	0.49
4:G:382:TRP:HB2	4:G:390:VAL:HG21	1.95	0.49
4:D:483:ASP:H	4:D:505:PRO:HG2	1.77	0.49
4:D:508:GLU:HB3	4:D:511:ALA:HB3	1.94	0.49
4:O:453:ASP:OD1	4:O:453:ASP:N	2.46	0.48
3:Q:54:TYR:N	3:Q:58:ALA:O	2.45	0.48
4:F:402:ASN:OD1	4:F:404:THR:OG1	2.26	0.48
1:B:233:PRO:HB3	1:B:262:PHE:HB3	1.94	0.48
4:E:364:LYS:HD2	4:E:410:GLU:HG3	1.95	0.48
4:R:427:THR:HG22	4:R:438:LYS:HG2	1.96	0.48
1:A:263:THR:O	1:A:324:HIS:NE2	2.36	0.48
3:Q:153:LEU:HD22	3:Q:154:PRO:HA	1.94	0.48
4:N:472:ILE:HD11	4:N:528:TRP:HE1	1.78	0.48
4:G:470:ALA:N	4:G:523:VAL:O	2.43	0.48
4:F:480:SER:H	4:F:540:HIS:CE1	2.32	0.48
4:K:379:THR:OG1	4:K:429:THR:OG1	2.31	0.48
3:Q:7:SER:OG	3:Q:21:THR:OG1	2.32	0.47
4:E:384:ARG:HD3	4:E:388:GLU:HB2	1.96	0.47
4:T:496:SER:HB3	4:T:499:LYS:HG2	1.96	0.47
4:R:454:VAL:O	4:R:550:ARG:NH1	2.47	0.47
4:N:486:VAL:HG22	4:N:538:VAL:HG12	1.96	0.47
4:N:566:LEU:HA	5:J:60:PHE:HB2	1.96	0.47
2:S:33:LYS:HB2	2:S:93:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:372:LEU:HD23	4:N:372:LEU:H	1.78	0.47
3:H:7:SER:OG	3:H:21:THR:OG1	2.32	0.47
4:O:355:ALA:HA	4:O:485:PHE:HB2	1.97	0.47
4:C:564:VAL:HB	4:D:564:VAL:HG13	1.97	0.47
4:D:463:GLN:HE22	4:D:471:THR:HG23	1.79	0.47
4:K:464:LEU:HD22	4:K:525:GLU:HG3	1.96	0.47
4:C:564:VAL:O	4:D:565:SER:N	2.46	0.47
4:R:454:VAL:HG13	4:R:476:VAL:HG22	1.97	0.47
3:Q:16:GLN:HG2	3:Q:17:THR:H	1.80	0.46
4:F:425:THR:HG21	4:F:438:LYS:HB3	1.98	0.46
3:H:18:LEU:HB3	3:H:84:LEU:HB3	1.97	0.46
4:N:374:THR:HA	4:N:405:PHE:HB2	1.98	0.46
4:D:476:VAL:HG11	4:D:538:VAL:HG21	1.96	0.46
5:J:57:ARG:NH2	5:J:59:ARG:O	2.32	0.46
2:L:60:PRO:HB2	2:L:62:ARG:HG2	1.97	0.46
4:G:369:VAL:HG21	4:G:428:VAL:HG21	1.98	0.46
3:Q:18:LEU:HB3	3:Q:84:LEU:HB3	1.97	0.46
3:Q:163:TYR:HD2	3:Q:167:SER:HB2	1.80	0.46
2:L:62:ARG:NH1	2:L:83:ASP:OD2	2.49	0.46
4:N:564:VAL:HB	4:O:564:VAL:HA	1.98	0.46
4:D:566:LEU:HD13	4:G:562:TYR:CZ	2.50	0.46
4:O:454:VAL:HG21	4:O:538:VAL:HG11	1.98	0.46
4:T:452:PRO:HD2	4:T:543:LEU:HD21	1.98	0.46
4:O:487:GLN:HG3	4:O:537:VAL:HG23	1.98	0.46
4:T:559:PRO:HG2	4:T:562:TYR:CZ	2.50	0.46
1:B:263:THR:O	1:B:324:HIS:NE2	2.44	0.46
2:S:60:PRO:HB2	2:S:62:ARG:HG2	1.98	0.45
4:G:556:THR:O	4:R:461:ARG:NH1	2.38	0.45
4:C:473:THR:HB	4:C:520:ILE:HG22	1.97	0.45
2:S:199:HIS:HB3	2:S:202:LEU:HD13	1.97	0.45
4:F:382:TRP:HE1	4:F:409:GLY:HA3	1.80	0.45
4:T:347:VAL:HG22	4:T:369:VAL:HG12	1.98	0.45
4:F:470:ALA:N	4:F:523:VAL:O	2.46	0.45
5:J:46:ARG:HG3	5:J:52:PRO:HA	1.99	0.45
3:H:59:LYS:HD3	3:H:61:TYR:HE2	1.82	0.45
3:Q:59:LYS:HD3	3:Q:61:TYR:HE2	1.81	0.45
4:O:381:SER:OG	4:O:427:THR:OG1	2.35	0.45
5:J:104:ASP:HB3	5:J:107:LYS:HB3	1.98	0.45
4:N:455:TYR:HB2	4:N:475:LEU:HB3	1.99	0.45
4:E:397:SER:OG	4:E:406:SER:O	2.35	0.45
3:H:146:GLY:HA2	3:H:189:GLN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:163:TYR:HD2	3:H:167:SER:HB2	1.81	0.45
4:G:452:PRO:HB3	4:G:479:PHE:HB3	1.99	0.45
4:E:452:PRO:HD2	4:E:543:LEU:HD21	1.99	0.44
4:F:537:VAL:HG11	4:G:545:ASN:ND2	2.32	0.44
4:T:490:GLN:HE21	4:T:532:GLU:HG2	1.82	0.44
2:S:56:ALA:HB3	2:S:59:ILE:HD13	1.99	0.44
2:L:56:ALA:HB3	2:L:59:ILE:HD13	1.99	0.44
4:N:561:LEU:HD11	7:O:601:NAG:H81	2.00	0.44
4:G:508:GLU:HB3	4:G:511:ALA:HB3	1.99	0.44
2:L:199:HIS:HB3	2:L:202:LEU:HD13	1.99	0.44
2:S:62:ARG:NH1	2:S:83:ASP:OD2	2.48	0.44
4:O:382:TRP:HB2	4:O:390:VAL:HG11	1.99	0.44
4:D:543:LEU:HB2	4:D:546:ARG:HA	1.98	0.44
1:A:238:PHE:HB2	1:A:256:ILE:HB	1.99	0.44
4:D:365:LEU:H	4:D:365:LEU:HD23	1.83	0.44
3:H:16:GLN:HG2	3:H:17:THR:H	1.81	0.44
4:N:372:LEU:HG	4:N:405:PHE:HB3	1.99	0.44
4:T:553:ASP:OD1	4:T:554:LYS:N	2.44	0.44
4:C:383:THR:OG1	4:C:425:THR:OG1	2.35	0.44
4:C:379:THR:HB	4:C:429:THR:HB	1.98	0.44
4:F:476:VAL:HG11	4:F:538:VAL:HG21	2.00	0.44
4:F:543:LEU:HB2	4:F:546:ARG:HA	2.00	0.44
4:D:426:CYS:HB3	4:D:439:GLN:HB3	2.00	0.43
4:F:532:GLU:HB3	4:F:534:TYR:CZ	2.53	0.43
5:J:13:LYS:HD2	5:J:67:LEU:HD23	1.99	0.43
2:L:121:PRO:HD3	2:L:133:VAL:HG22	2.00	0.43
4:O:364:LYS:HD2	4:O:410:GLU:HB3	1.99	0.43
4:F:483:ASP:H	4:F:505:PRO:HG2	1.82	0.43
4:R:487:GLN:HG3	4:R:537:VAL:HG13	2.00	0.43
4:K:383:THR:HG1	4:K:425:THR:HG1	1.66	0.43
4:K:560:THR:HG22	4:T:560:THR:HA	2.01	0.43
5:J:10:ASN:HD21	5:J:12:CYS:HB3	1.83	0.43
4:N:357:ILE:HG23	4:N:363:THR:HB	2.01	0.43
4:N:456:LEU:HD21	4:N:536:CYS:HB2	2.01	0.43
4:T:414:CYS:SG	4:T:415:GLU:N	2.91	0.43
2:S:133:VAL:HB	2:S:180:LEU:HB3	1.99	0.43
5:J:57:ARG:HD2	5:J:57:ARG:HA	1.92	0.43
4:D:537:VAL:HG12	4:D:549:GLU:HG2	2.01	0.43
4:E:487:GLN:HB3	4:E:537:VAL:HG23	2.01	0.43
2:S:92:TYR:CG	3:Q:106:GLU:HG3	2.54	0.43
2:S:161:GLN:HE21	3:Q:178:VAL:HG11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:116:VAL:HG12	5:J:121:THR:HA	2.01	0.43
4:K:526:GLU:O	4:K:530:THR:OG1	2.25	0.42
2:L:92:TYR:CG	3:H:106:GLU:HG3	2.54	0.42
4:N:379:THR:O	4:N:429:THR:OG1	2.31	0.42
4:D:553:ASP:OD1	4:D:556:THR:OG1	2.23	0.42
4:K:561:LEU:HD23	4:K:561:LEU:H	1.83	0.42
3:H:117:THR:HG21	3:H:153:LEU:HD21	2.01	0.42
4:R:399:SER:OG	4:R:404:THR:O	2.30	0.42
4:K:394:THR:OG1	4:K:395:ASN:N	2.52	0.42
3:Q:223:PRO:O	3:Q:224:VAL:HG22	2.19	0.42
4:R:365:LEU:HD23	4:R:365:LEU:H	1.84	0.42
3:Q:132:VAL:HG23	3:Q:223:PRO:HG3	2.01	0.42
4:K:355:ALA:HA	4:K:485:PHE:HB2	2.02	0.42
4:K:383:THR:OG1	4:K:425:THR:OG1	2.35	0.42
4:K:563:ASN:N	4:T:562:TYR:O	2.50	0.42
4:G:527:GLU:HG3	4:G:532:GLU:HG2	2.02	0.42
3:Q:158:THR:HB	3:Q:210:GLN:HE21	1.84	0.42
4:C:365:LEU:HD23	4:C:365:LEU:H	1.85	0.42
4:F:563:ASN:OD1	7:F:601:NAG:N2	2.53	0.42
4:T:508:GLU:HB3	4:T:511:ALA:HB3	2.01	0.42
3:H:54:TYR:N	3:H:58:ALA:O	2.45	0.42
3:Q:216:LYS:H	3:Q:216:LYS:HD2	1.85	0.42
4:C:459:PRO:HD3	4:C:472:ILE:HG12	2.01	0.42
4:N:349:ALA:HB1	4:N:441:ILE:HD11	2.02	0.42
4:D:521:LEU:HG	4:D:523:VAL:HG13	2.02	0.42
4:T:345:ILE:HG13	4:T:372:LEU:HA	2.01	0.41
2:S:84:PHE:HA	2:S:105:VAL:HG23	2.02	0.41
4:T:398:GLU:O	4:T:406:SER:OG	2.36	0.41
4:N:543:LEU:HB2	4:N:546:ARG:HA	2.02	0.41
4:D:419:ASN:OD1	4:D:443:ARG:NH1	2.54	0.41
4:T:374:THR:HA	4:T:405:PHE:HB2	2.01	0.41
1:B:274:ASP:OD2	1:B:316:ASN:ND2	2.53	0.41
4:N:383:THR:HG1	4:N:425:THR:HG1	1.67	0.41
4:T:383:THR:O	4:T:425:THR:OG1	2.31	0.41
3:H:158:THR:HB	3:H:210:GLN:HE21	1.84	0.41
7:T:601:NAG:O4	5:J:20:ARG:NH2	2.50	0.41
4:N:521:LEU:HG	4:N:523:VAL:HG13	2.02	0.41
4:D:384:ARG:NH1	4:D:389:ALA:O	2.44	0.41
3:Q:211:HIS:HD2	3:Q:213:ASN:HB2	1.85	0.41
1:B:313:LEU:HD13	4:N:431:THR:HA	2.02	0.41
3:H:211:HIS:HD2	3:H:213:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:367:CYS:HB2	4:D:382:TRP:CZ2	2.55	0.41
4:E:532:GLU:O	4:E:533:THR:OG1	2.32	0.41
4:O:394:THR:HG22	4:O:395:ASN:H	1.86	0.41
4:O:473:THR:HB	4:O:520:ILE:HG22	2.01	0.41
4:E:394:THR:OG1	4:E:395:ASN:N	2.54	0.41
4:R:521:LEU:HG	4:R:523:VAL:HG13	2.03	0.41
2:L:191:LYS:NZ	2:L:212:ARG:O	2.50	0.41
4:N:508:GLU:HB3	4:N:511:ALA:HB3	2.03	0.41
4:T:532:GLU:O	4:T:533:THR:HG22	2.20	0.41
3:Q:100:THR:HG22	3:Q:107:PHE:H	1.86	0.40
4:N:544:PRO:HD3	5:J:134:TYR:CZ	2.56	0.40
4:C:347:VAL:HG13	4:C:369:VAL:HG22	2.03	0.40
4:E:559:PRO:O	4:E:560:THR:HG22	2.21	0.40
2:L:91:GLN:HE21	2:L:91:GLN:HB2	1.66	0.40
4:R:463:GLN:NE2	4:R:471:THR:OG1	2.40	0.40
4:K:365:LEU:HB3	4:K:382:TRP:CH2	2.57	0.40
2:L:165:THR:HG22	3:H:175:PHE:HA	2.03	0.40
3:H:100:THR:HG22	3:H:107:PHE:H	1.87	0.40
4:O:347:VAL:HG13	4:O:369:VAL:HG22	2.03	0.40
4:R:453:ASP:HB3	4:R:455:TYR:HE2	1.87	0.40
4:T:384:ARG:HD2	4:T:388:GLU:HB2	2.03	0.40
2:S:129:GLY:HA2	2:S:184:LYS:HD2	2.04	0.40
4:O:482:ALA:HB1	4:O:505:PRO:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/117 (87%)	101 (99%)	1 (1%)	0	100	100
1	B	91/117 (78%)	90 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	213/215 (99%)	208 (98%)	4 (2%)	1 (0%)	29	69
2	S	213/215 (99%)	208 (98%)	4 (2%)	1 (0%)	29	69
3	H	223/226 (99%)	216 (97%)	5 (2%)	2 (1%)	17	57
3	Q	223/226 (99%)	217 (97%)	4 (2%)	2 (1%)	17	57
4	C	223/383 (58%)	208 (93%)	15 (7%)	0	100	100
4	D	222/383 (58%)	214 (96%)	8 (4%)	0	100	100
4	E	222/383 (58%)	210 (95%)	12 (5%)	0	100	100
4	F	217/383 (57%)	209 (96%)	8 (4%)	0	100	100
4	G	222/383 (58%)	213 (96%)	9 (4%)	0	100	100
4	K	226/383 (59%)	217 (96%)	9 (4%)	0	100	100
4	N	230/383 (60%)	219 (95%)	11 (5%)	0	100	100
4	O	225/383 (59%)	213 (95%)	12 (5%)	0	100	100
4	R	226/383 (59%)	218 (96%)	8 (4%)	0	100	100
4	T	224/383 (58%)	211 (94%)	13 (6%)	0	100	100
5	J	102/136 (75%)	91 (89%)	11 (11%)	0	100	100
All	All	3404/5082 (67%)	3263 (96%)	135 (4%)	6 (0%)	50	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	199	GLN
3	H	224	VAL
3	Q	224	VAL
3	Q	199	GLN
2	L	162	GLU
2	S	162	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	98/104 (94%)	97 (99%)	1 (1%)	76	86
1	B	91/104 (88%)	90 (99%)	1 (1%)	73	84
2	L	186/186 (100%)	181 (97%)	5 (3%)	44	65
2	S	186/186 (100%)	181 (97%)	5 (3%)	44	65
3	H	197/198 (100%)	191 (97%)	6 (3%)	41	63
3	Q	197/198 (100%)	190 (96%)	7 (4%)	35	59
4	C	201/331 (61%)	197 (98%)	4 (2%)	55	74
4	D	200/331 (60%)	200 (100%)	0	100	100
4	E	200/331 (60%)	195 (98%)	5 (2%)	47	68
4	F	198/331 (60%)	194 (98%)	4 (2%)	55	74
4	G	200/331 (60%)	197 (98%)	3 (2%)	65	80
4	K	205/331 (62%)	202 (98%)	3 (2%)	65	80
4	N	206/331 (62%)	201 (98%)	5 (2%)	49	69
4	O	203/331 (61%)	200 (98%)	3 (2%)	65	80
4	R	205/331 (62%)	204 (100%)	1 (0%)	88	93
4	T	204/331 (62%)	195 (96%)	9 (4%)	28	53
5	J	100/128 (78%)	99 (99%)	1 (1%)	76	86
All	All	3077/4414 (70%)	3014 (98%)	63 (2%)	57	74

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	LYS
1	B	315	LEU
2	L	90	GLN
2	L	91	GLN
2	L	143	ARG
2	L	155	LEU
2	L	161	GLN
3	H	29	LEU
3	H	59	LYS
3	H	172	THR
3	H	204	HIS
3	H	210	GLN
3	H	216	LYS
2	S	90	GLN
2	S	91	GLN

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Mol	Chain	Res	Type
2	S	143	ARG
2	S	155	LEU
2	S	161	GLN
3	Q	29	LEU
3	Q	59	LYS
3	Q	172	THR
3	Q	204	HIS
3	Q	210	GLN
3	Q	216	LYS
3	Q	220	VAL
4	N	363	THR
4	N	394	THR
4	N	404	THR
4	N	426	CYS
4	N	562	TYR
4	O	394	THR
4	O	522	THR
4	O	530	THR
4	C	394	THR
4	C	522	THR
4	C	530	THR
4	C	533	THR
4	E	374	THR
4	E	404	THR
4	E	426	CYS
4	E	473	THR
4	E	522	THR
4	F	367	CYS
4	F	388	GLU
4	F	433	LEU
4	F	473	THR
4	G	366	THR
4	G	473	THR
4	G	560	THR
4	R	367	CYS
4	K	363	THR
4	K	392	THR
4	K	575	CYS
4	T	369	VAL
4	T	386	ASN
4	T	426	CYS
4	T	429	THR

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Mol	Chain	Res	Type
4	T	522	THR
4	T	533	THR
4	T	551	THR
4	T	556	THR
4	T	571	THR
5	J	129	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	332	ASN
1	B	297	GLN
2	L	90	GLN
2	L	91	GLN
2	L	101	GLN
2	L	138	ASN
2	L	156	GLN
2	L	159	ASN
2	L	161	GLN
2	L	199	HIS
2	L	200	GLN
3	H	56	ASN
3	H	66	GLN
3	H	112	GLN
3	H	189	GLN
3	H	199	GLN
2	S	90	GLN
2	S	91	GLN
2	S	101	GLN
2	S	156	GLN
2	S	159	ASN
2	S	161	GLN
2	S	199	HIS
2	S	200	GLN
3	Q	56	ASN
3	Q	66	GLN
3	Q	112	GLN
3	Q	199	GLN
3	Q	210	GLN
4	O	385	GLN
4	O	419	ASN

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Mol	Chain	Res	Type
4	O	487	GLN
4	O	510	GLN
4	C	393	HIS
4	C	439	GLN
4	C	493	GLN
4	C	510	GLN
4	C	545	ASN
4	D	385	GLN
4	D	439	GLN
4	D	463	GLN
4	D	487	GLN
4	D	493	GLN
4	E	395	ASN
4	E	545	ASN
4	F	487	GLN
4	G	463	GLN
4	G	545	ASN
4	R	510	GLN
4	K	402	ASN
4	K	430	HIS
4	K	465	ASN
4	K	545	ASN
4	T	386	ASN
4	T	439	GLN
4	T	510	GLN

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](#)

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	I	1	3,6	14,14,15	0.21	0	17,19,21	0.41	0
6	NAG	I	2	6	14,14,15	1.02	2 (14%)	17,19,21	0.86	1 (5%)
6	NAG	M	1	3,6	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	M	2	6	14,14,15	1.01	2 (14%)	17,19,21	0.87	1 (5%)
6	NAG	P	1	6,5	14,14,15	0.25	0	17,19,21	0.41	0
6	NAG	P	2	6	14,14,15	0.27	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	NAG	M	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	M	2	6	-	0/6/23/26	0/1/1/1
6	NAG	P	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	2	NAG	O5-C1	3.09	1.48	1.43
6	I	2	NAG	O5-C1	3.05	1.48	1.43
6	I	2	NAG	C1-C2	2.11	1.55	1.52
6	M	2	NAG	C1-C2	2.05	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	2	NAG	C1-O5-C5	3.32	116.70	112.19
6	I	2	NAG	C1-O5-C5	3.29	116.66	112.19

There are no chirality outliers.

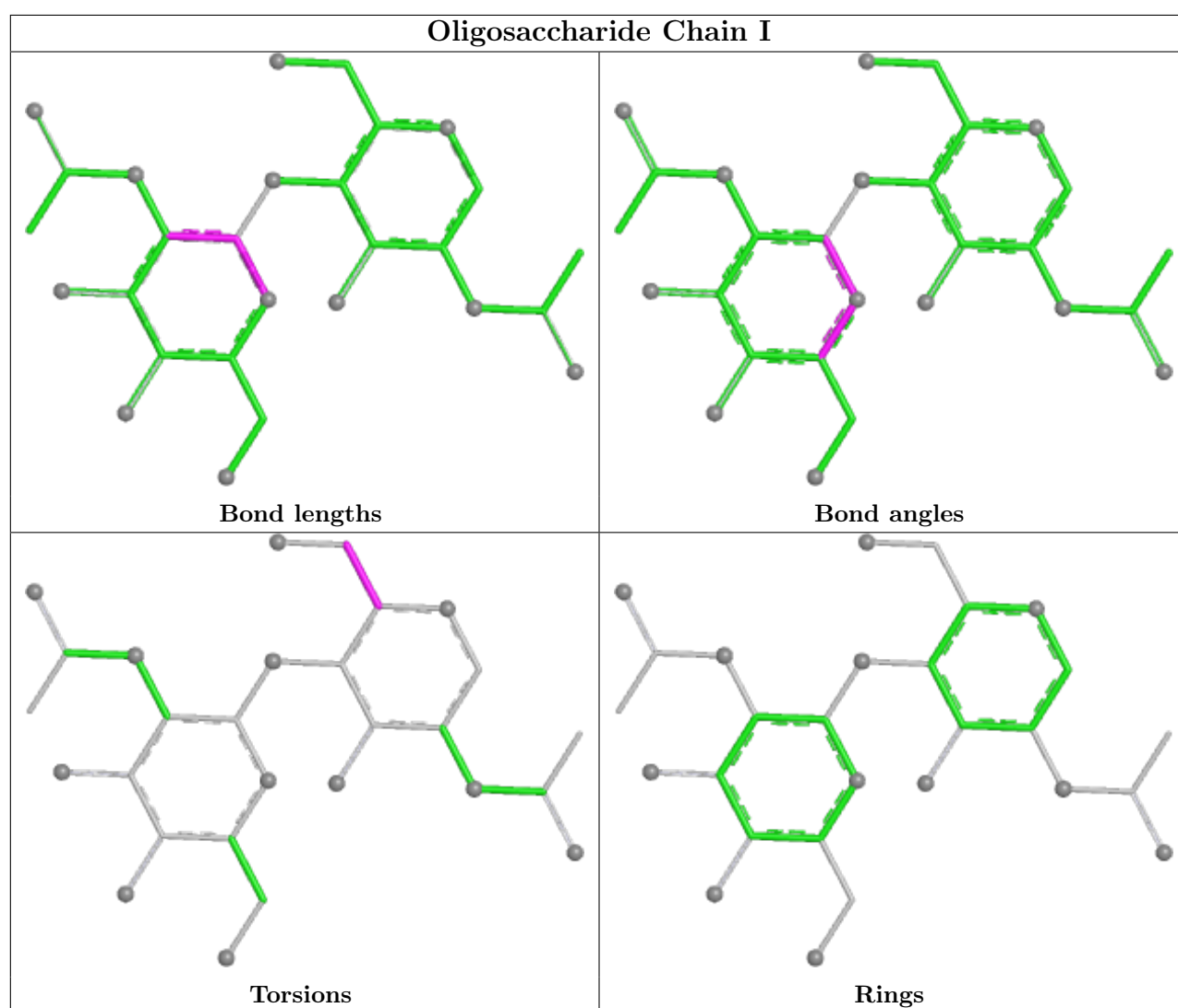
All (6) torsion outliers are listed below:

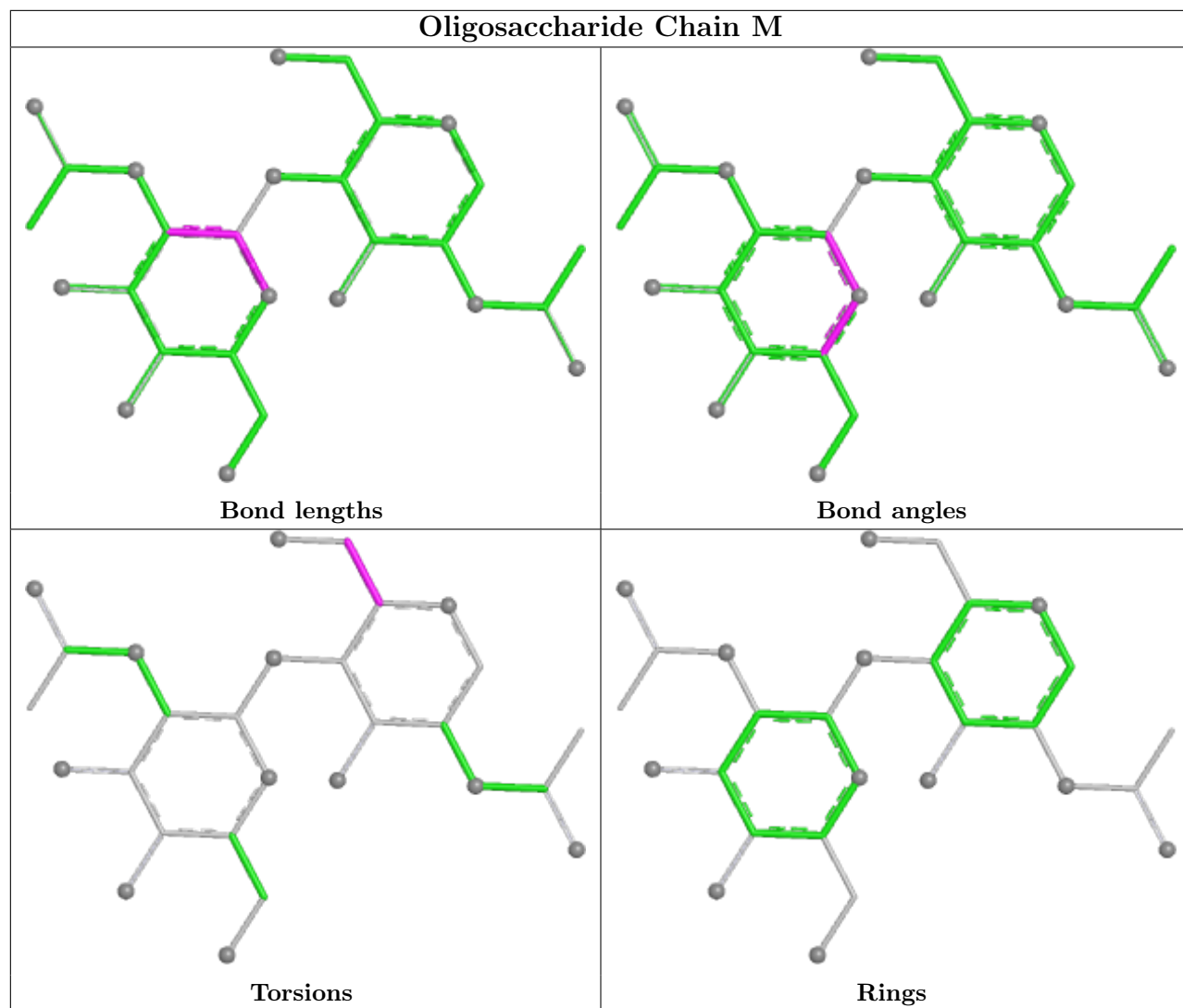
Mol	Chain	Res	Type	Atoms
6	M	1	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6

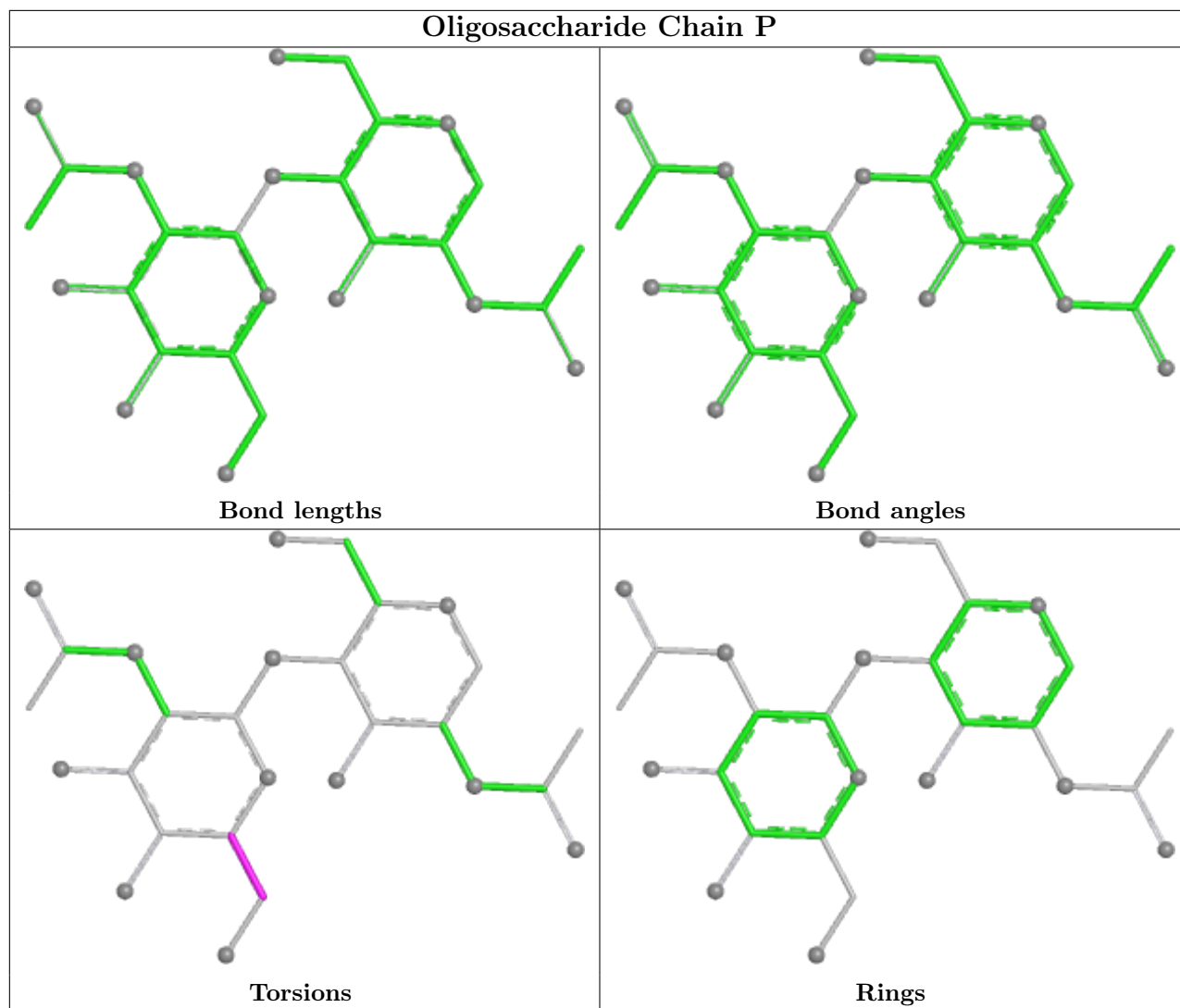
There are no ring outliers.

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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	G	601	4	14,14,15	0.28	0	17,19,21	0.42	0
7	NAG	K	601	4	14,14,15	0.23	0	17,19,21	0.36	0
7	NAG	F	601	4	14,14,15	0.35	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	T	601	4	14,14,15	0.22	0	17,19,21	0.43	0
7	NAG	C	601	4	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	E	601	4	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	D	601	4	14,14,15	0.23	0	17,19,21	0.40	0
7	NAG	O	601	4	14,14,15	0.22	0	17,19,21	0.41	0
7	NAG	R	601	4	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	N	601	4	14,14,15	0.22	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	601	4	-	2/6/23/26	0/1/1/1
7	NAG	K	601	4	-	2/6/23/26	0/1/1/1
7	NAG	F	601	4	-	2/6/23/26	0/1/1/1
7	NAG	T	601	4	-	2/6/23/26	0/1/1/1
7	NAG	C	601	4	-	4/6/23/26	0/1/1/1
7	NAG	E	601	4	-	2/6/23/26	0/1/1/1
7	NAG	D	601	4	-	2/6/23/26	0/1/1/1
7	NAG	O	601	4	-	2/6/23/26	0/1/1/1
7	NAG	R	601	4	-	2/6/23/26	0/1/1/1
7	NAG	N	601	4	-	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 (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	O	601	NAG	O5-C5-C6-O6
7	F	601	NAG	O5-C5-C6-O6
7	G	601	NAG	O5-C5-C6-O6
7	D	601	NAG	C4-C5-C6-O6
7	C	601	NAG	O5-C5-C6-O6
7	R	601	NAG	O5-C5-C6-O6
7	F	601	NAG	C4-C5-C6-O6
7	O	601	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	G	601	NAG	C4-C5-C6-O6
7	R	601	NAG	C4-C5-C6-O6
7	C	601	NAG	C8-C7-N2-C2
7	C	601	NAG	O7-C7-N2-C2
7	K	601	NAG	C8-C7-N2-C2
7	K	601	NAG	O7-C7-N2-C2
7	C	601	NAG	C4-C5-C6-O6
7	E	601	NAG	O5-C5-C6-O6
7	T	601	NAG	O5-C5-C6-O6
7	D	601	NAG	O5-C5-C6-O6
7	T	601	NAG	C4-C5-C6-O6
7	E	601	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	601	NAG	1	0
7	F	601	NAG	1	0
7	T	601	NAG	1	0
7	O	601	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.

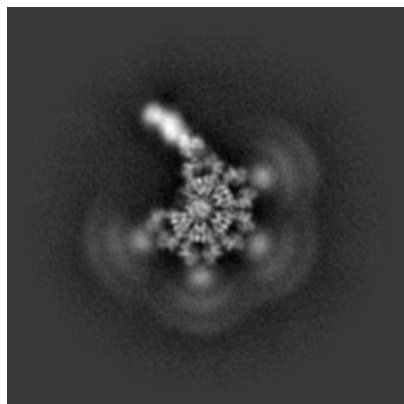
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15380. These allow visual inspection of the internal detail of the map and identification of artifacts.

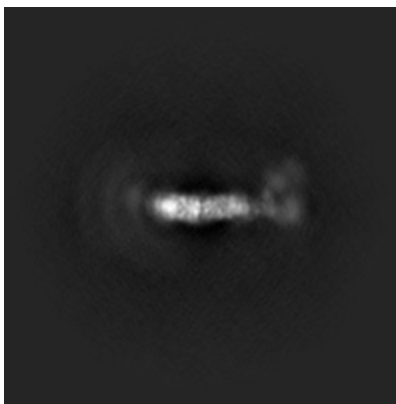
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

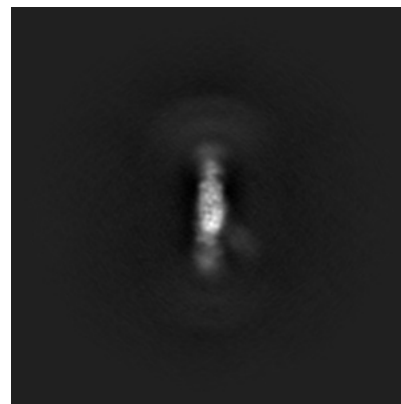
6.1.1 Primary map



X

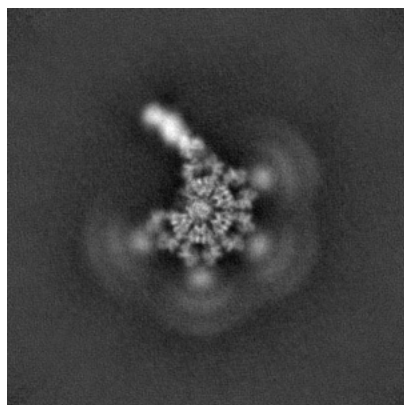


Y

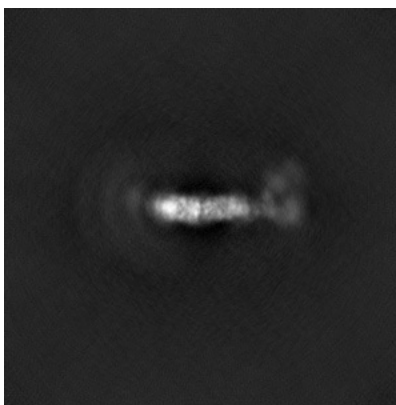


Z

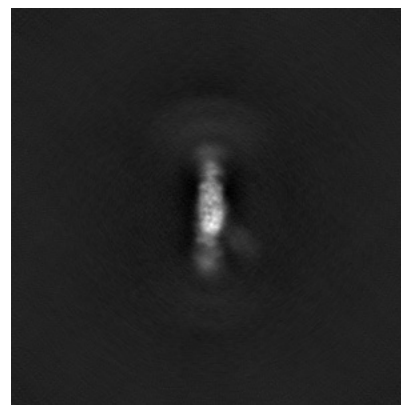
6.1.2 Raw map



X



Y

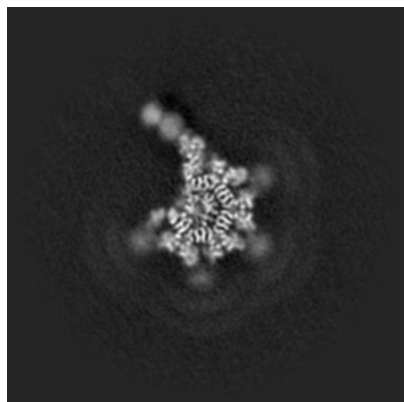


Z

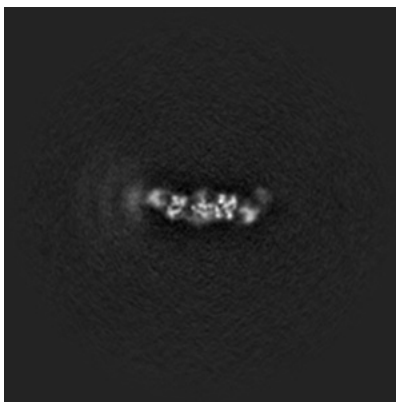
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

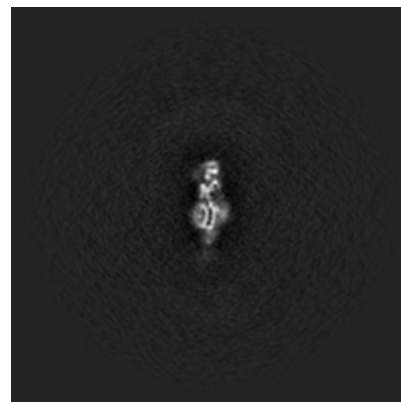
6.2.1 Primary map



X Index: 150

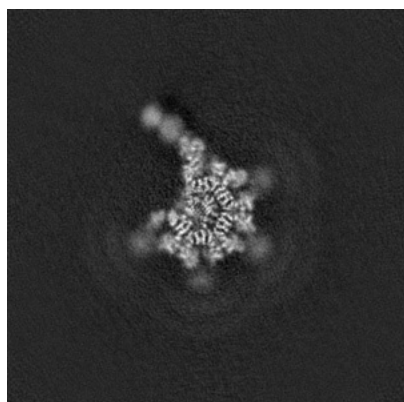


Y Index: 150

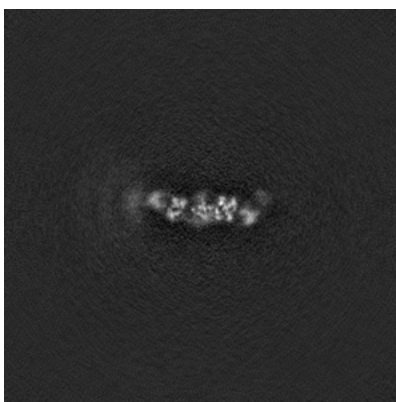


Z Index: 150

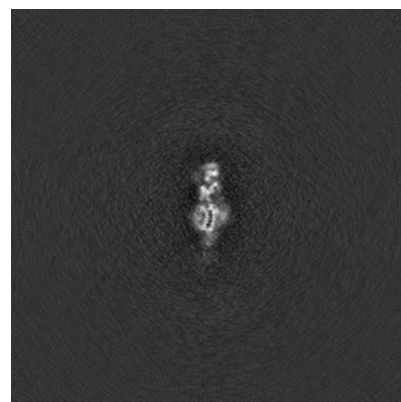
6.2.2 Raw map



X Index: 150



Y Index: 150

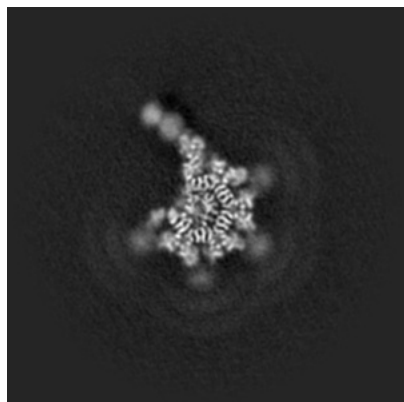


Z Index: 150

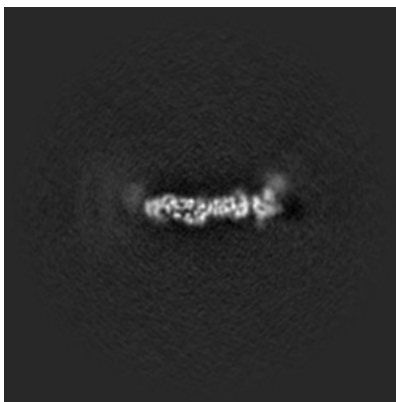
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

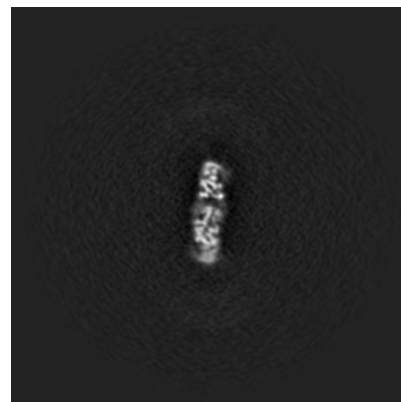
6.3.1 Primary map



X Index: 150

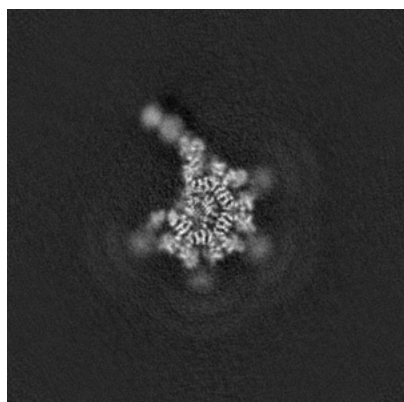


Y Index: 136

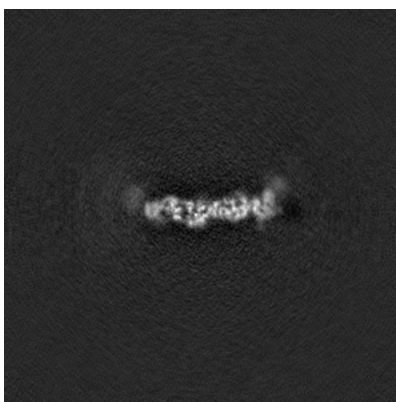


Z Index: 143

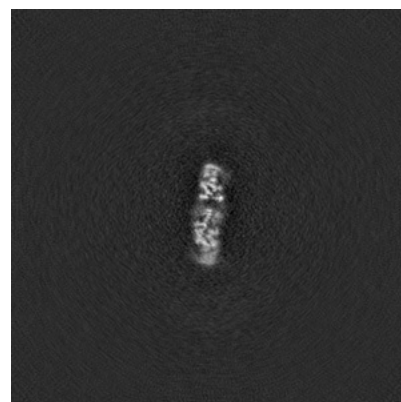
6.3.2 Raw map



X Index: 150



Y Index: 137

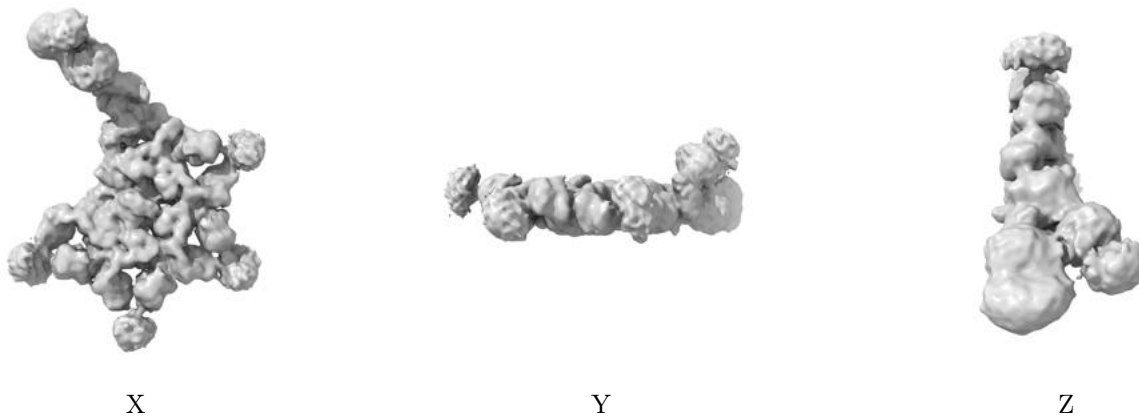


Z Index: 143

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

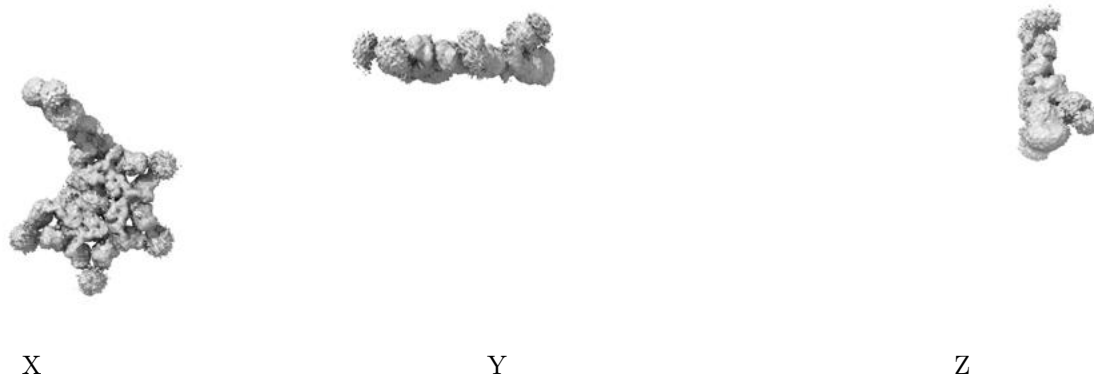
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

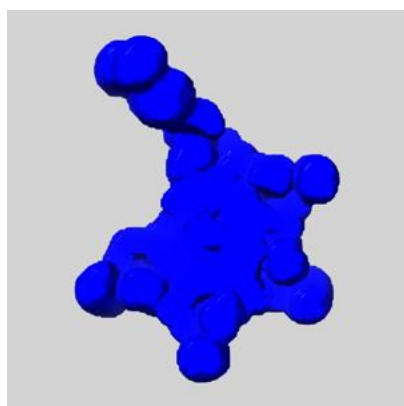
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

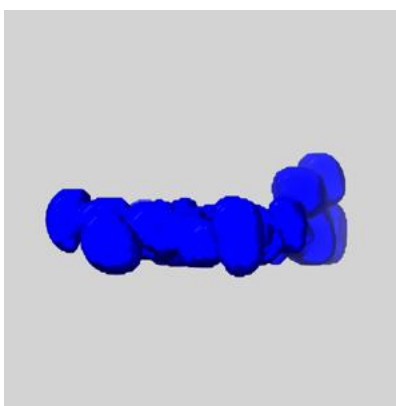
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

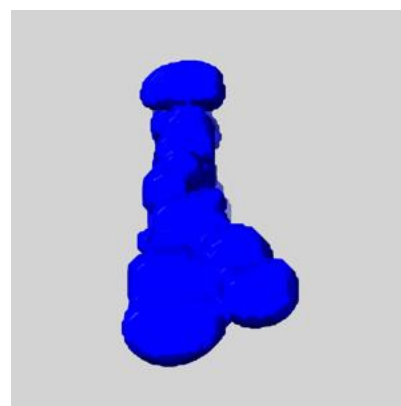
6.5.1 emd_15380_msk_1.map [i](#)



X



Y

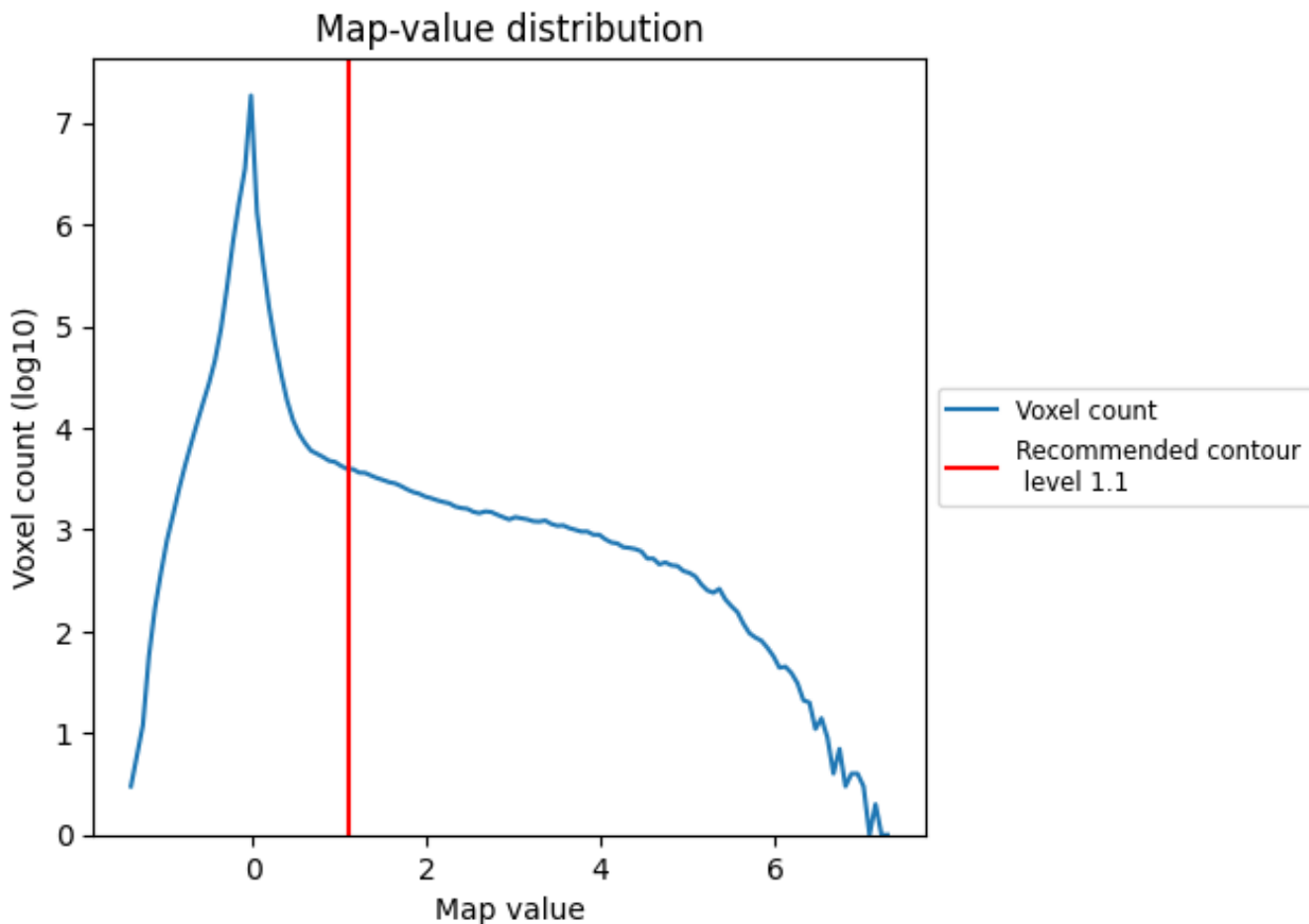


Z

7 Map analysis [i](#)

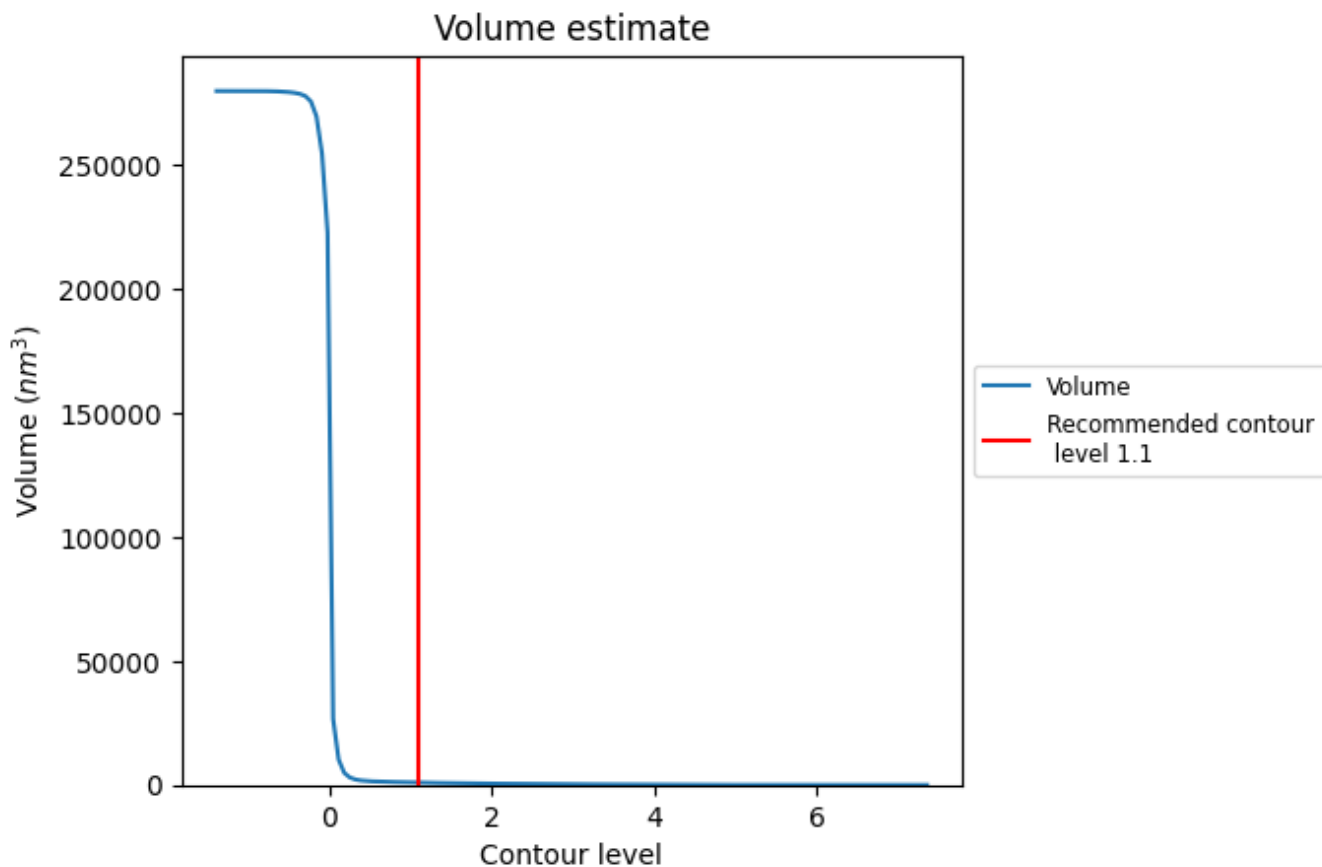
This section contains the results of statistical analysis of the map.

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.

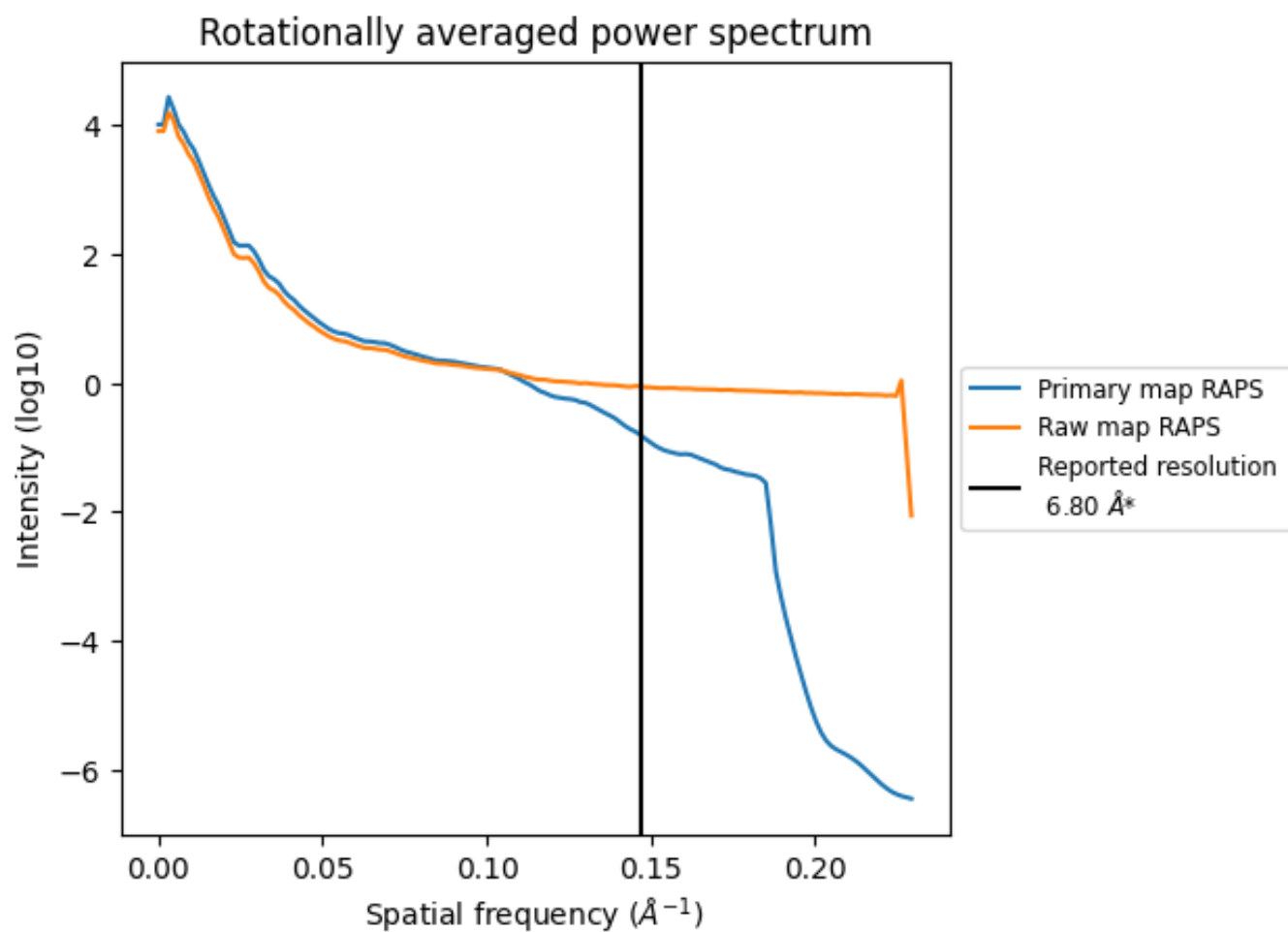
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 956 nm^3 ; this corresponds to an approximate mass of 864 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

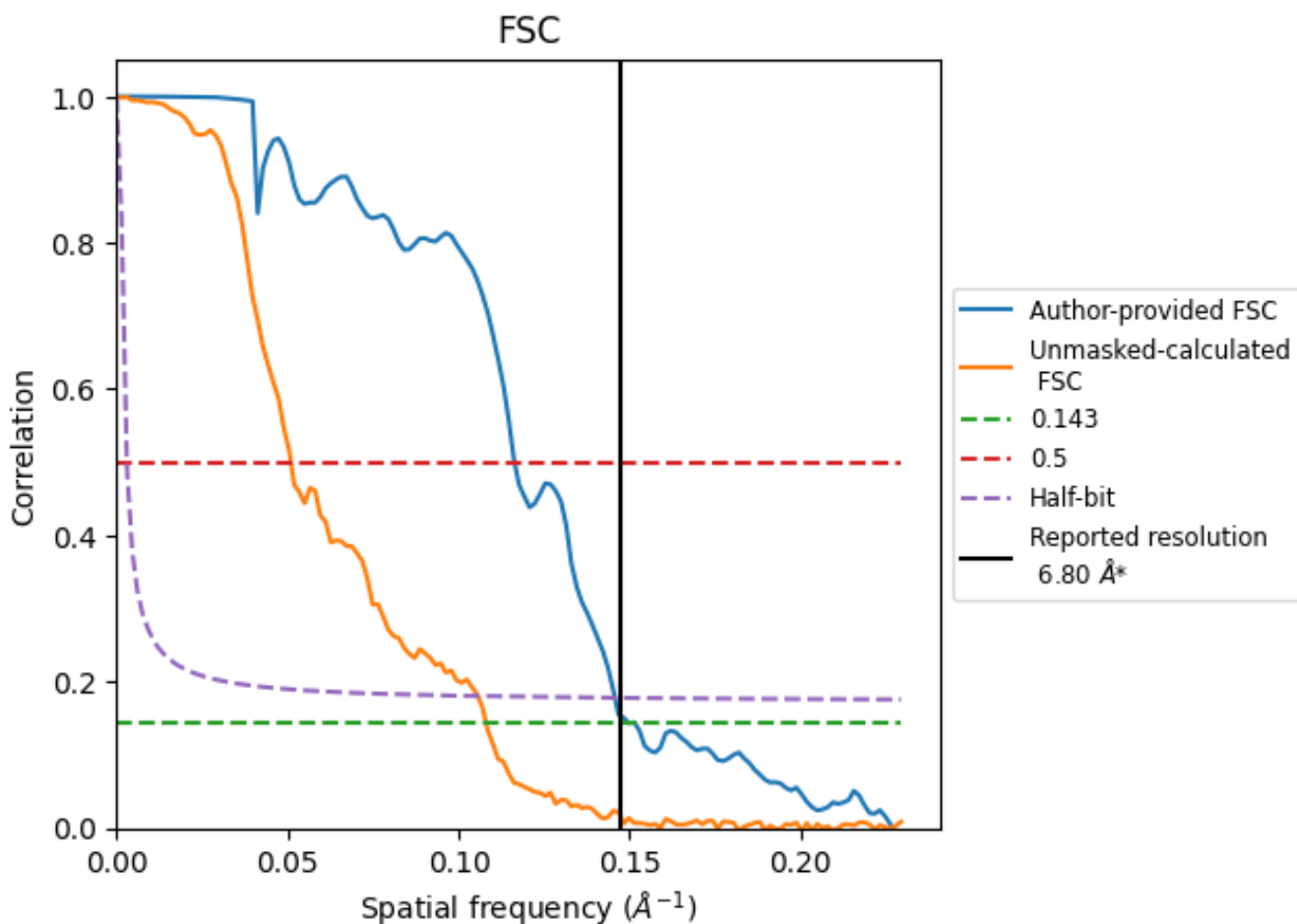


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

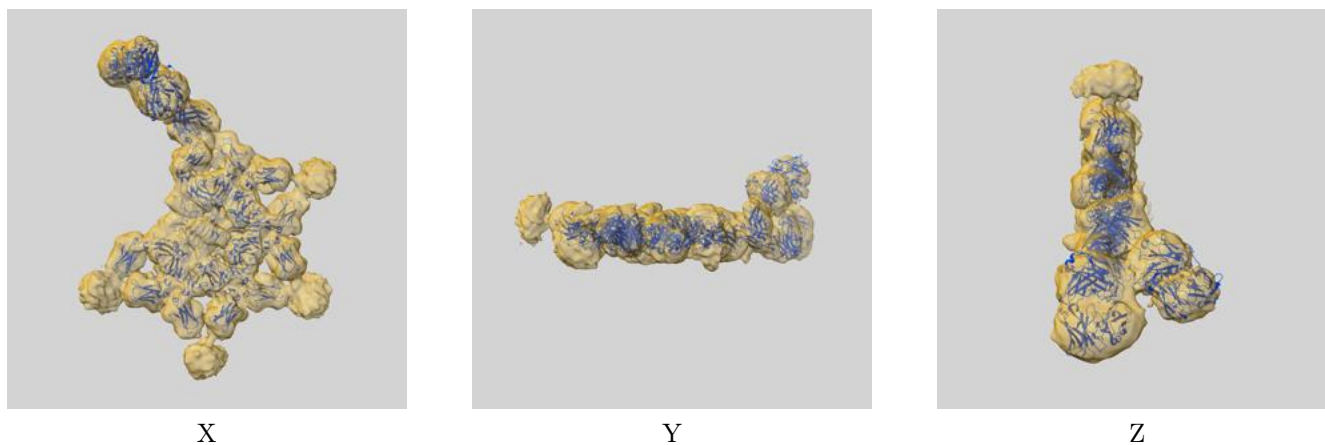
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.68	8.59	6.86
Unmasked-calculated*	9.25	19.61	9.46

*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 9.25 differs from the reported value 6.8 by more than 10 %

9 Map-model fit [i](#)

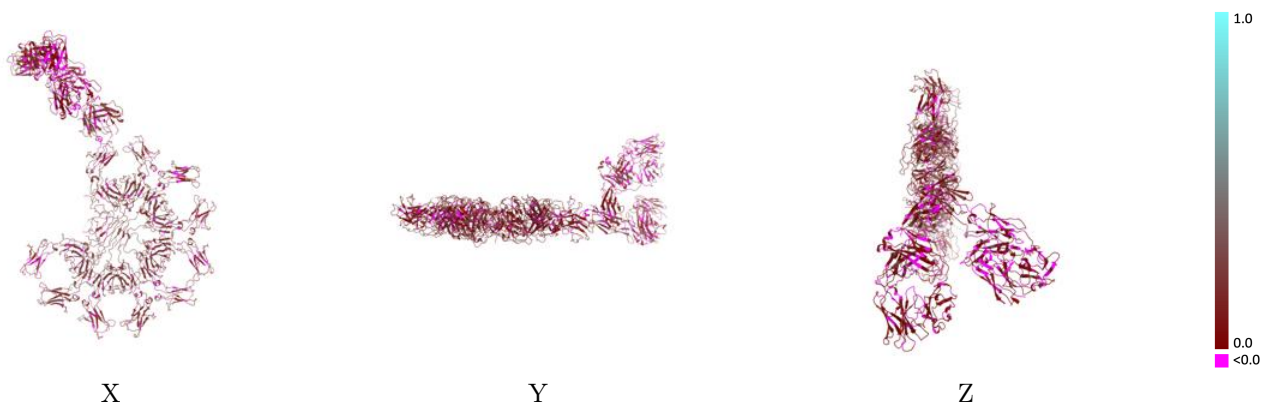
This section contains information regarding the fit between EMDB map EMD-15380 and PDB model 8AE3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.1 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](#)



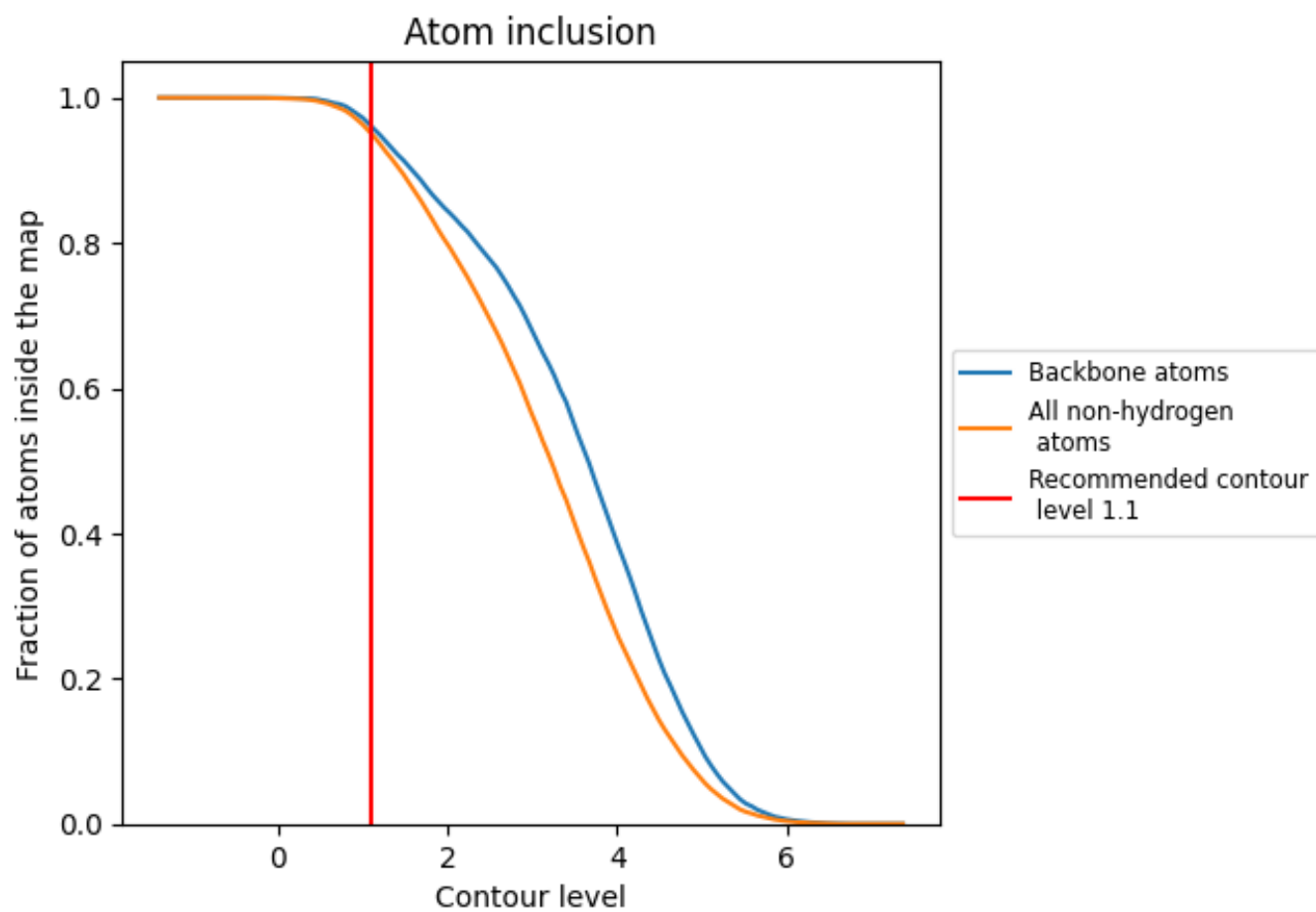
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9507	 0.1150
A	 0.9816	 0.0970
B	 0.9894	 0.0970
C	 0.9890	 0.1480
D	 0.9942	 0.1480
E	 0.9872	 0.1400
F	 0.9672	 0.1260
G	 0.9919	 0.1430
H	 0.9529	 0.0670
I	 1.0000	 0.0160
J	 0.9855	 0.1450
K	 0.9898	 0.1490
L	 0.9009	 0.0510
M	 0.1429	 0.0250
N	 0.9955	 0.1420
O	 0.9983	 0.1530
P	 1.0000	 0.2530
Q	 0.7095	 0.0300
R	 0.9932	 0.1400
S	 0.8166	 0.0420
T	 0.9675	 0.1190

