



Full wwPDB EM Validation Report ⓘ

Dec 4, 2024 – 12:39 PM EST

PDB ID : 9B8J
EMDB ID : EMD-44347
Title : GP38-GnH-DS-Gc in the pre-fusion conformation
Authors : McFadden, E.; McLellan, J.S.
Deposited on : 2024-03-30
Resolution : 3.40 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

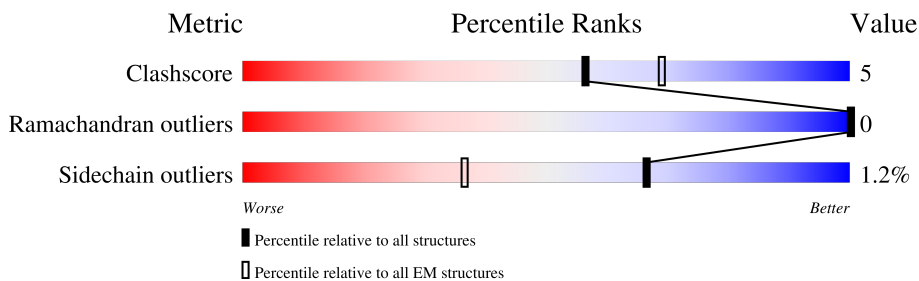
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	268	
2	B	98	
3	D	535	
4	E	480	
5	F	235	
6	H	471	
7	L	237	
8	C	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	G	3	 33% 67%

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 7610 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 GP38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	243	1949	1248	334	357	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	CYS	GLN	engineered mutation	UNP Q8JSZ3

- Molecule 2 is a protein called Glycoprotein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	52	398	243	73	79	3	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	516	SER	ARG	engineered mutation	UNP Q8JSZ3
B	562	CYS	VAL	engineered mutation	UNP Q8JSZ3
B	588	GLU	-	expression tag	UNP Q8JSZ3
B	589	ASN	-	expression tag	UNP Q8JSZ3
B	590	LEU	-	expression tag	UNP Q8JSZ3
B	591	TYR	-	expression tag	UNP Q8JSZ3
B	592	PHE	-	expression tag	UNP Q8JSZ3
B	593	GLN	-	expression tag	UNP Q8JSZ3
B	594	GLY	-	expression tag	UNP Q8JSZ3
B	595	GLY	-	expression tag	UNP Q8JSZ3
B	596	GLY	-	expression tag	UNP Q8JSZ3
B	597	GLY	-	expression tag	UNP Q8JSZ3
B	598	SER	-	expression tag	UNP Q8JSZ3
B	599	GLY	-	expression tag	UNP Q8JSZ3
B	600	GLY	-	expression tag	UNP Q8JSZ3
B	601	GLY	-	expression tag	UNP Q8JSZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	602	SER	-	expression tag	UNP Q8JSZ3
B	603	GLY	-	expression tag	UNP Q8JSZ3
B	604	GLY	-	expression tag	UNP Q8JSZ3
B	605	GLY	-	expression tag	UNP Q8JSZ3
B	606	SER	-	expression tag	UNP Q8JSZ3
B	607	GLU	-	expression tag	UNP Q8JSZ3
B	608	ASN	-	expression tag	UNP Q8JSZ3
B	609	LEU	-	expression tag	UNP Q8JSZ3
B	610	TYR	-	expression tag	UNP Q8JSZ3
B	611	PHE	-	expression tag	UNP Q8JSZ3
B	612	GLN	-	expression tag	UNP Q8JSZ3
B	613	GLY	-	expression tag	UNP Q8JSZ3

- Molecule 3 is a protein called Glycoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	217	1735	1096	296	323	20	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1546	GLY	-	expression tag	UNP Q8JSZ3
D	1547	SER	-	expression tag	UNP Q8JSZ3
D	1548	LEU	-	expression tag	UNP Q8JSZ3
D	1549	GLU	-	expression tag	UNP Q8JSZ3
D	1550	VAL	-	expression tag	UNP Q8JSZ3
D	1551	LEU	-	expression tag	UNP Q8JSZ3
D	1552	PHE	-	expression tag	UNP Q8JSZ3
D	1553	GLN	-	expression tag	UNP Q8JSZ3
D	1554	GLY	-	expression tag	UNP Q8JSZ3
D	1555	PRO	-	expression tag	UNP Q8JSZ3
D	1556	GLY	-	expression tag	UNP Q8JSZ3
D	1557	HIS	-	expression tag	UNP Q8JSZ3
D	1558	HIS	-	expression tag	UNP Q8JSZ3
D	1559	HIS	-	expression tag	UNP Q8JSZ3
D	1560	HIS	-	expression tag	UNP Q8JSZ3
D	1561	HIS	-	expression tag	UNP Q8JSZ3
D	1562	HIS	-	expression tag	UNP Q8JSZ3
D	1563	HIS	-	expression tag	UNP Q8JSZ3
D	1564	HIS	-	expression tag	UNP Q8JSZ3
D	1565	SER	-	expression tag	UNP Q8JSZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1566	ALA	-	expression tag	UNP Q8JSZ3
D	1567	TRP	-	expression tag	UNP Q8JSZ3
D	1568	SER	-	expression tag	UNP Q8JSZ3
D	1569	HIS	-	expression tag	UNP Q8JSZ3
D	1570	PRO	-	expression tag	UNP Q8JSZ3
D	1571	GLN	-	expression tag	UNP Q8JSZ3
D	1572	PHE	-	expression tag	UNP Q8JSZ3
D	1573	GLU	-	expression tag	UNP Q8JSZ3
D	1574	LYS	-	expression tag	UNP Q8JSZ3
D	1575	GLY	-	expression tag	UNP Q8JSZ3
D	1576	GLY	-	expression tag	UNP Q8JSZ3
D	1577	GLY	-	expression tag	UNP Q8JSZ3
D	1578	SER	-	expression tag	UNP Q8JSZ3
D	1579	GLY	-	expression tag	UNP Q8JSZ3
D	1580	GLY	-	expression tag	UNP Q8JSZ3
D	1581	GLY	-	expression tag	UNP Q8JSZ3
D	1582	GLY	-	expression tag	UNP Q8JSZ3
D	1583	SER	-	expression tag	UNP Q8JSZ3
D	1584	GLY	-	expression tag	UNP Q8JSZ3
D	1585	GLY	-	expression tag	UNP Q8JSZ3
D	1586	SER	-	expression tag	UNP Q8JSZ3
D	1587	ALA	-	expression tag	UNP Q8JSZ3
D	1588	TRP	-	expression tag	UNP Q8JSZ3
D	1589	SER	-	expression tag	UNP Q8JSZ3
D	1590	HIS	-	expression tag	UNP Q8JSZ3
D	1591	PRO	-	expression tag	UNP Q8JSZ3
D	1592	GLN	-	expression tag	UNP Q8JSZ3
D	1593	PHE	-	expression tag	UNP Q8JSZ3
D	1594	GLU	-	expression tag	UNP Q8JSZ3
D	1595	LYS	-	expression tag	UNP Q8JSZ3

- Molecule 4 is a protein called ADI-46152 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O	S	
4	E	122	951	604	160	183	4	0

- Molecule 5 is a protein called ADI-46152 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O	S	
5	F	107	805	510	134	159	2	0

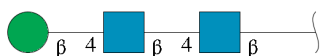
- Molecule 6 is a protein called ADI-36125 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	113	865	539	157	165	4	0	0

- Molecule 7 is a protein called ADI-36125 light chain.

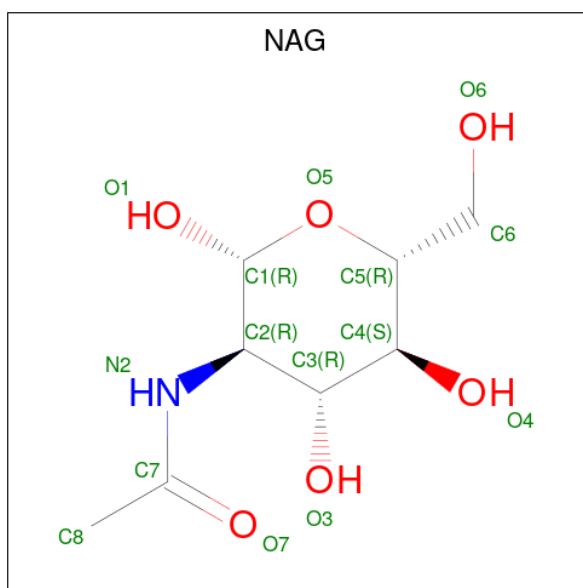
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	L	107	815	517	132	164	2	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	C	3	39	22	2	15	0	0
8	G	3	39	22	2	15	0	0

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

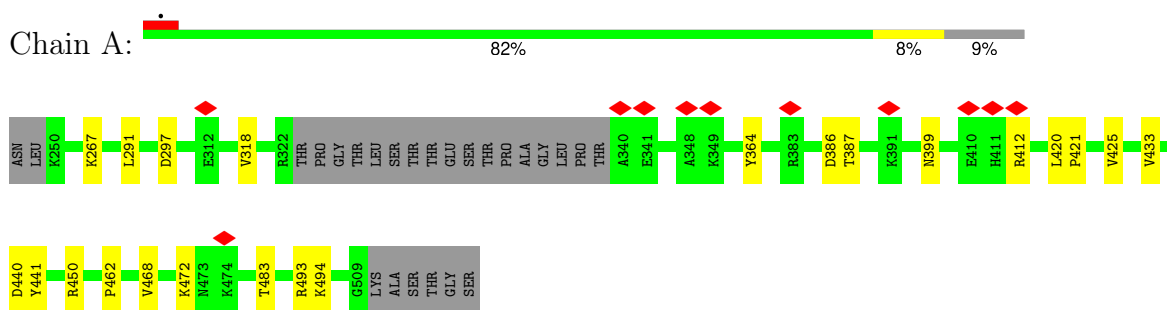


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	A	1	14	8	1	5	0

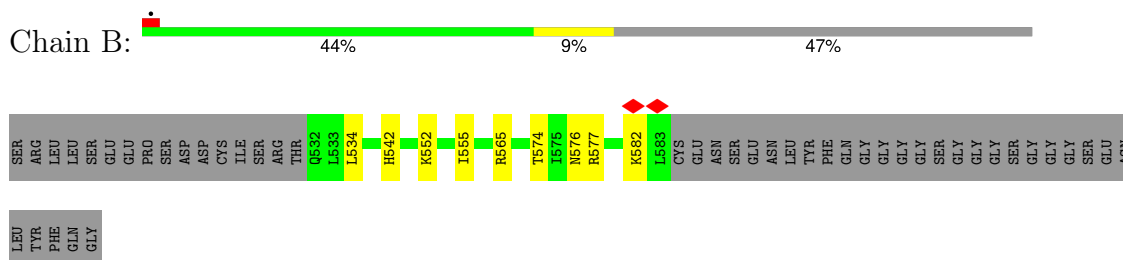
3 Residue-property plots [i](#)

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

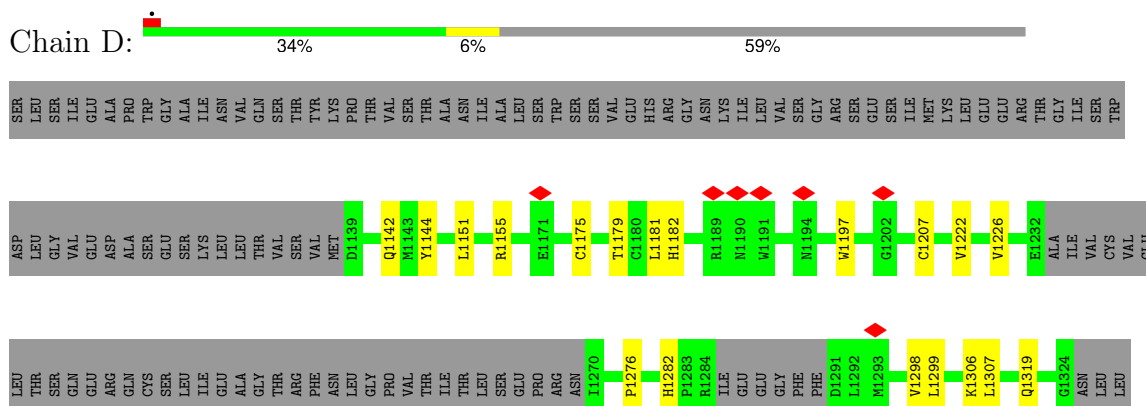
- Molecule 1: GP38

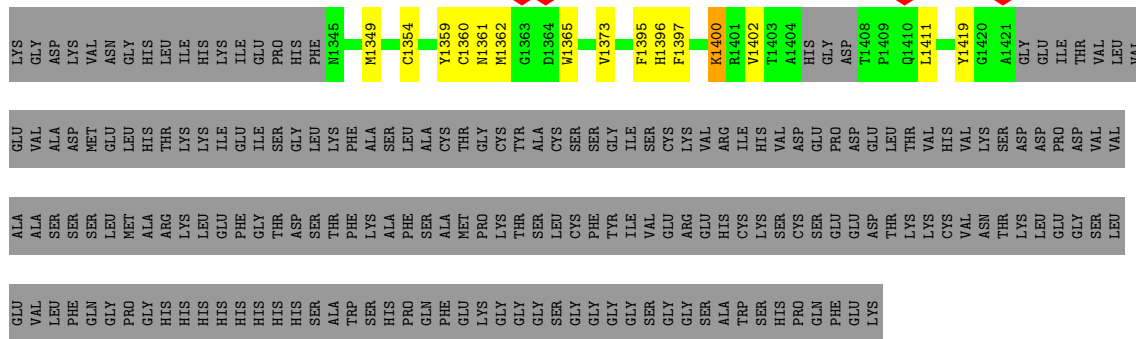


- Molecule 2: Glycoprotein N

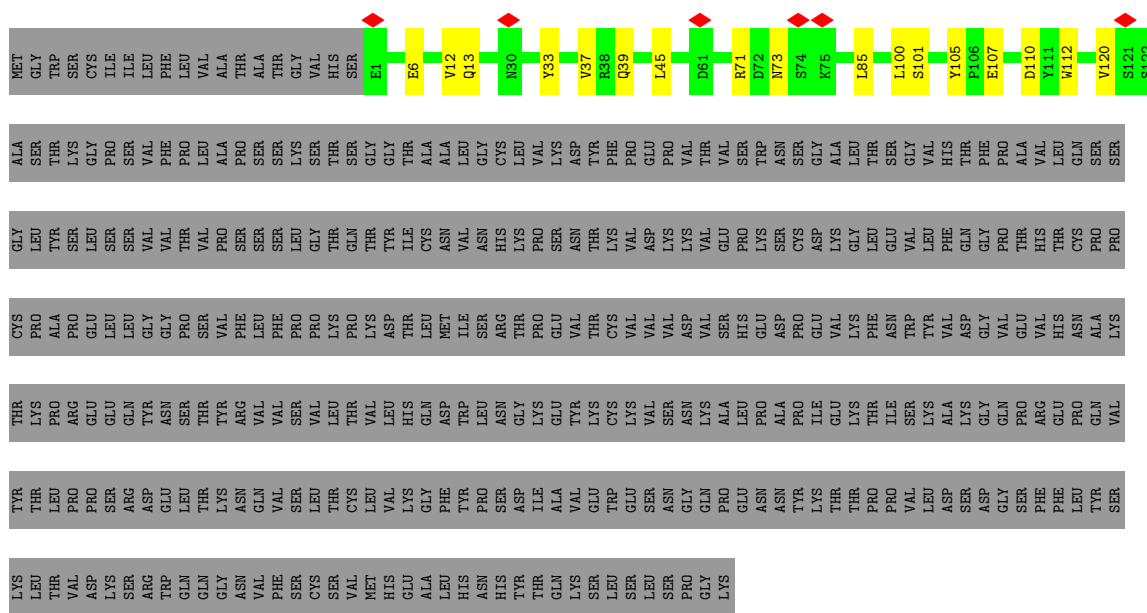


- Molecule 3: Glycoprotein C

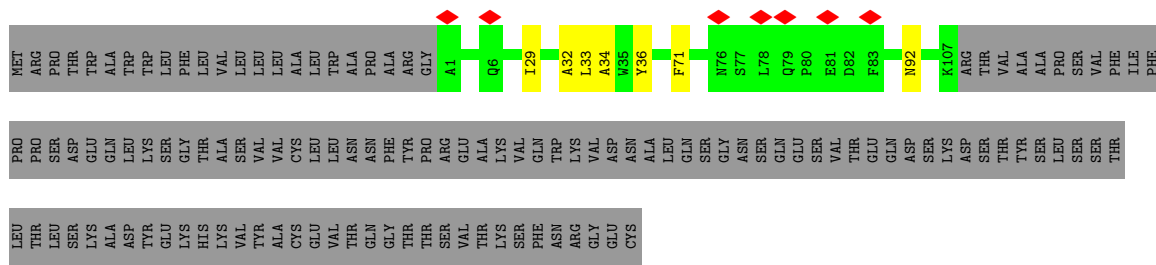




● Molecule 4: ADI-46152 heavy chain

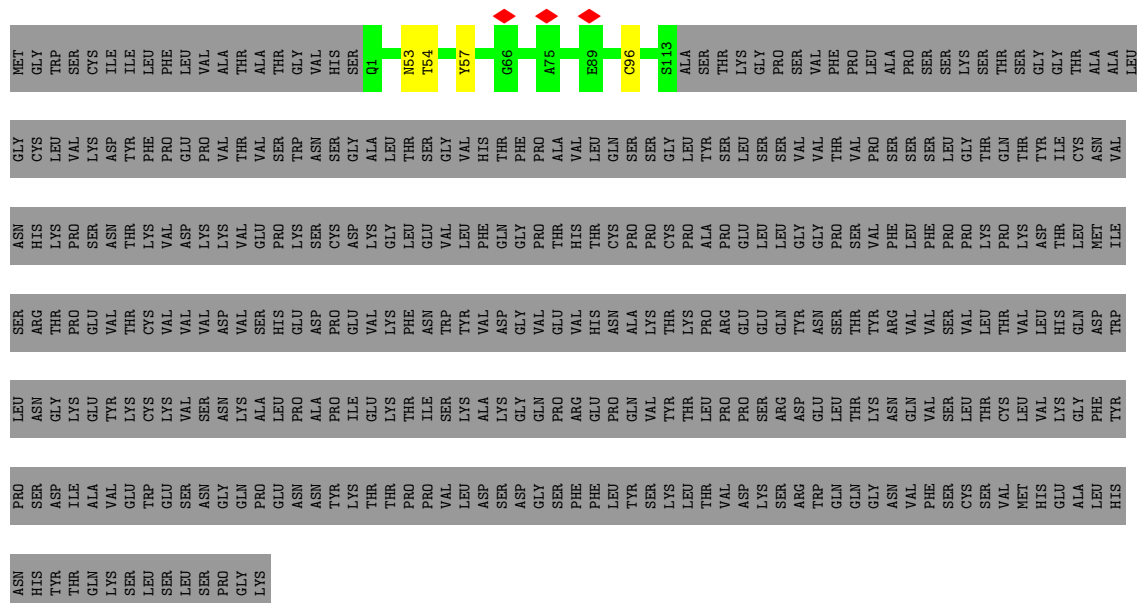


● Molecule 5: ADI-46152 light chain

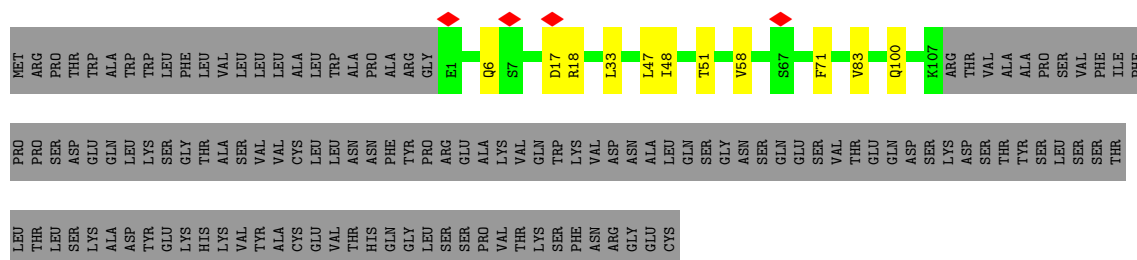
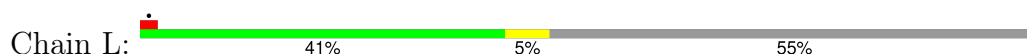


● Molecule 6: ADI-36125 heavy chain





- Molecule 7: ADI-36125 light chain



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



- Molecule 8: beta-D-mannopyranose-(1-4)-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	728031	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 ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.022	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.112	Depositor
Map size (Å)	399.93597, 399.93597, 399.93597	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8331999, 0.8331999, 0.8331999	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, BMA

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	0.27	0/1984	0.47	0/2672
2	B	0.28	0/402	0.54	0/540
3	D	0.27	0/1786	0.46	0/2429
4	E	0.29	0/974	0.50	0/1325
5	F	0.29	0/823	0.49	0/1119
6	H	0.29	0/883	0.51	0/1193
7	L	0.29	0/834	0.48	0/1137
All	All	0.28	0/7686	0.49	0/10415

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	1949	0	1973	21	0
2	B	398	0	388	12	0
3	D	1735	0	1620	23	0
4	E	951	0	915	11	0
5	F	805	0	790	7	0
6	H	865	0	843	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	815	0	802	6	0
8	C	39	0	34	0	0
8	G	39	0	34	0	0
9	A	14	0	13	0	0
All	All	7610	0	7412	70	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 (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:LYS:HE2	2:B:574:THR:HG21	1.15	1.13
1:A:494:LYS:HD3	3:D:1362:MET:CE	1.79	1.12
1:A:494:LYS:HD3	3:D:1362:MET:HE2	1.37	1.05
2:B:552:LYS:CE	2:B:574:THR:HG21	1.91	0.99
1:A:493:ARG:NH1	3:D:1197:TRP:CH2	2.34	0.96
2:B:552:LYS:HE2	2:B:574:THR:CG2	1.96	0.95
1:A:412:ARG:HD2	1:A:472:LYS:HE2	1.49	0.94
1:A:493:ARG:NH1	3:D:1197:TRP:CZ3	2.44	0.85
1:A:494:LYS:CD	3:D:1362:MET:CE	2.59	0.80
5:F:29:ILE:HD12	5:F:33:LEU:HD11	1.66	0.77
3:D:1402:VAL:HG22	3:D:1411:LEU:HD12	1.67	0.76
2:B:552:LYS:CE	2:B:574:THR:CG2	2.61	0.70
5:F:29:ILE:CD1	5:F:33:LEU:HD11	2.24	0.67
1:A:412:ARG:HD2	1:A:472:LYS:CE	2.25	0.66
4:E:71:ARG:NH1	4:E:73:ASN:OD1	2.31	0.63
3:D:1298:VAL:HG21	3:D:1397:PHE:CE1	2.34	0.62
1:A:386:ASP:OD1	1:A:387:THR:N	2.33	0.60
3:D:1361:ASN:ND2	3:D:1365:TRP:O	2.34	0.60
2:B:565:ARG:O	3:D:1365:TRP:NE1	2.37	0.58
7:L:47:LEU:HA	7:L:58:VAL:HG21	1.86	0.57
6:H:53:ASN:OD1	6:H:54:THR:N	2.38	0.56
3:D:1151:LEU:HD13	3:D:1222:VAL:HG22	1.90	0.55
4:E:13:GLN:N	4:E:13:GLN:OE1	2.41	0.54
1:A:291:LEU:HD21	1:A:318:VAL:HG11	1.89	0.54
3:D:1226:VAL:N	3:D:1276:PRO:O	2.42	0.53
4:E:12:VAL:HG21	4:E:85:LEU:HD13	1.90	0.53
4:E:6:GLU:N	4:E:6:GLU:OE1	2.42	0.52
1:A:493:ARG:CZ	3:D:1197:TRP:CH2	2.93	0.52
7:L:33:LEU:HD22	7:L:71:PHE:CD1	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:32:ALA:O	5:F:33:LEU:HD12	2.10	0.52
1:A:441:TYR:OH	1:A:450:ARG:O	2.23	0.51
3:D:1142:GLN:OE1	3:D:1144:TYR:OH	2.25	0.51
4:E:39:GLN:HB2	4:E:45:LEU:HD23	1.92	0.51
3:D:1307:LEU:HD13	6:H:57:TYR:CZ	2.46	0.51
7:L:83:VAL:O	7:L:83:VAL:HG23	2.11	0.51
1:A:364:TYR:OH	1:A:440:ASP:OD2	2.28	0.50
4:E:120:VAL:O	4:E:120:VAL:HG23	2.12	0.50
4:E:110:ASP:OD1	4:E:110:ASP:N	2.41	0.49
1:A:425:VAL:HG13	1:A:483:THR:HG22	1.94	0.49
5:F:33:LEU:HD13	5:F:71:PHE:CZ	2.48	0.49
7:L:48:ILE:HG22	7:L:51:THR:O	2.13	0.48
3:D:1306:LYS:O	3:D:1319:GLN:NE2	2.42	0.48
3:D:1397:PHE:HB2	3:D:1400:LYS:HE3	1.95	0.48
4:E:37:VAL:HG21	4:E:112:TRP:CZ3	2.48	0.48
3:D:1307:LEU:HD13	6:H:57:TYR:CE1	2.49	0.48
3:D:1354:CYS:SG	3:D:1373:VAL:HG22	2.55	0.47
2:B:552:LYS:HE3	2:B:574:THR:CG2	2.43	0.47
1:A:494:LYS:HD3	3:D:1362:MET:HE1	1.86	0.46
5:F:34:ALA:HB1	5:F:36:TYR:CE1	2.52	0.45
2:B:552:LYS:HG2	2:B:576:ASN:HA	1.98	0.45
1:A:433:VAL:O	1:A:468:VAL:HG22	2.17	0.44
1:A:421:PRO:HG2	1:A:462:PRO:O	2.18	0.44
3:D:1179:THR:HG23	3:D:1349:MET:CB	2.48	0.44
1:A:494:LYS:CD	3:D:1362:MET:HE3	2.46	0.44
4:E:101:SER:OG	4:E:107:GLU:OE2	2.33	0.44
1:A:399:ASN:OD1	1:A:399:ASN:N	2.51	0.44
2:B:534:LEU:O	2:B:582:LYS:N	2.45	0.44
3:D:1181:LEU:HD23	3:D:1182:HIS:N	2.33	0.43
1:A:267:LYS:NZ	1:A:297:ASP:OD1	2.50	0.43
4:E:33:TYR:CE1	4:E:100:LEU:HD11	2.53	0.43
2:B:576:ASN:OD1	2:B:577:ARG:N	2.52	0.43
4:E:105:TYR:OH	5:F:92:ASN:OD1	2.37	0.43
2:B:542:HIS:HD2	2:B:552:LYS:NZ	2.17	0.42
7:L:17:ASP:OD1	7:L:18:ARG:N	2.52	0.42
1:A:412:ARG:HD2	1:A:472:LYS:HG2	2.01	0.42
3:D:1395:PHE:O	3:D:1396:HIS:C	2.57	0.42
7:L:6:GLN:O	7:L:100:GLN:NE2	2.53	0.41
2:B:552:LYS:HE3	2:B:574:THR:HG22	2.02	0.41
1:A:420:LEU:HD21	2:B:555:ILE:HG13	2.01	0.41
5:F:32:ALA:C	5:F:33:LEU:HD12	2.42	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	239/268 (89%)	234 (98%)	5 (2%)	0	100	100
2	B	50/98 (51%)	49 (98%)	1 (2%)	0	100	100
3	D	207/535 (39%)	196 (95%)	11 (5%)	0	100	100
4	E	120/480 (25%)	116 (97%)	4 (3%)	0	100	100
5	F	105/235 (45%)	98 (93%)	7 (7%)	0	100	100
6	H	111/471 (24%)	108 (97%)	3 (3%)	0	100	100
7	L	105/237 (44%)	98 (93%)	7 (7%)	0	100	100
All	All	937/2324 (40%)	899 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	219/240 (91%)	219 (100%)	0	100	100
2	B	44/79 (56%)	44 (100%)	0	100	100
3	D	196/468 (42%)	187 (95%)	9 (5%)	23	49
4	E	102/423 (24%)	102 (100%)	0	100	100
5	F	88/200 (44%)	88 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	H	93/414 (22%)	92 (99%)	1 (1%)	70	81
7	L	93/207 (45%)	93 (100%)	0	100	100
All	All	835/2031 (41%)	825 (99%)	10 (1%)	66	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1155	ARG
3	D	1175	CYS
3	D	1207	CYS
3	D	1282	HIS
3	D	1299	LEU
3	D	1359	TYR
3	D	1360	CYS
3	D	1400	LYS
3	D	1419	TYR
6	H	96	CYS

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

Mol	Chain	Res	Type
1	A	431	HIS
2	B	542	HIS
3	D	1187	HIS
3	D	1361	ASN
5	F	89	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
8	NAG	C	1	1,8	14,14,15	0.70	0	17,19,21	0.84	0
8	NAG	C	2	8	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
8	BMA	C	3	8	11,11,12	0.82	0	15,15,17	2.31	4 (26%)
8	NAG	G	1	2,8	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
8	NAG	G	2	8	14,14,15	0.72	0	17,19,21	0.87	0
8	BMA	G	3	8	11,11,12	0.80	0	15,15,17	2.25	4 (26%)

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
8	NAG	C	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	NAG	G	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	G	2	8	-	0/6/23/26	0/1/1/1
8	BMA	G	3	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	3	BMA	C1-O5-C5	6.95	121.51	112.19
8	G	3	BMA	C1-O5-C5	6.65	121.09	112.19
8	G	3	BMA	C3-C4-C5	3.02	115.70	110.23
8	C	3	BMA	C3-C4-C5	2.96	115.60	110.23
8	C	3	BMA	C2-C3-C4	2.37	115.03	110.86
8	G	3	BMA	C2-C3-C4	2.33	114.95	110.86
8	C	2	NAG	O5-C1-C2	-2.22	107.85	111.29
8	C	3	BMA	O4-C4-C3	-2.18	105.24	110.38
8	G	3	BMA	O4-C4-C3	-2.15	105.31	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1	NAG	O5-C1-C2	-2.10	108.04	111.29

There are no chirality outliers.

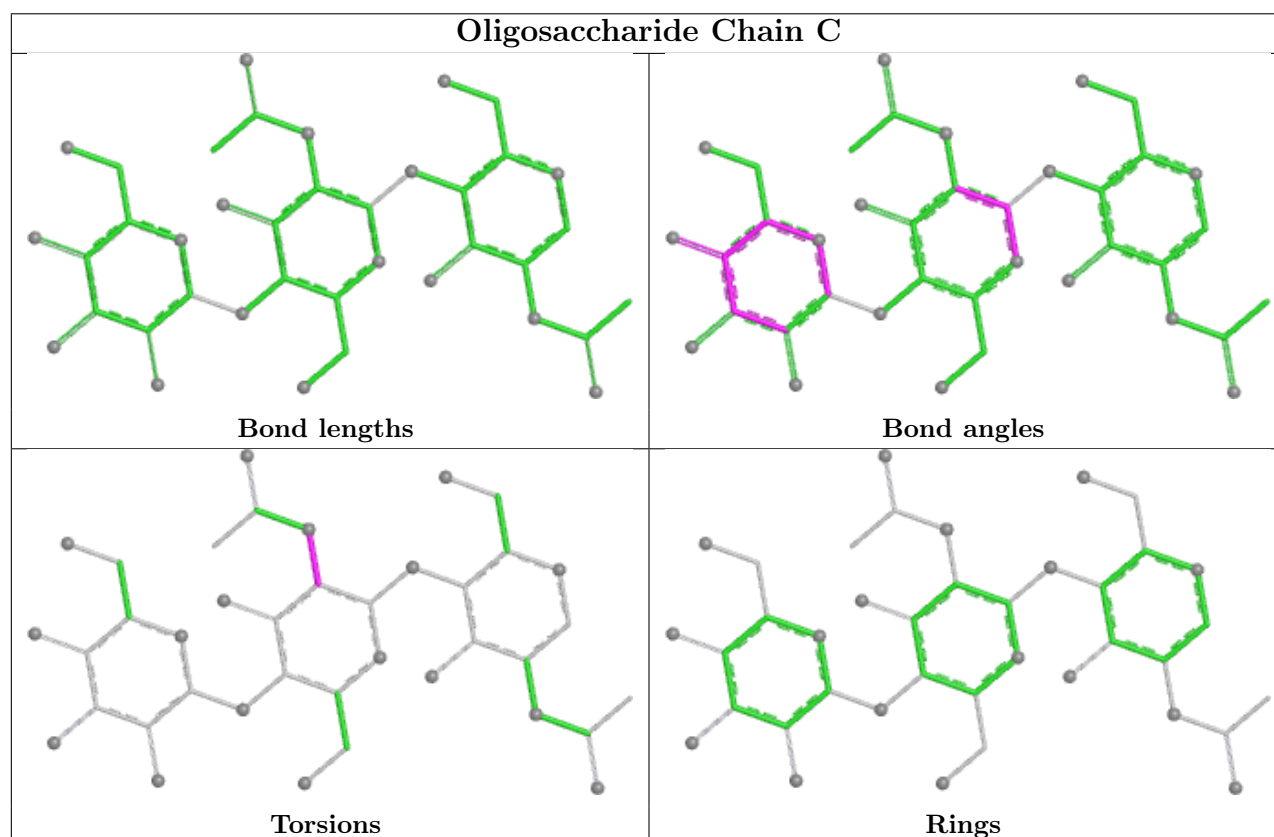
All (3) torsion outliers are listed below:

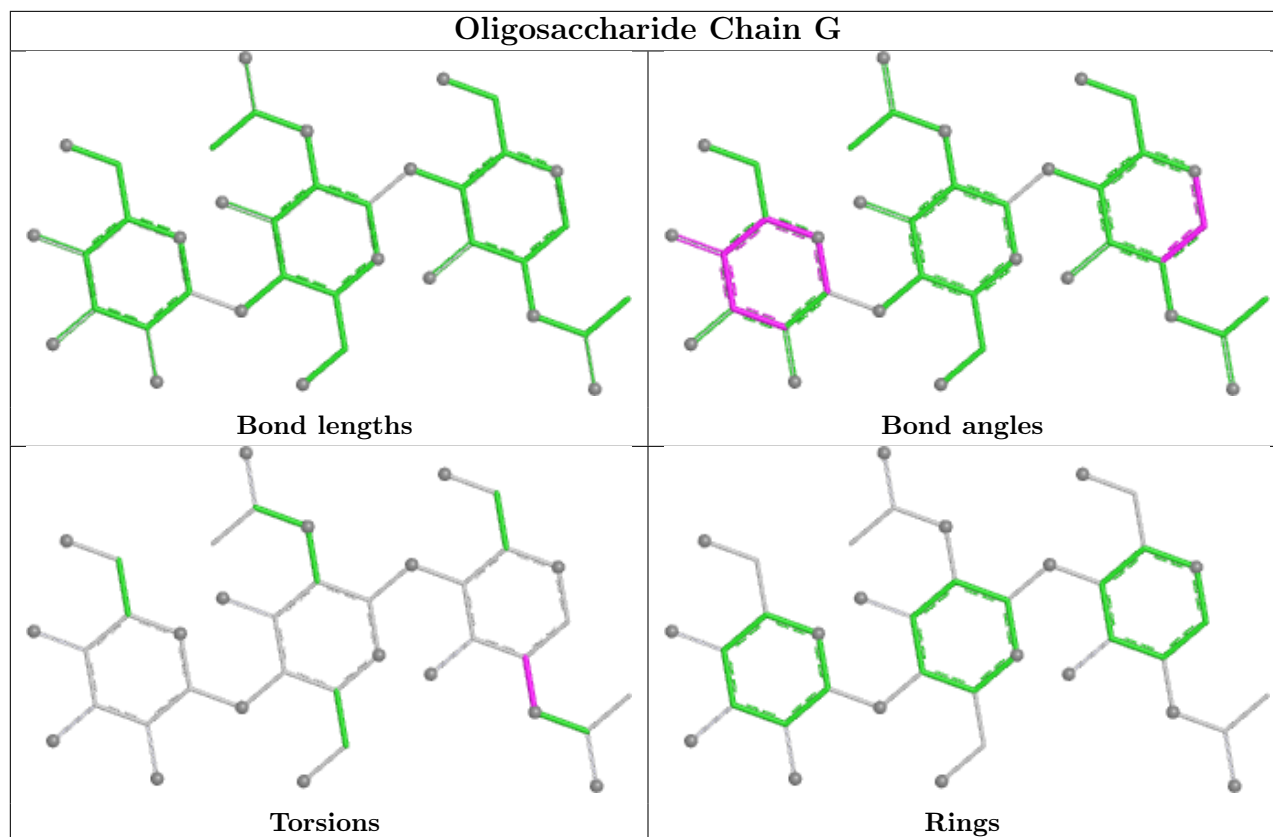
Mol	Chain	Res	Type	Atoms
8	C	2	NAG	C1-C2-N2-C7
8	G	1	NAG	C3-C2-N2-C7
8	G	1	NAG	C1-C2-N2-C7

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	601	1	14,14,15	0.72	0	17,19,21	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	NAG	C4-C5-C6-O6
9	A	601	NAG	O5-C5-C6-O6

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 [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44347. These allow visual inspection of the internal detail of the map and identification of artifacts.

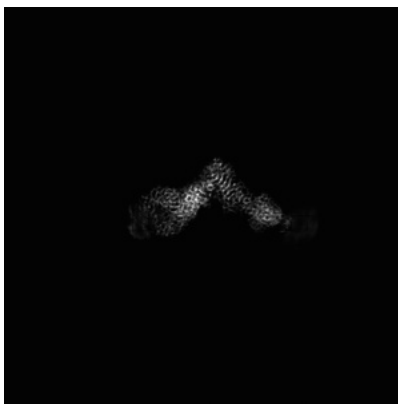
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

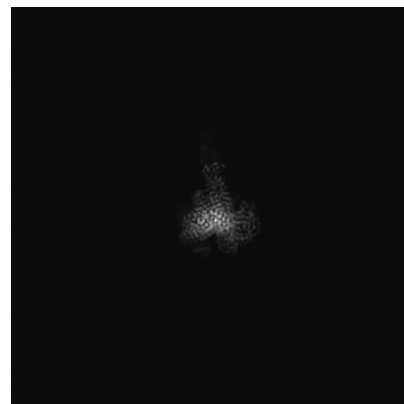
6.1.1 Primary map



X

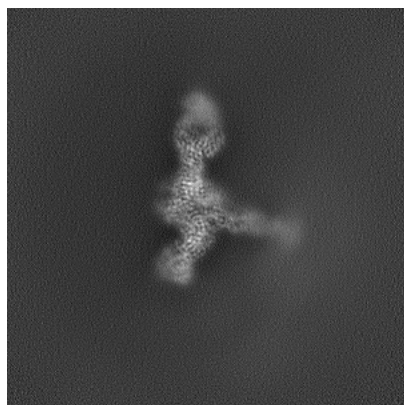


Y

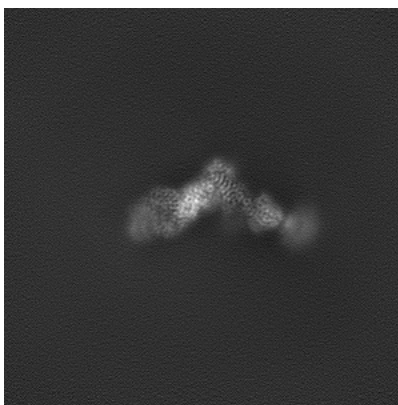


Z

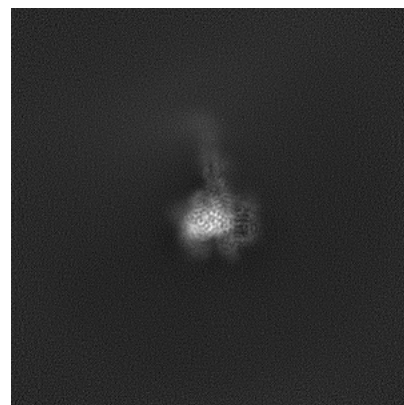
6.1.2 Raw map



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: 240



Y Index: 240

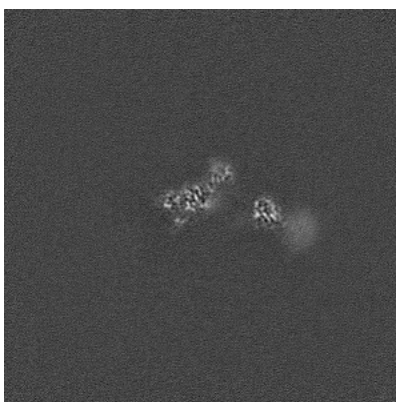


Z Index: 240

6.2.2 Raw map



X Index: 240



Y Index: 240

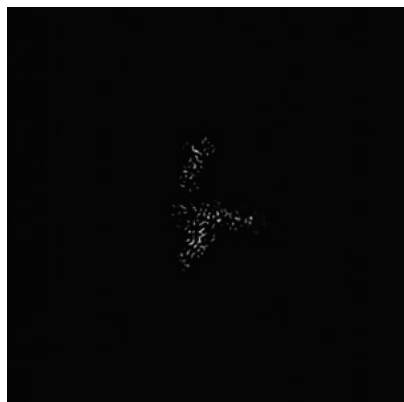


Z Index: 240

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

6.3 Largest variance slices [i](#)

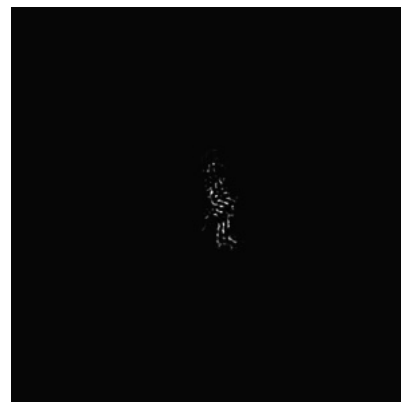
6.3.1 Primary map



X Index: 246

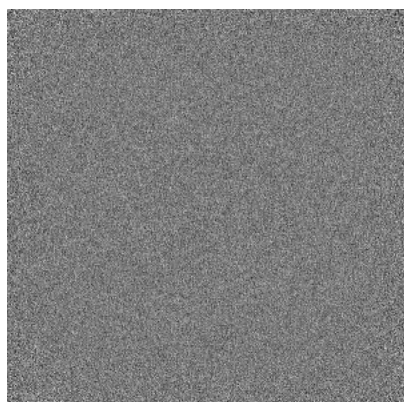


Y Index: 220

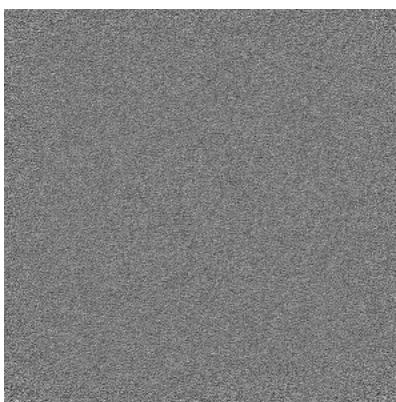


Z Index: 231

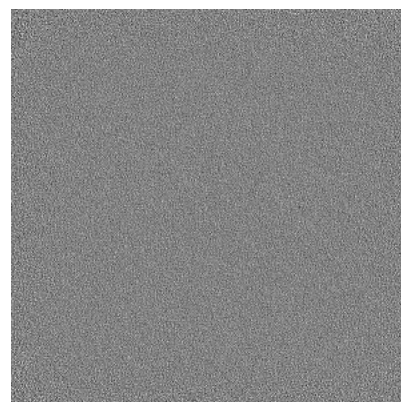
6.3.2 Raw map



X Index: 0



Y Index: 0

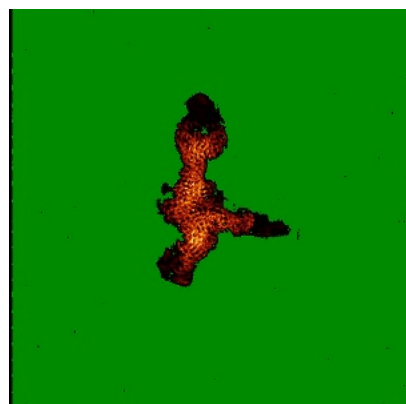


Z Index: 0

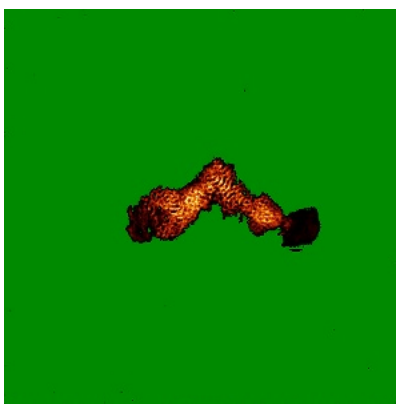
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

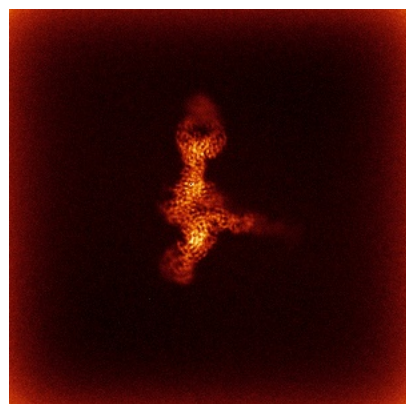


Y

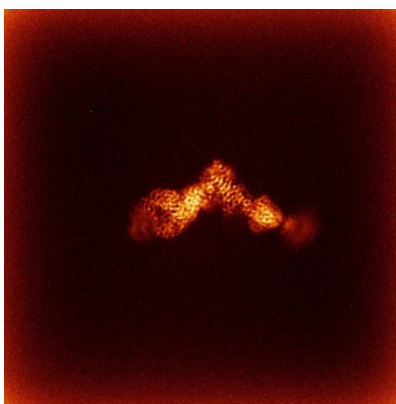


Z

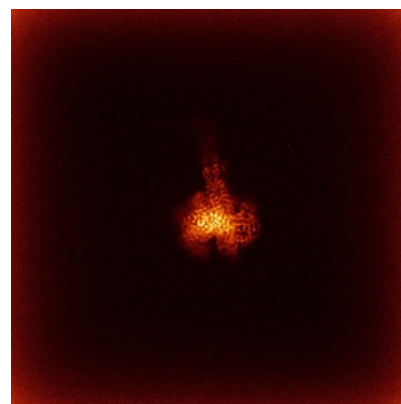
6.4.2 Raw map



X



Y

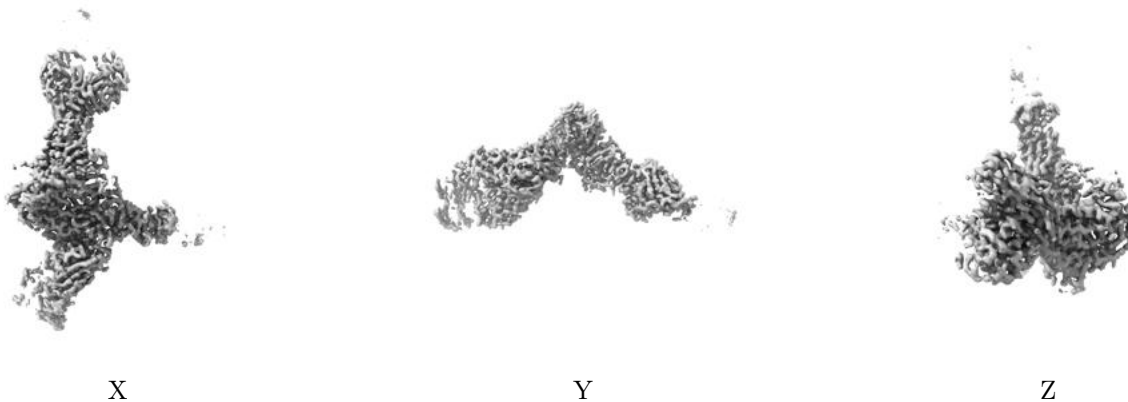


Z

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.

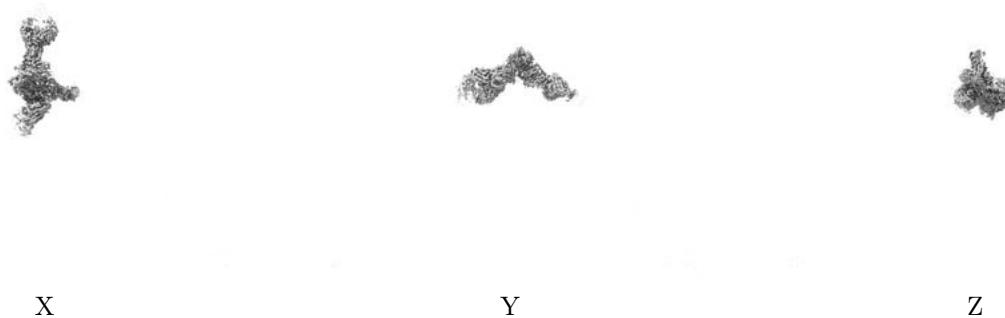
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.112. 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.

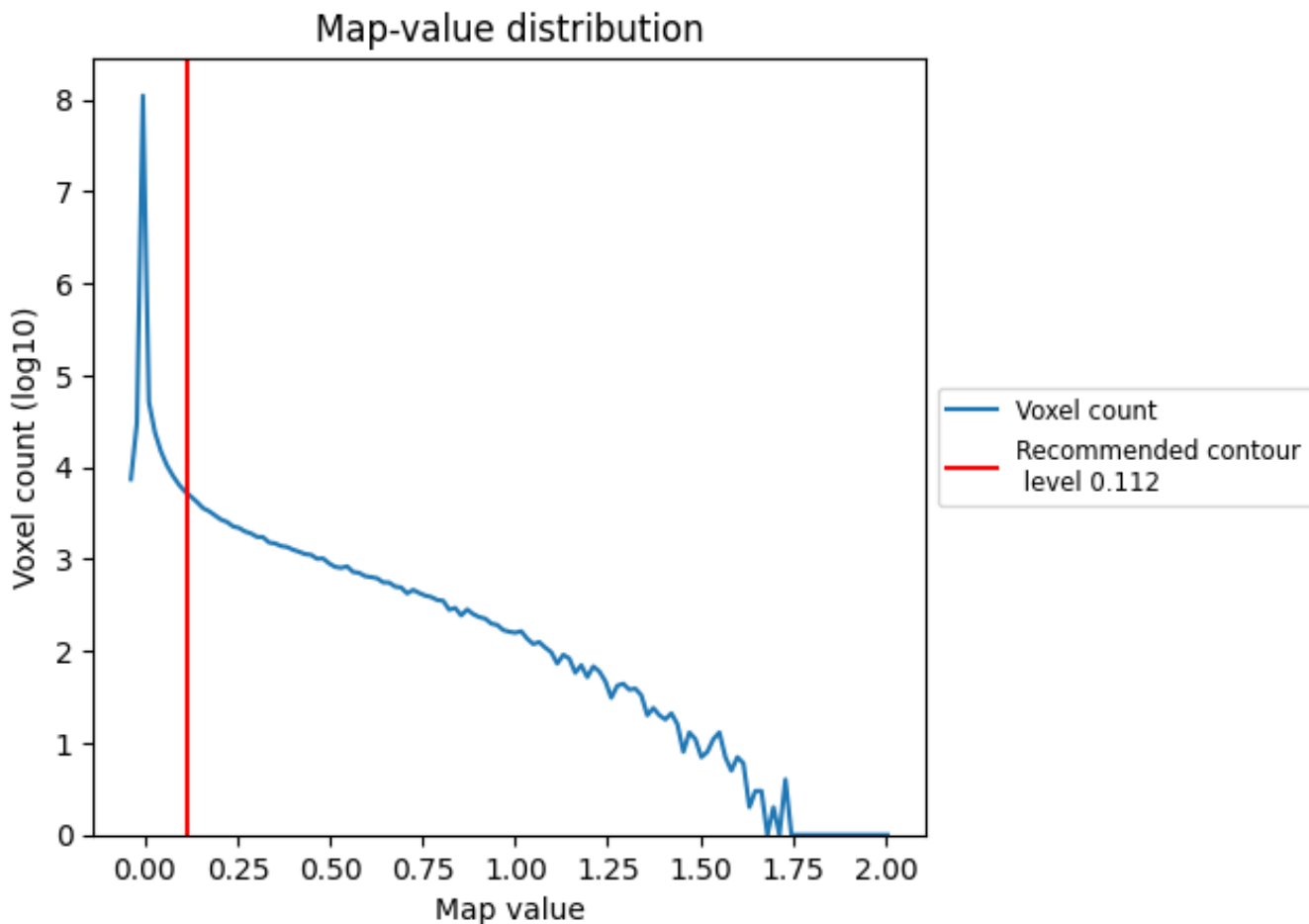
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

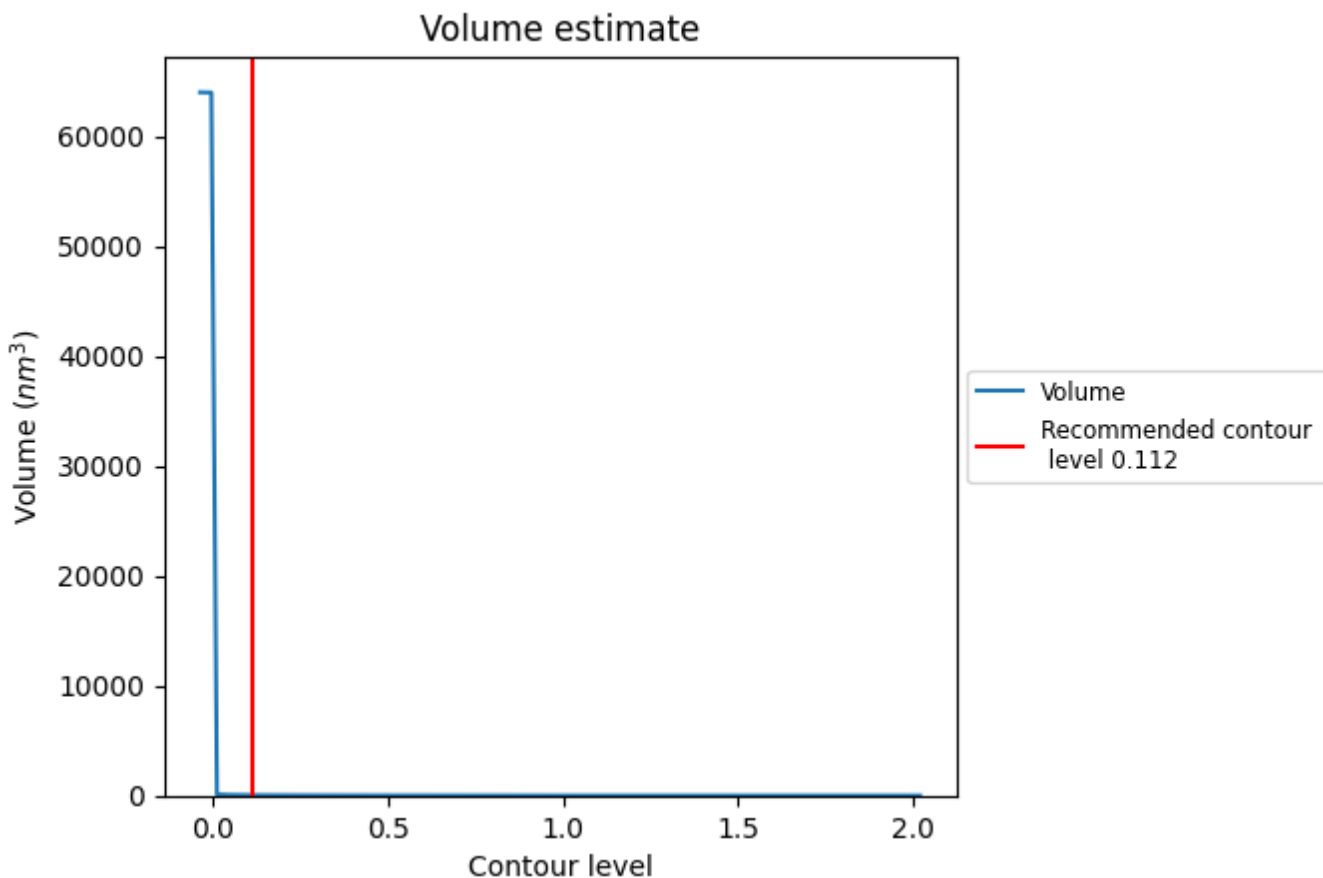
This section contains the results of statistical analysis of the map.

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.

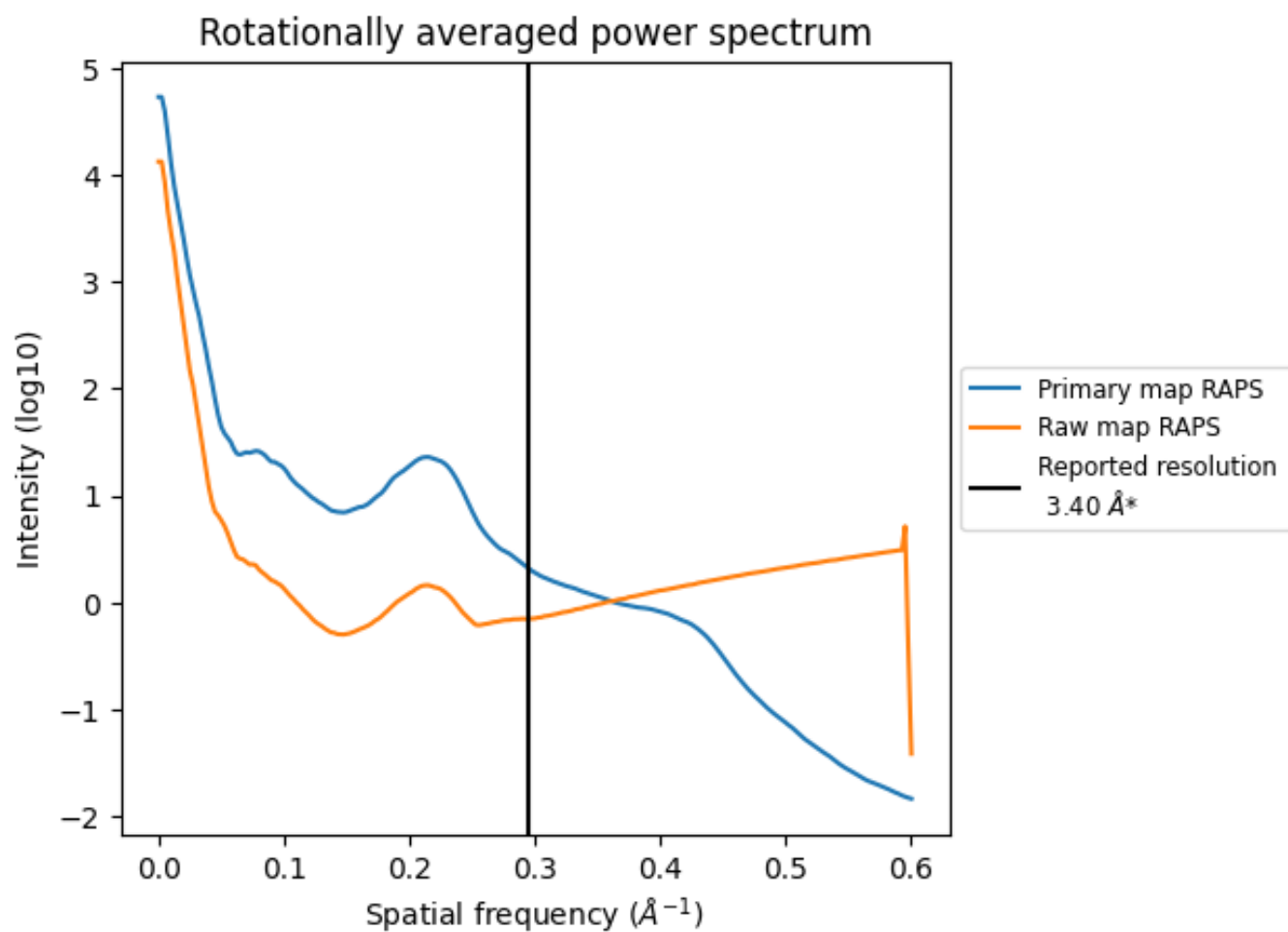
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm³; this corresponds to an approximate mass of 36 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

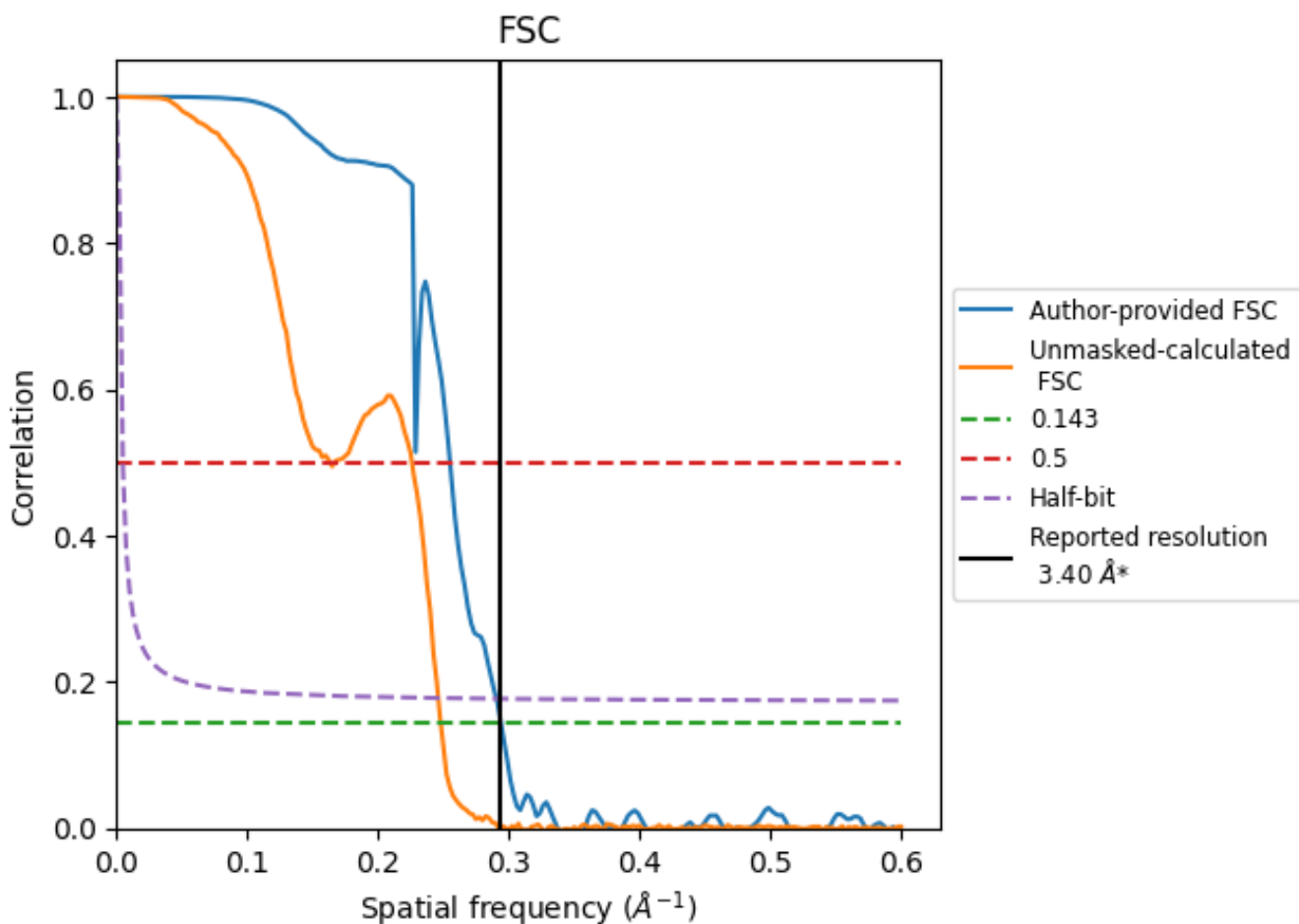


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

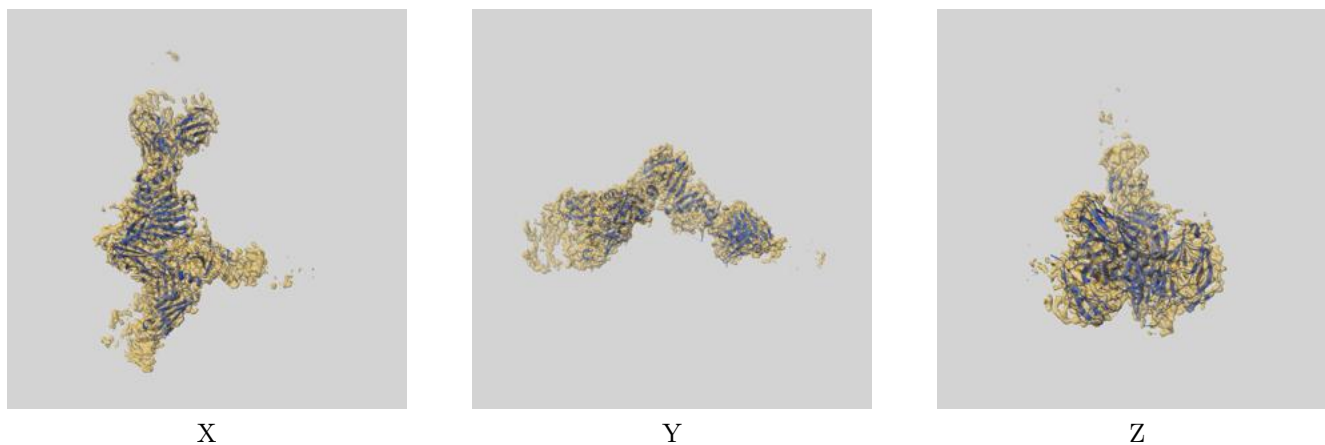
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.92	3.44
Unmasked-calculated*	4.03	6.12	4.06

*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 4.03 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

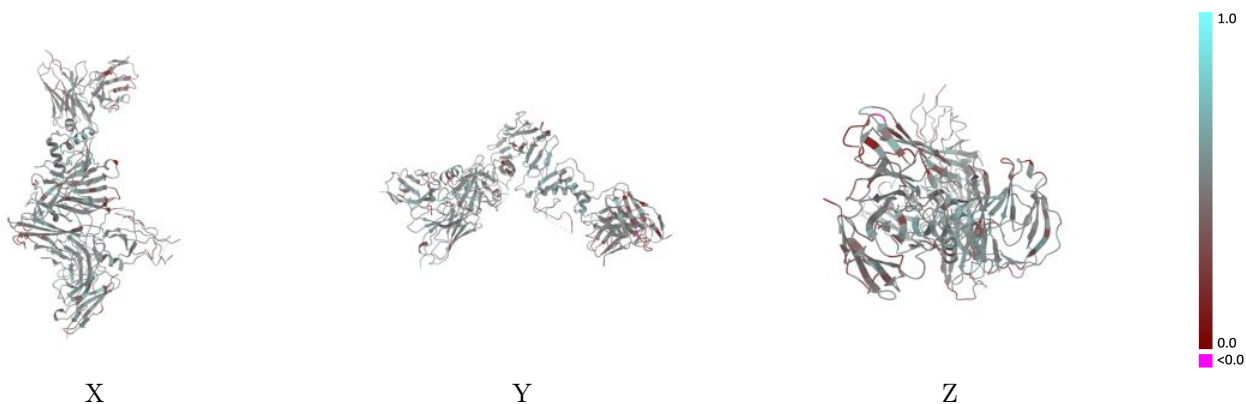
This section contains information regarding the fit between EMDB map EMD-44347 and PDB model 9B8J. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



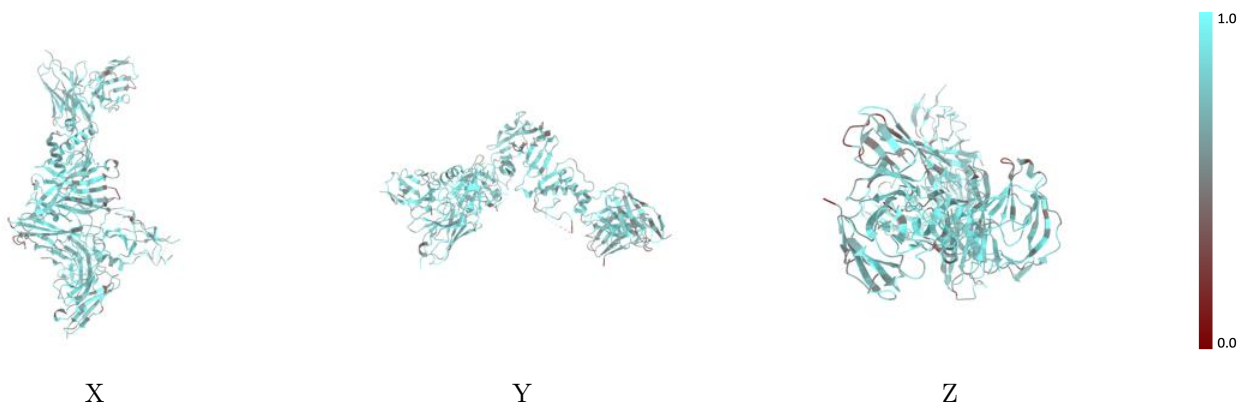
The images above show the 3D surface view of the map at the recommended contour level 0.112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



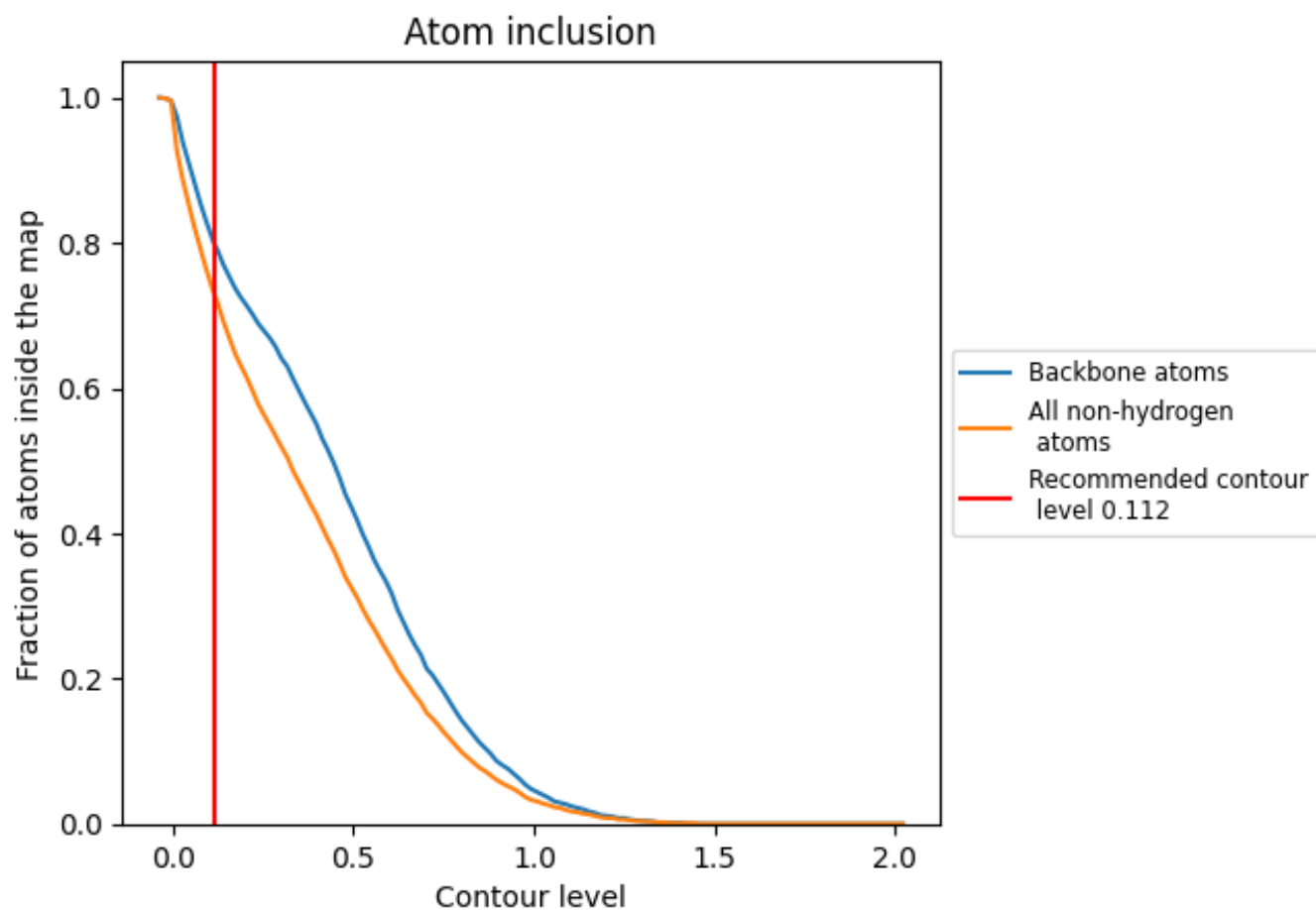
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.112).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% 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 (0.112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7320	 0.4740
A	 0.7310	 0.4820
B	 0.7580	 0.4850
C	 0.4100	 0.4340
D	 0.7400	 0.4720
E	 0.7170	 0.4530
F	 0.6810	 0.4250
G	 0.7180	 0.4420
H	 0.7740	 0.5070
L	 0.7430	 0.4970

