WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Mar 21, 2023 – 02:22 PM EDT

PDB ID	:	8D74
EMDB ID	:	EMD-27227
Title	:	Cryo-EM structure of human CNTF signaling complex: model containing the interaction core region
Authors	:	Zhou, Y.; Franklin, M.C.
Deposited on	:	2022-06-07
Resolution	:	3.03 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 (i) 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 (i)) were used in the production of this report:

|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), 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)	:	2.32.1

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 3.03 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.1%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
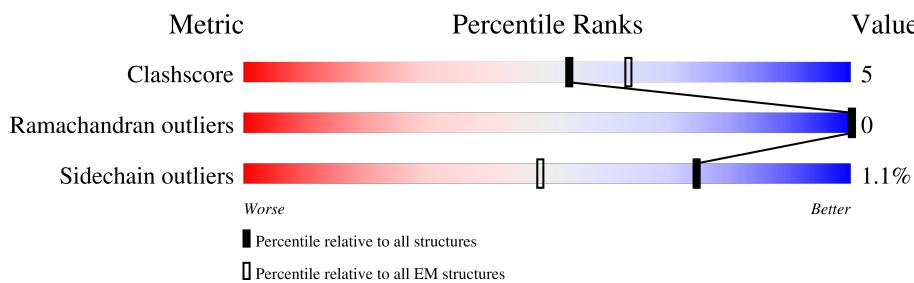
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	625	· 51% 12% 37%
2	D	214	69% 13% 19%
3	C	320	57% 5% 38%
4	B	817	5% 40% 8% 51%
5	E	2	50% 100%
5	F	2	50% 50%
5	G	2	100%
5	H	2	100%
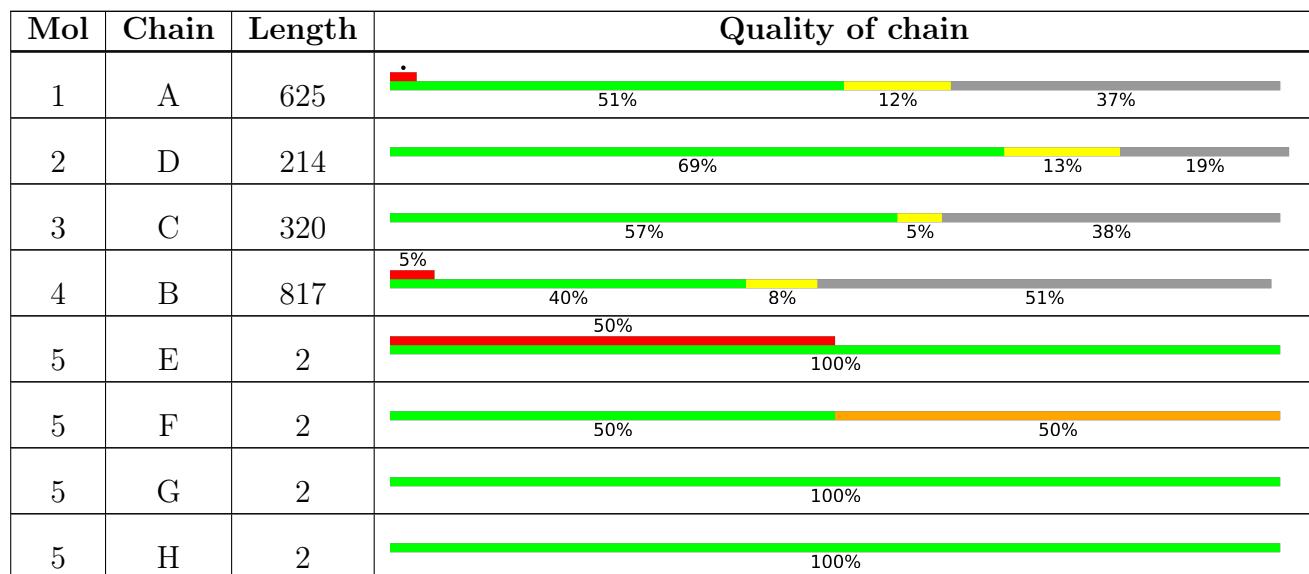
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Mol	Chain	Length	Quality of chain
5	I	2	100%
5	J	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9639 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 Interleukin-6 receptor subunit beta.

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

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
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 2 is a protein called Ciliary neurotrophic factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	174	1416	897	252	263	4	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	187	GLU	-	expression tag	UNP P26441
D	188	GLN	-	expression tag	UNP P26441
D	189	LYS	-	expression tag	UNP P26441
D	190	LEU	-	expression tag	UNP P26441
D	191	ILE	-	expression tag	UNP P26441
D	192	SER	-	expression tag	UNP P26441
D	193	GLU	-	expression tag	UNP P26441
D	194	GLU	-	expression tag	UNP P26441
D	195	ASP	-	expression tag	UNP P26441
D	196	LEU	-	expression tag	UNP P26441
D	197	GLY	-	expression tag	UNP P26441
D	198	GLY	-	expression tag	UNP P26441
D	199	GLU	-	expression tag	UNP P26441
D	200	GLN	-	expression tag	UNP P26441
D	201	LYS	-	expression tag	UNP P26441
D	202	LEU	-	expression tag	UNP P26441
D	203	ILE	-	expression tag	UNP P26441
D	204	SER	-	expression tag	UNP P26441
D	205	GLU	-	expression tag	UNP P26441
D	206	GLU	-	expression tag	UNP P26441
D	207	ASP	-	expression tag	UNP P26441
D	208	LEU	-	expression tag	UNP P26441
D	209	HIS	-	expression tag	UNP P26441
D	210	HIS	-	expression tag	UNP P26441
D	211	HIS	-	expression tag	UNP P26441
D	212	HIS	-	expression tag	UNP P26441
D	213	HIS	-	expression tag	UNP P26441
D	214	HIS	-	expression tag	UNP P26441

- Molecule 3 is a protein called Ciliary neurotrophic factor receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	199	1607	1037	272	292	6	0	0

- Molecule 4 is a protein called Leukemia inhibitory factor receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	398	3197	2047	541	597	12	0	0

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
B	859	HIS	-	expression tag	UNP P42702
B	860	HIS	-	expression tag	UNP P42702
B	861	HIS	-	expression tag	UNP P42702

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
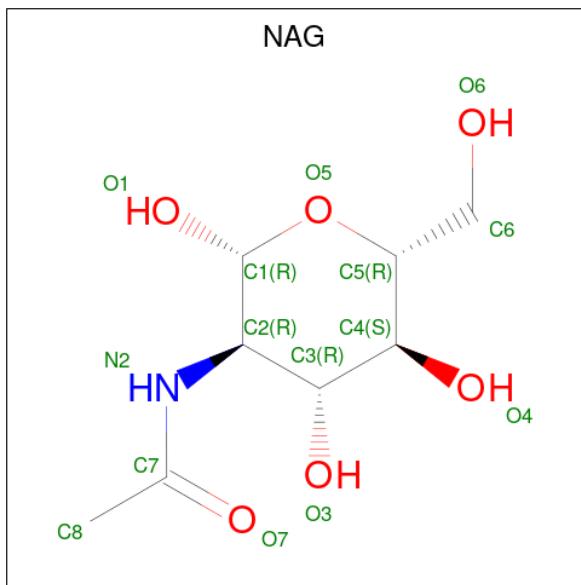
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

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

3 Residue-property plots ⓘ

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: Interleukin-6 receptor subunit beta
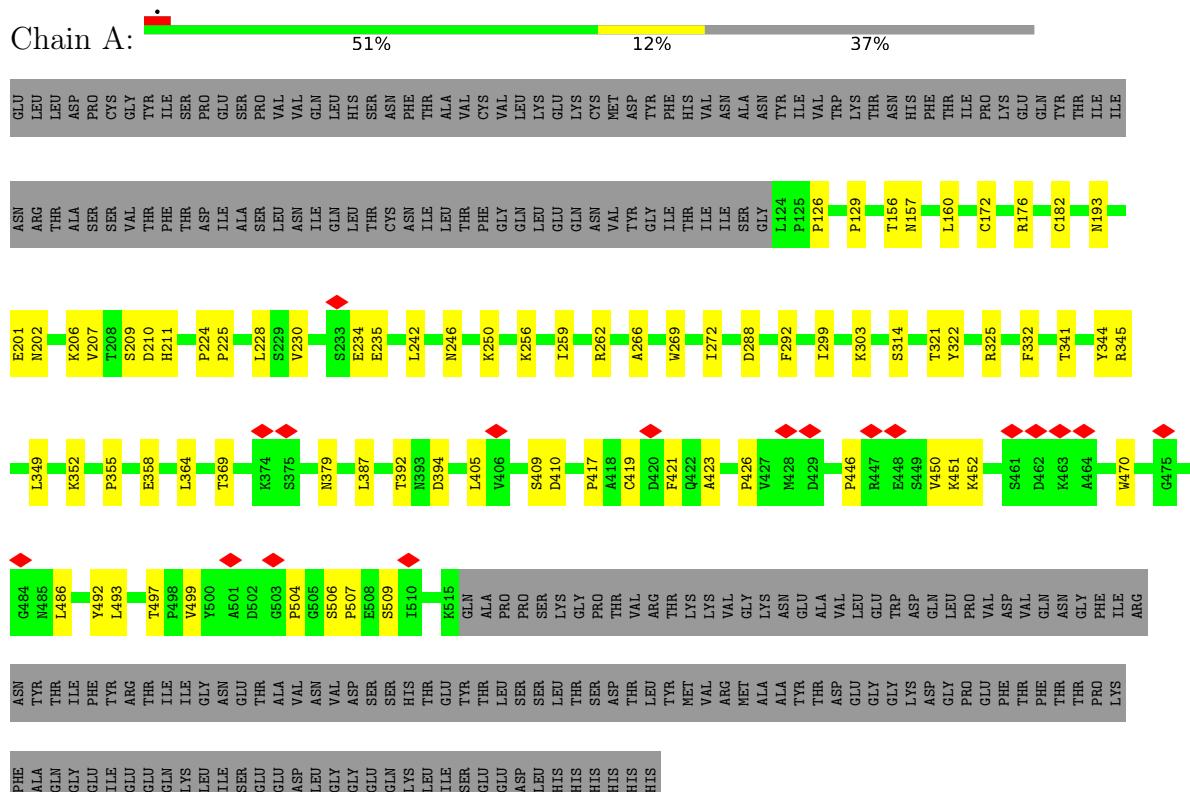
Chain A:

• Molecule 2: Ciliary neurotrophic factor
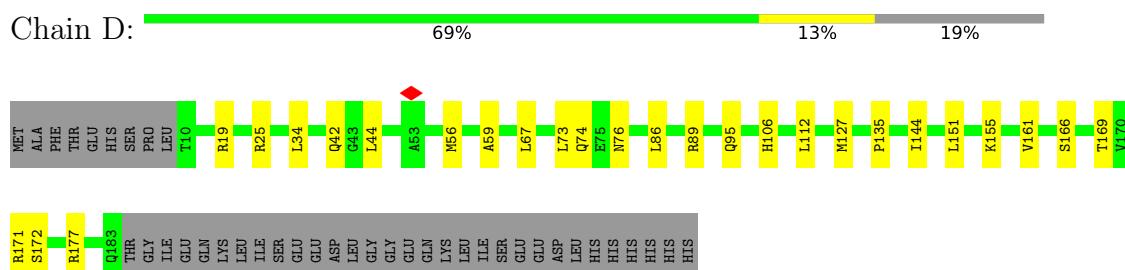
Chain D:

• Molecule 3: Ciliary neurotrophic factor receptor subunit alpha

Chain C:

57%　　　　　5%　　　　　38%

GLN ARG HIS SER PRO GLN GLU ALA PRO HIS VAL GLN TYR GLU ARG LEU GLY SER ASP VAL THR LEU PRO CYS GLY THR ALA ASN TRP ASP ALA ALA VAL THR TRP ARG VAL ASN GLY THR ASP LEU ALA PRO ASP LEU LEU ASN GLY SER GLN LEU VAL LEU HIS GLY LEU GLU LEU GLY

HIS SER GLY LEU TYR ALA CYS PHE HIS ARG ASP SER TRP HIS LEU ARG HIS GLN VAL LEU LEU HIS VAL GLY L107 T135 Y136 I137 P158 A159 L160 C164 H165 I166 R167 Y168 N190 S217 N218 P219 R220 V224 F243 I278 D284 N285 W290 E305 PRO

ARG HIS LEU THR GLU GLN ALA GLN ALA ALA GLU GLU THR THR THR SER THR SER SER LEU ALA PRO PRO THR THR LYS ILE CYS ASP PRO GLY GLU LEU GLY SER

● Molecule 4: Leukemia inhibitory factor receptor

5%

Chain B:

40%　　　　　8%　　　　　51%

GLN LYS LYS GLY ALA PRO HIS ASP LEU LYS CYS VAL THR ASN ASN LEU GLN VAL TRP ASN CYS SER TRP LYS ALA PRO SER GLY THR GLY ARG GLY THR ASP TYR GLU VAL CYS ILE GLU VAL ASN ARG ARG SER CYS TYR GLN LEU GLU LYS THR SER ILE LYS PRO ALA LEU SER

HIS GLY ASP TYR GLU ILE THR ILE ASN SER LEU HIS ASP PHE GLY SER SER THR SER LYS PHE THR LEU ASN ASN GLN GLN ASN V132 I135 P139 L142 N143 L144 L155 K156 W157 N158 F164 R167 S168 N169 E173 L177 S181 L184 V185 N195 D198

H201 R221 D225 N226 F229 L281 I282 G283 H284 T285 N286 E295 T318 E319 D320 N321 V326 T343 H344 D345 I349 L361 R365 Y369 E373 S374 F375 K383 R384 A385 GLU ALA PRO THR N390 F397 N402 L410 T435 P436 T437

S438 F439 K440 V441 K442 D443 I444 N445 S446 T447 A448 V449 A460 C466 I470 K471 K472 S473 N474 S475 V476 Q477 E478 Q479 R480 K485 G486 N489 L493 V494 A495 L496 D497 N500 P501 Y502 T503 L504 Y505 R508 I509 R510 C511 S512 T513 E514 K521 W522 S523 N524 K525

H528 L529 E532 A533 SER PRO SER LYS GLY PRO ASP THR ARG GLU TRP SER SER GLY LYS ASN LEU ILE ILE TYR TRP LYS PRO LEU PRO ILE ALA ASN GLY LYS ILE LEU SER TYR ASN VAL SER CYS SER SER ASP GLU GLU THR GLN SER LEU SER GLU LEU ILE SER GLU GLU ASP LEU HIS HIS HIS HIS HIS HIS

PRO ASP PRO GLN HIS LYS ALA GLU ILE ARG LEU ASP LYS ASN ASP TYR ILE ILE SER VAL ALA LYS ASN SER VAL GLY SER SER PRO CYS LEU MET ASP TRP ARG LYS PRO SER VAL ASN SER THR GLU VAL ILE GLU PRO ASN ASP ASP GLU LYS ILE GLN GLU VAL VAL MET GLY LYS ILE LEU LEU THR TRP

HIS TYR ASP THR ASN MET THR CYS ASP TYR VAL ILE GLY TYR ILE LEU GLU GLU ALA PRO ILE VAL ALA PRO ASN PHE THR VAL GLU ASP TRP ARG LYS VAL PRO SER ASN SER THR ALA ASP SER LEU LEU VAL LYS TRP GLU ASP ILE PRO VAL GLU GLU LEU ARG GLY PHE ARG TYR ASN PHE PHE LEU TYR GLY ARG ASN GLN

GLY TYR GLN LEU LEU ARG SER MET ILE GLY TYR ILE GLU GLU LEU ALA PRO ILE VAL ALA PRO ASN PHE THR VAL GLU ASP TRP ARG LYS VAL PRO SER ASN SER THR ALA ASP SER LEU LEU VAL LYS TRP GLU LYS ILE PRO VAL GLU GLU LEU ARG GLY PHE LEU ARG GLY TYR LEU PHE TYR PHE GLY LYS GLY GLU

ARG ASP THR SER LYS MET ARG VAL LEU GLU SER GLY ARG SER ASP ILE LYS VAL ASN ILE THR ASP ILE SER GLN LYS THR LEU ARG ILE ALA ASP LEU GLN GLY LYS THR SER TYR HIS LEU VAL LEU ARG ALA TYR THR ASP GLY GLY VAL GLY PRO GLU LYS SER MET TYR VAL

VAL THR LYS GLU ASN SER GLU GLN LYS LEU ILE SER GLU GLU ASP LEU GLU HIS HIS HIS HIS HIS HIS

● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

50%

Chain E:

100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain F: 50% 50%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain G: 100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain H: 100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain I: 100%

NAG1 NAG2

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain J: 100%

NAG1 NAG2
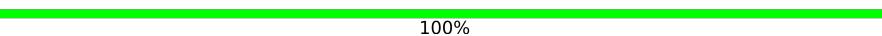
4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	250735	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 $(e^-/\text{Å}^2)$	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	1.385	Depositor
Minimum map value	-0.645	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.23	0/3256	0.44	0/4442
2	D	0.23	0/1446	0.36	0/1959
3	C	0.23	0/1664	0.42	0/2284
4	B	0.24	0/3279	0.45	0/4467
All	All	0.23	0/9645	0.43	0/13152

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 ⓘ

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	3167	0	3101	42	0
2	D	1416	0	1402	14	0
3	C	1607	0	1556	9	0
4	B	3197	0	3159	42	0
5	E	28	0	25	0	0
5	F	28	0	25	1	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	28	0	25	0	0
6	A	70	0	65	1	0
6	C	14	0	13	0	0
All	All	9639	0	9446	104	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 (104) 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:B:466:CYS:HA	4:B:511:CYS:HB3	1.49	0.93
4:B:349:ILE:HB	4:B:397:PHE:HB3	1.73	0.69
1:A:325:ARG:HH21	1:A:409:SER:HA	1.61	0.66
1:A:499:VAL:HA	1:A:504:PRO:HA	1.80	0.64
4:B:144:LEU:HD12	4:B:155:LEU:HD13	1.79	0.64
1:A:345:ARG:HH22	1:A:419:CYS:HB3	1.63	0.64
2:D:42:GLN:HE21	2:D:155:LYS:HG2	1.63	0.64
4:B:466:CYS:CA	4:B:511:CYS:HB3	2.26	0.63
1:A:423:ALA:HB1	1:A:426:PRO:HG3	1.82	0.62
4:B:510:ARG:HD2	4:B:522:TRP:HE1	1.64	0.62
4:B:177:LEU:HB3	4:B:181:SER:HA	1.80	0.62
4:B:435:THR:HB	4:B:521:LYS:HB3	1.80	0.62
2:D:151:LEU:HB2	4:B:326:VAL:HG21	1.81	0.61
4:B:318:THR:HG22	4:B:319:GLU:H	1.66	0.61
1:A:341:THR:OG1	1:A:344:TYR:O	2.18	0.59
1:A:349:LEU:HD22	1:A:387:LEU:HD22	1.85	0.58
4:B:320:ASP:OD1	4:B:321:ASN:ND2	2.37	0.58
1:A:160:LEU:HB3	1:A:172:CYS:HB3	1.87	0.57
1:A:156:THR:HG22	1:A:202:ASN:HB3	1.87	0.57
2:D:73:LEU:HD13	2:D:127:MET:HG2	1.87	0.56
3:C:190:ASN:HB3	5:F:1:NAG:C7	2.35	0.56
4:B:184:LEU:HD13	4:B:185:VAL:HG13	1.87	0.56
1:A:193:ASN:OD1	2:D:19:ARG:NH1	2.36	0.56
1:A:262:ARG:NH1	1:A:266:ALA:O	2.39	0.56
1:A:228:LEU:HD12	1:A:242:LEU:HD11	1.87	0.55
1:A:364:LEU:HD11	1:A:405:LEU:HD22	1.88	0.55
4:B:502:TYR:HD2	4:B:529:LEU:HD23	1.71	0.54
4:B:369:TYR:HB3	4:B:410:LEU:HD11	1.90	0.54
4:B:466:CYS:HA	4:B:511:CYS:CB	2.32	0.54
1:A:246:ASN:HB2	1:A:250:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:O	6:A:704:NAG:O3	2.20	0.52
4:B:283:GLY:O	4:B:285:THR:OG1	2.24	0.52
4:B:173:GLU:OE2	4:B:221:ARG:NE	2.35	0.52
1:A:256:LYS:NZ	1:A:303:LYS:O	2.39	0.52
4:B:361:LEU:HB3	4:B:365:ARG:HG3	1.91	0.52
4:B:282:ILE:HG23	4:B:283:GLY:H	1.75	0.52
2:D:89:ARG:HG2	2:D:144:ILE:HD11	1.92	0.51
1:A:209:SER:OG	1:A:210:ASP:N	2.44	0.51
1:A:493:LEU:HD11	1:A:509:SER:HB2	1.93	0.51
2:D:76:ASN:ND2	2:D:172:SER:OG	2.44	0.50
4:B:281:LEU:HB3	4:B:286:ASN:H	1.76	0.50
4:B:470:ILE:HG13	4:B:480:ARG:HH21	1.76	0.50
1:A:292:PHE:N	1:A:321:THR:OG1	2.46	0.49
2:D:34:LEU:HD23	2:D:112:LEU:HD22	1.95	0.49
1:A:230:VAL:HG22	1:A:242:LEU:HD13	1.94	0.48
1:A:451:LYS:HE3	1:A:499:VAL:HG12	1.95	0.48
3:C:284:ASP:OD1	3:C:285:ASN:N	2.45	0.48
4:B:142:LEU:HG	4:B:157:TRP:HA	1.96	0.48
1:A:392:THR:HG23	1:A:394:ASP:H	1.79	0.47
4:B:443:ASP:HB3	4:B:449:VAL:HA	1.95	0.47
1:A:369:THR:HA	1:A:379:ASN:HA	1.97	0.47
4:B:508:ARG:NE	4:B:523:SER:O	2.48	0.47
1:A:157:ASN:HB3	1:A:176:ARG:HH22	1.78	0.47
2:D:74:GLN:HE22	2:D:135:PRO:HD3	1.79	0.47
1:A:497:THR:HB	1:A:507:PRO:HB3	1.96	0.47
4:B:510:ARG:HB3	4:B:522:TRP:CD1	2.50	0.47
2:D:59:ALA:HA	2:D:171:ARG:HH21	1.80	0.46
4:B:226:ASN:HD22	4:B:229:PHE:HB2	1.81	0.46
4:B:501:PRO:O	4:B:503:THR:HG22	2.16	0.46
1:A:201:GLU:HG3	1:A:206:LYS:HB2	1.98	0.46
1:A:452:LYS:HE2	1:A:499:VAL:HG11	1.97	0.46
4:B:472:LYS:HD2	4:B:505:TYR:HE1	1.81	0.46
1:A:446:PRO:HG2	1:A:450:VAL:HB	1.98	0.46
2:D:25:ARG:HH22	2:D:177:ARG:HH22	1.64	0.45
2:D:166:SER:O	2:D:169:THR:OG1	2.33	0.45
1:A:288:ASP:OD1	3:C:220:ARG:NH2	2.39	0.45
4:B:513:THR:OG1	4:B:514:GLU:N	2.50	0.45
3:C:224:VAL:HG11	3:C:278:ILE:HG21	1.99	0.45
3:C:217:SER:OG	3:C:218:ASN:OD1	2.34	0.44
1:A:355:PRO:HD2	1:A:358:GLU:HB2	1.99	0.44
1:A:259:ILE:HB	1:A:272:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:LEU:HD11	2:D:155:LYS:HB3	2.00	0.44
4:B:447:THR:HG22	4:B:448:ALA:H	1.82	0.44
1:A:409:SER:OG	1:A:410:ASP:N	2.50	0.44
4:B:349:ILE:N	4:B:397:PHE:O	2.51	0.44
4:B:500:ASN:HB3	4:B:505:TYR:CE2	2.53	0.44
1:A:210:ASP:OD1	1:A:211:HIS:N	2.51	0.43
3:C:243:PHE:HB2	3:C:290:TRP:CZ3	2.54	0.43
4:B:169:ASN:HB2	4:B:225:ASP:HB2	2.01	0.43
4:B:139:PRO:HG3	4:B:221:ARG:HA	2.01	0.43
4:B:508:ARG:HH11	4:B:525:LYS:HE2	1.84	0.42
1:A:234:GLU:O	1:A:235:GLU:HG2	2.18	0.42
4:B:500:ASN:HB3	4:B:505:TYR:HE2	1.85	0.42
1:A:262:ARG:HB3	1:A:269:TRP:HA	2.02	0.42
1:A:129:PRO:HD2	1:A:209:SER:HB2	2.01	0.42
1:A:352:LYS:HG2	1:A:470:TRP:CH2	2.54	0.42
4:B:383:LYS:HA	4:B:383:LYS:HD2	1.87	0.42
2:D:86:LEU:HD23	2:D:161:VAL:HG22	2.02	0.42
3:C:190:ASN:N	3:C:190:ASN:OD1	2.52	0.42
4:B:343:THR:OG1	4:B:345:ASP:O	2.34	0.42
4:B:436:PRO:HG2	4:B:509:ILE:HD12	2.02	0.42
4:B:373:GLU:OE1	4:B:375:PHE:N	2.54	0.41
1:A:225:PRO:HG2	1:A:299:ILE:HG23	2.03	0.41
1:A:486:LEU:HB2	1:A:492:TYR:CZ	2.56	0.41
1:A:224:PRO:HB2	1:A:314:SER:HB3	2.02	0.41
3:C:135:THR:HG22	3:C:137:ILE:H	1.86	0.41
4:B:485:LYS:HG2	4:B:486:GLY:H	1.86	0.41
4:B:502:TYR:HA	4:B:529:LEU:HD23	2.02	0.41
2:D:95:GLN:HG2	2:D:106:HIS:CE1	2.57	0.40
4:B:158:ASN:HD21	4:B:198:ASP:HB3	1.86	0.40
1:A:417:PRO:HB2	1:A:421:PHE:HB2	2.03	0.40
1:A:426:PRO:HG3	1:A:506:SER:HB3	2.02	0.40
1:A:126:PRO:HG2	1:A:207:VAL:HG12	2.04	0.40
3:C:158:PRO:HG2	3:C:160:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/625 (62%)	367 (94%)	23 (6%)	0	100	100
2	D	172/214 (80%)	170 (99%)	2 (1%)	0	100	100
3	C	197/320 (62%)	190 (96%)	7 (4%)	0	100	100
4	B	394/817 (48%)	363 (92%)	31 (8%)	0	100	100
All	All	1153/1976 (58%)	1090 (94%)	63 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/566 (63%)	354 (99%)	3 (1%)	81	92
2	D	154/190 (81%)	152 (99%)	2 (1%)	69	88
3	C	180/281 (64%)	177 (98%)	3 (2%)	60	84
4	B	368/746 (49%)	364 (99%)	4 (1%)	73	90
All	All	1059/1783 (59%)	1047 (99%)	12 (1%)	74	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	CYS
1	A	322	TYR

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Mol	Chain	Res	Type
1	A	332	PHE
2	D	56	MET
2	D	67	LEU
3	C	164	CYS
3	C	166	ILE
3	C	168	TYR
4	B	164	PHE
4	B	201	HIS
4	B	295	GLU
4	B	511	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	271	GLN
1	A	376	HIS
1	A	485	ASN
2	D	12	HIS
2	D	42	GLN
2	D	76	ASN
2	D	107	GLN
2	D	122	GLN
2	D	145	ASN
2	D	163	GLN
2	D	174	HIS
2	D	182	HIS
3	C	162	ASN
3	C	255	GLN
3	C	256	HIS
4	B	166	HIS
4	B	226	ASN
4	B	313	ASN
4	B	321	ASN
4	B	390	ASN
4	B	403	GLN
4	B	458	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

12 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	$\#\|Z\| > 2$
5	NAG	E	1	5,1	14,14,15	0.54	0	17,19,21	0.65	0
5	NAG	E	2	5	14,14,15	0.30	0	17,19,21	0.51	0
5	NAG	F	1	5,3	14,14,15	0.39	0	17,19,21	0.67	1 (5%)
5	NAG	F	2	5	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	G	1	5,4	14,14,15	0.33	0	17,19,21	0.43	0
5	NAG	G	2	5	14,14,15	0.25	0	17,19,21	0.37	0
5	NAG	H	1	5,4	14,14,15	0.26	0	17,19,21	0.50	0
5	NAG	H	2	5	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	I	1	5,4	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	I	2	5	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	J	1	5,4	14,14,15	0.25	0	17,19,21	0.55	0
5	NAG	J	2	5	14,14,15	0.25	0	17,19,21	0.43	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	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1
5	NAG	F	1	5,3	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	5,4	-	3/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1
5	NAG	I	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5,4	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	E	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C1-C2-N2-C7
5	E	2	NAG	C3-C2-N2-C7
5	F	1	NAG	C3-C2-N2-C7
5	J	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	1	0

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

Oligosaccharide Chain E

Bond lengths   Bond angles

Torsions   **Rings**

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths · Bond angles · Torsions · Rings

5.6 Ligand geometry ⓘ

6 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	$\#|Z| > 2$
6	NAG	A	704	1	14,14,15	0.41	0	17,19,21	0.34	0
6	NAG	A	702	1	14,14,15	0.42	0	17,19,21	0.35	0
6	NAG	C	401	3	14,14,15	0.24	0	17,19,21	0.49	0
6	NAG	A	703	1	14,14,15	0.23	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	701	1	14,14,15	0.43	0	17,19,21	0.40	0
6	NAG	A	705	1	14,14,15	0.20	0	17,19,21	0.38	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	A	704	1	-	0/6/23/26	0/1/1/1
6	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	NAG	C	401	3	-	3/6/23/26	0/1/1/1
6	NAG	A	703	1	-	3/6/23/26	0/1/1/1
6	NAG	A	701	1	-	2/6/23/26	0/1/1/1
6	NAG	A	705	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	701	NAG	O5-C5-C6-O6
6	A	702	NAG	C4-C5-C6-O6
6	A	702	NAG	O5-C5-C6-O6
6	A	701	NAG	C4-C5-C6-O6
6	A	703	NAG	O5-C5-C6-O6
6	C	401	NAG	C4-C5-C6-O6
6	A	705	NAG	O5-C5-C6-O6
6	A	703	NAG	C4-C5-C6-O6
6	C	401	NAG	O5-C5-C6-O6
6	A	703	NAG	C3-C2-N2-C7
6	C	401	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	704	NAG	1	0

5.7　Other polymers　ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues　ⓘ

There are no chain breaks in this entry.

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-27227. 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 ⓘ
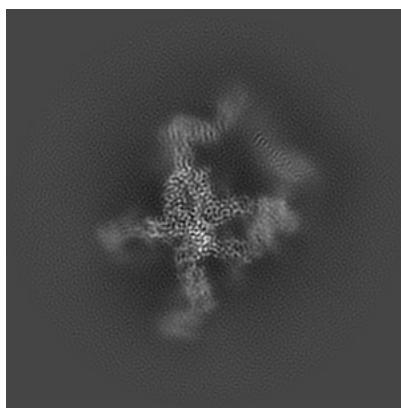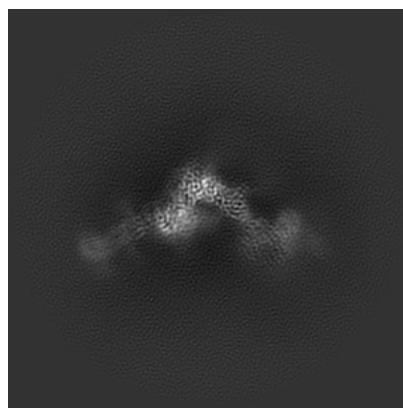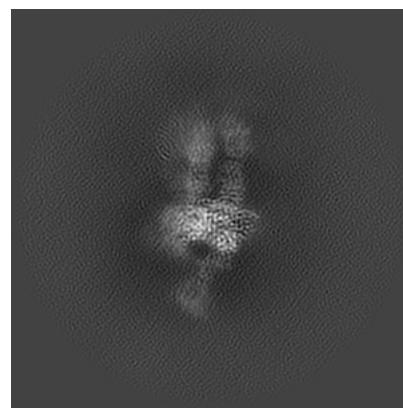
6.1.1　Primary map

X	Y	Z

6.1.2　Raw map

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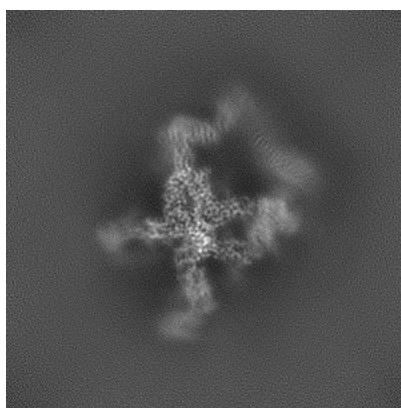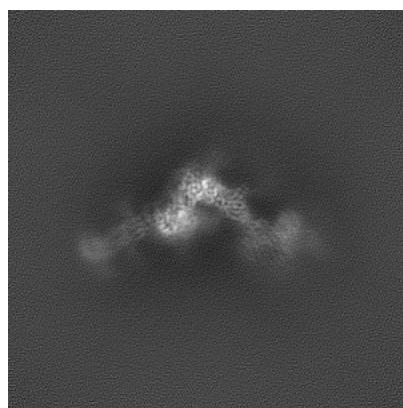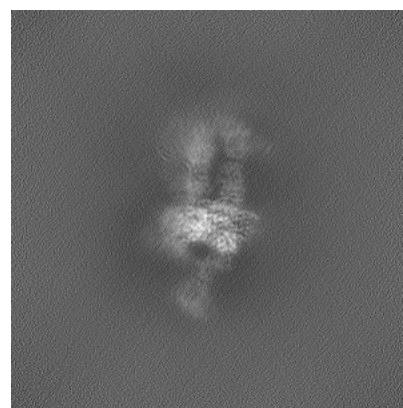
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
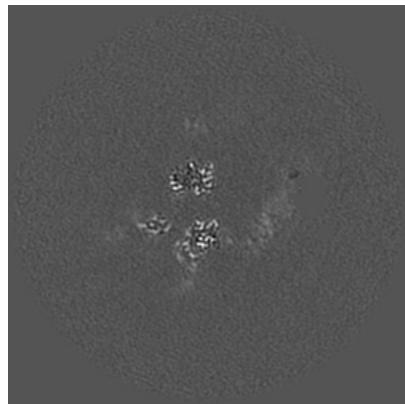
6.2.1 Primary map
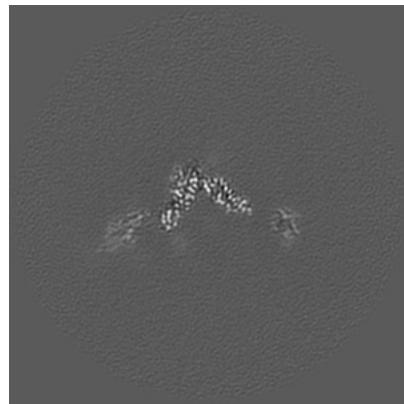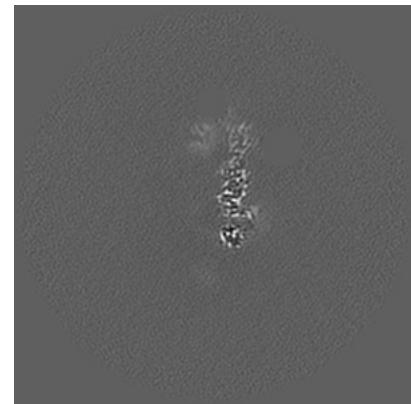
| X Index: 200 | Y Index: 200 | Z Index: 200 |

6.2.2 Raw map
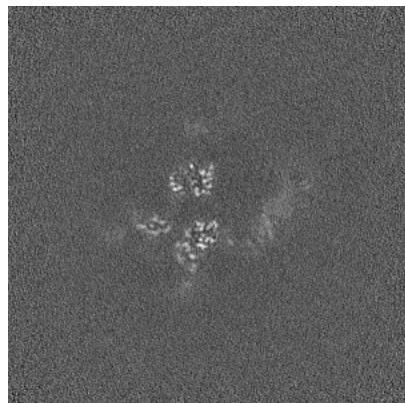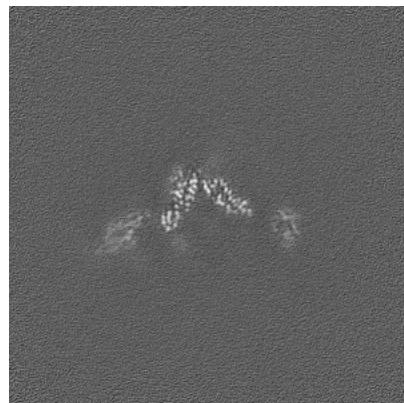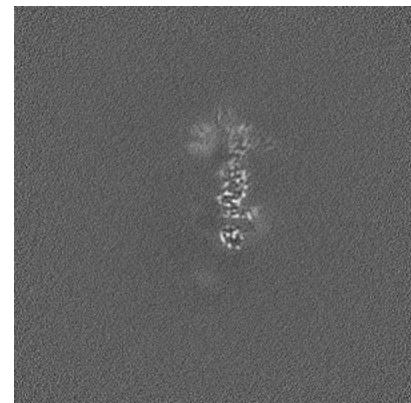
| X Index: 200 | Y Index: 200 | Z Index: 200 |

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

6.3 Largest variance slices ⓘ
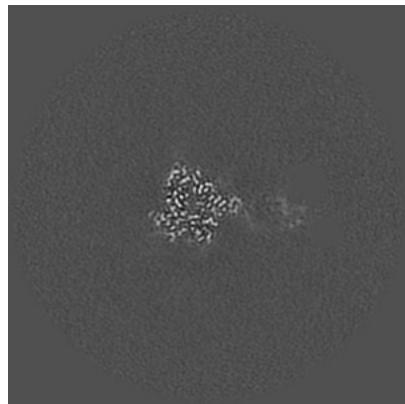
6.3.1 Primary map
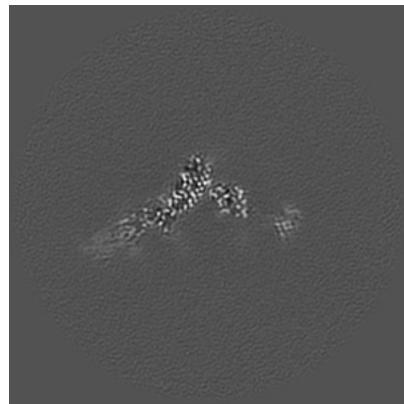
X Index: 213   Y Index: 190   Z Index: 185
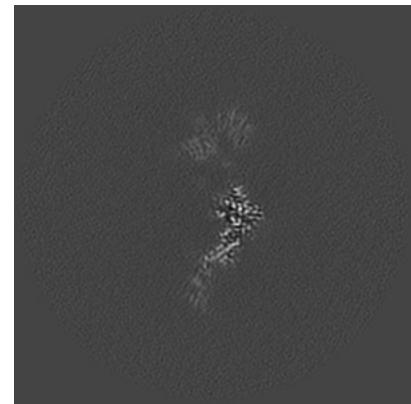
6.3.2 Raw map
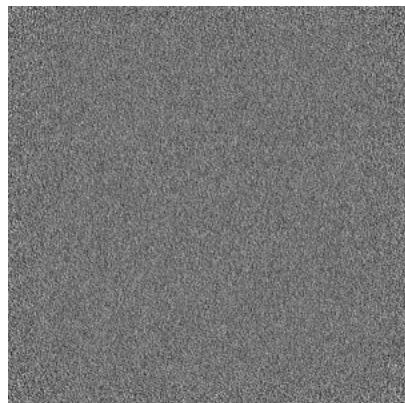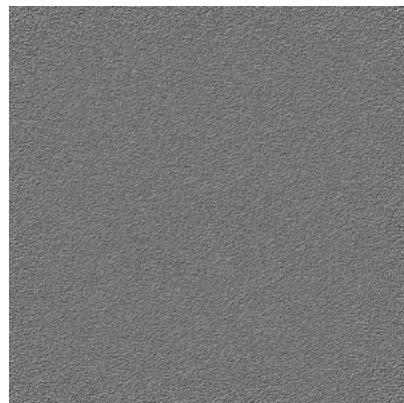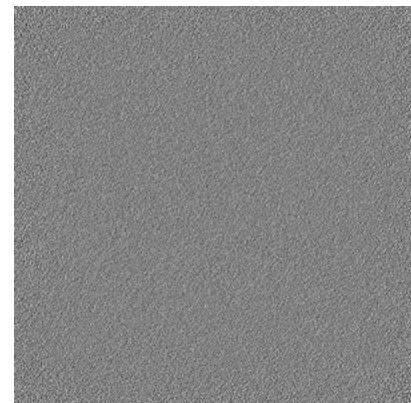
X Index: 0   Y Index: 0   Z Index: 399

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

| X | Y | Z |
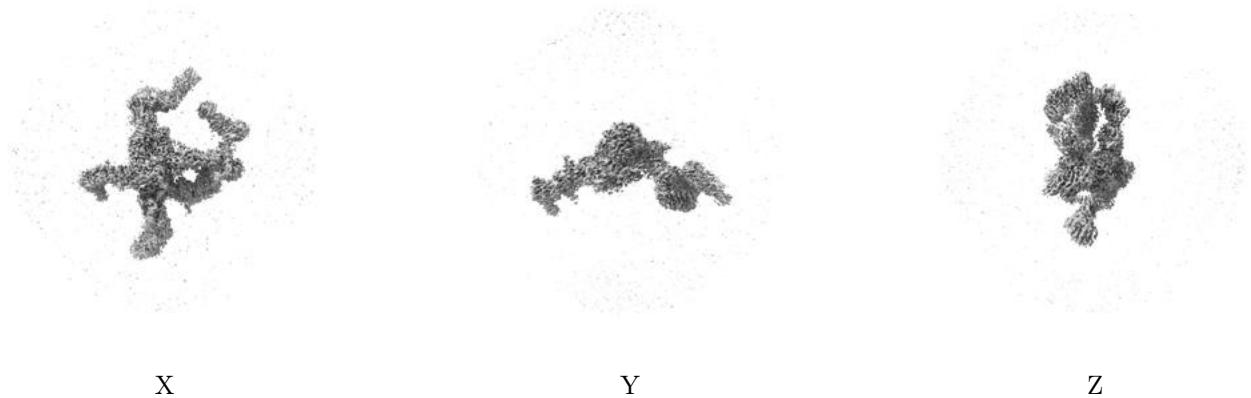
The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

| X | Y | Z |
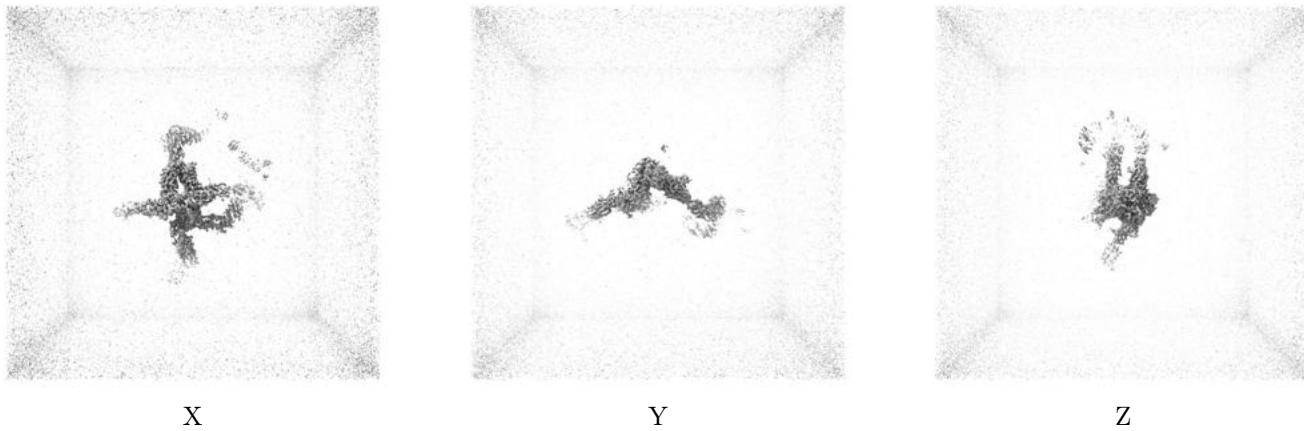
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
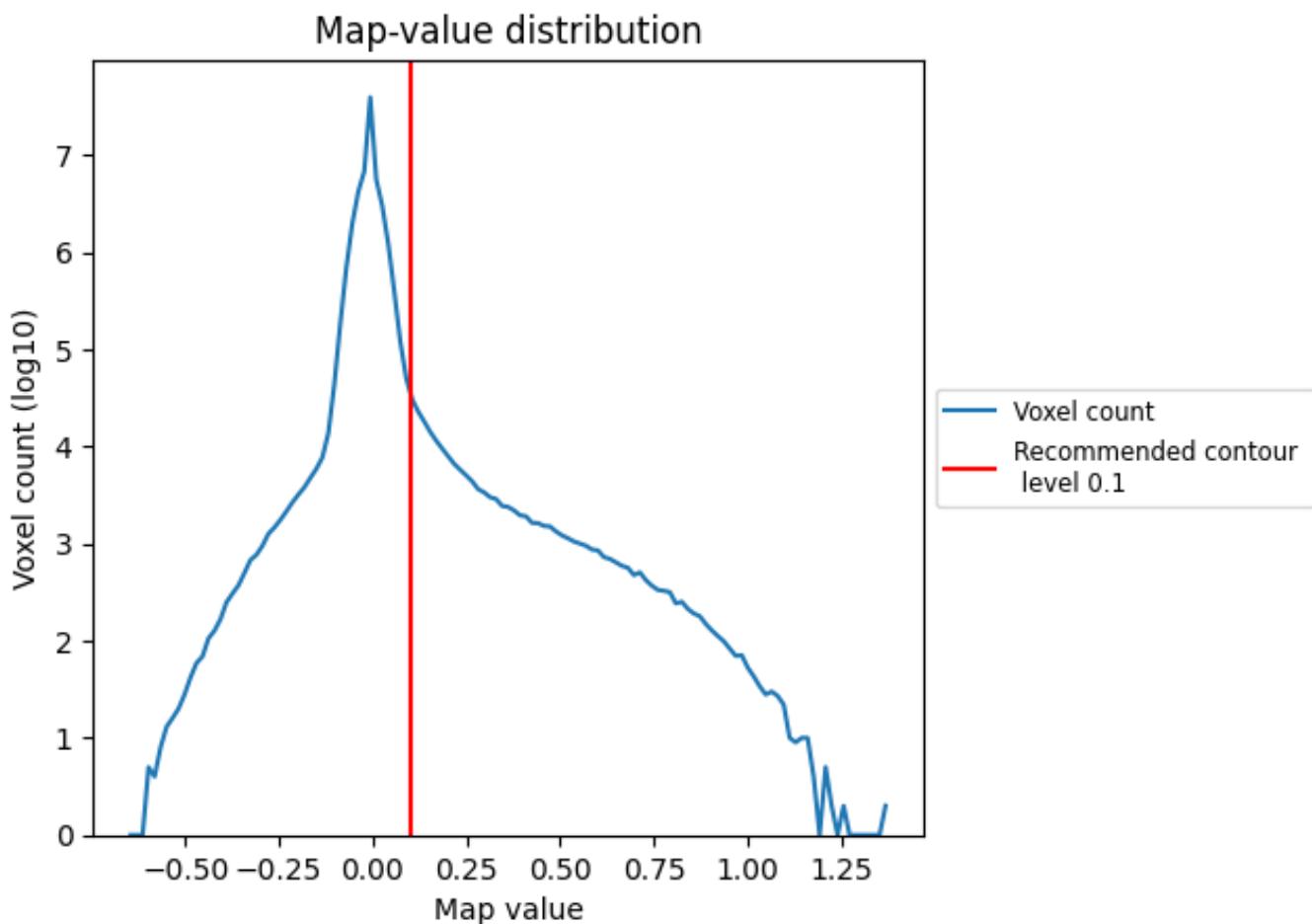
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
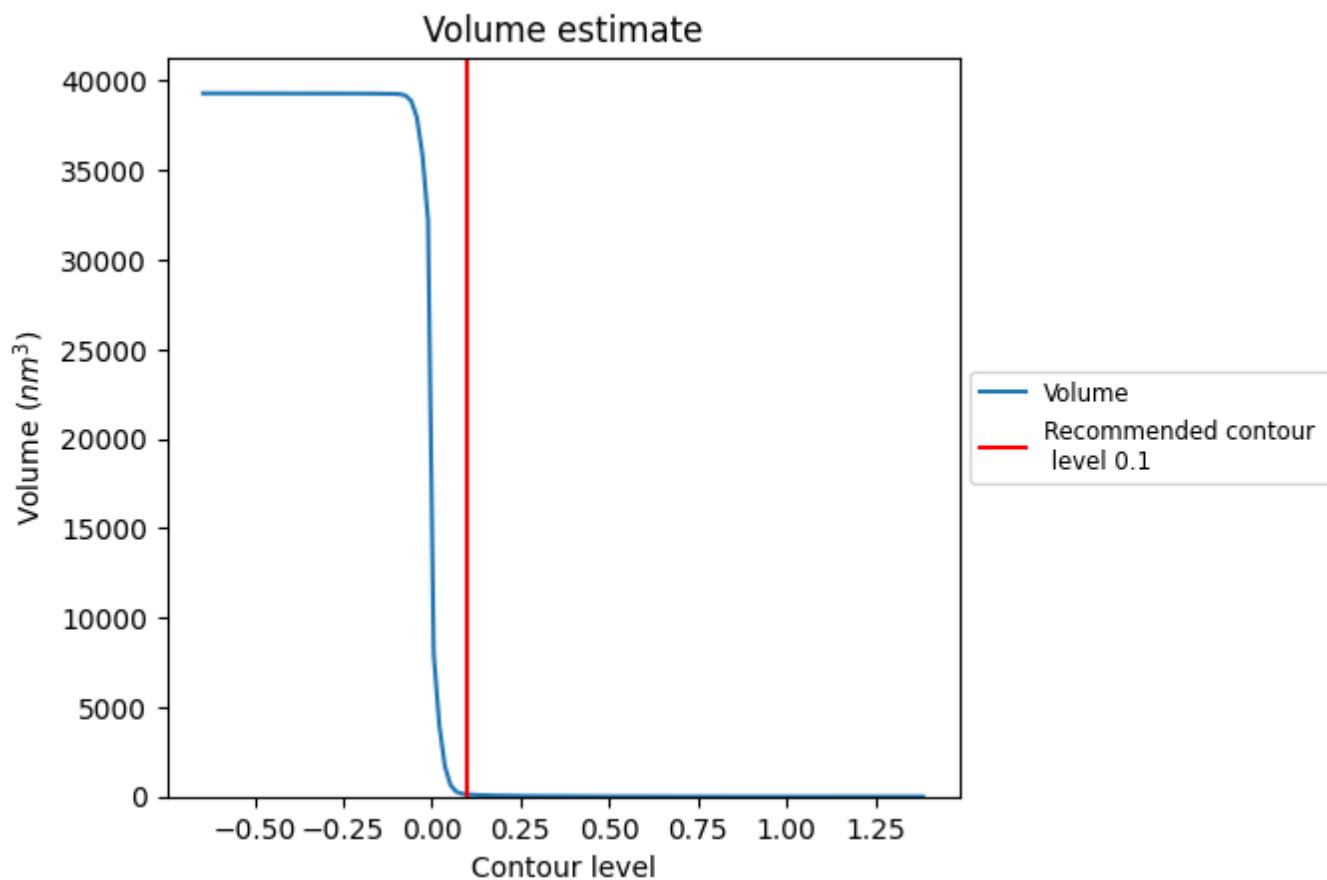
The volume at the recommended contour level is 122 nm^3; this corresponds to an approximate mass of 111 kDa.

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 ⓘ
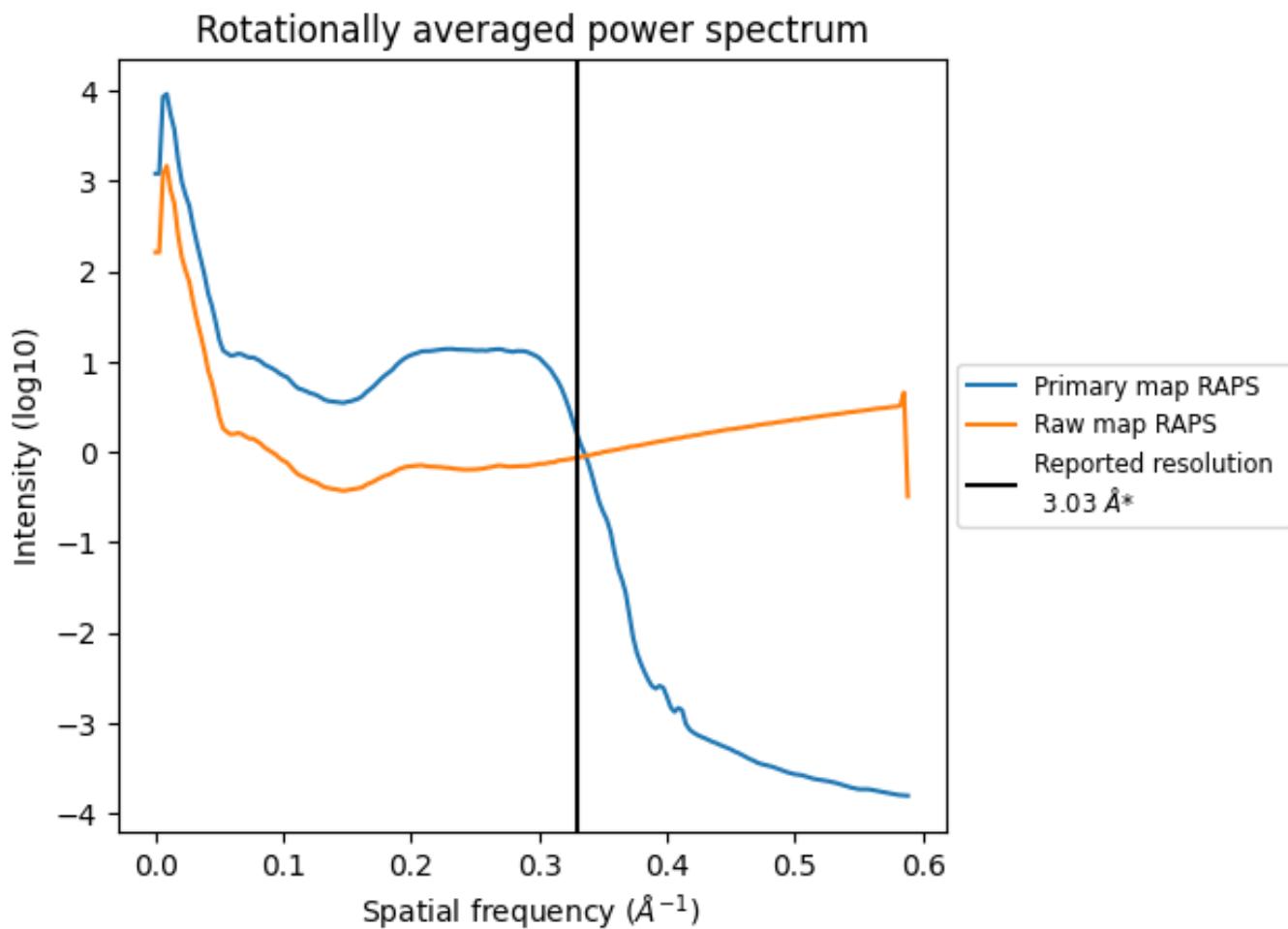
*Reported resolution corresponds to spatial frequency of 0.330 Å^{-1}

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)
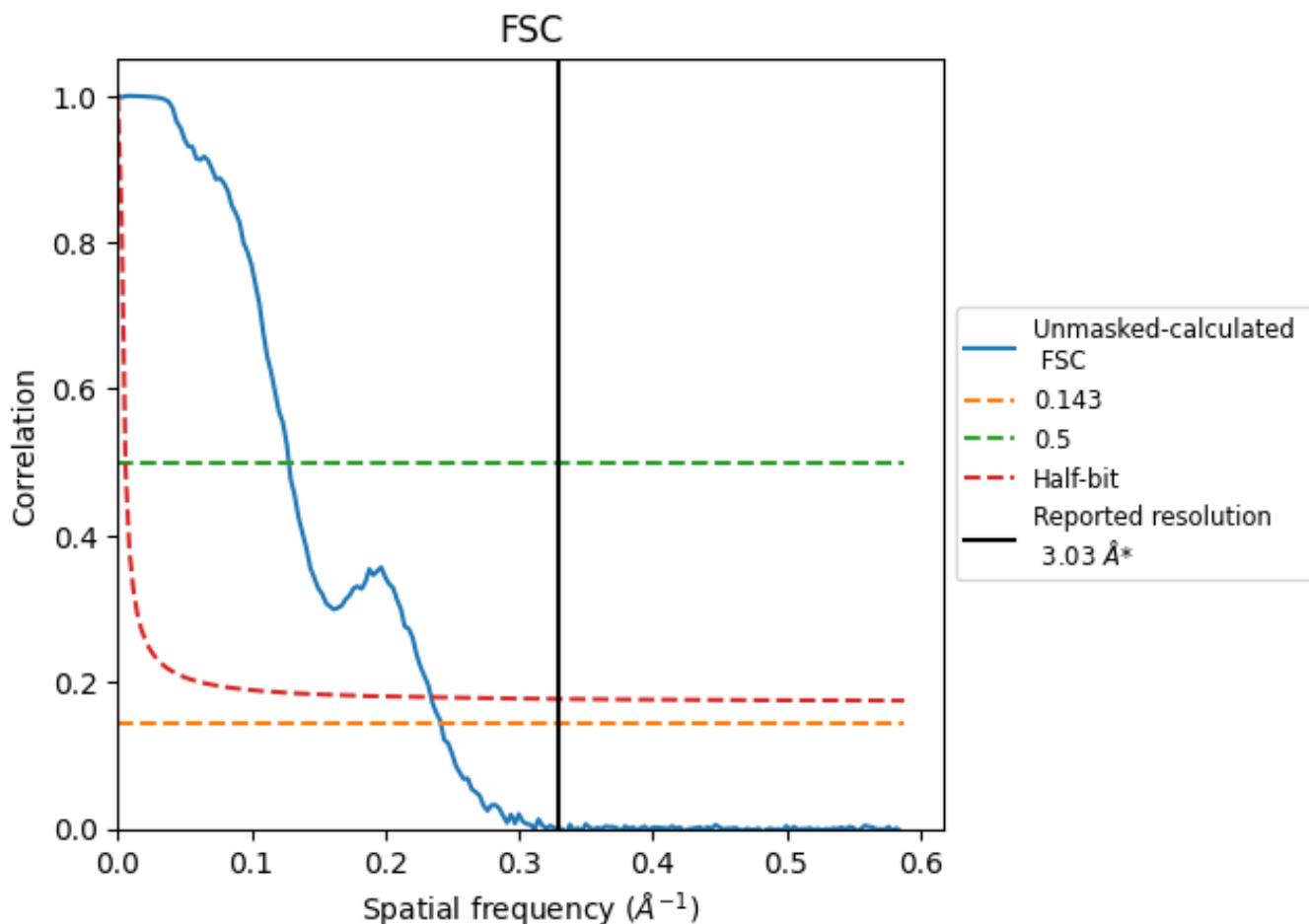
*Reported resolution corresponds to spatial frequency of 0.330 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	7.81	4.27

*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 4.14 differs from the reported value 3.03 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27227 and PDB model 8D74. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)

| X | Y | Z |

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

9.2 Q-score mapped to coordinate model ⓘ

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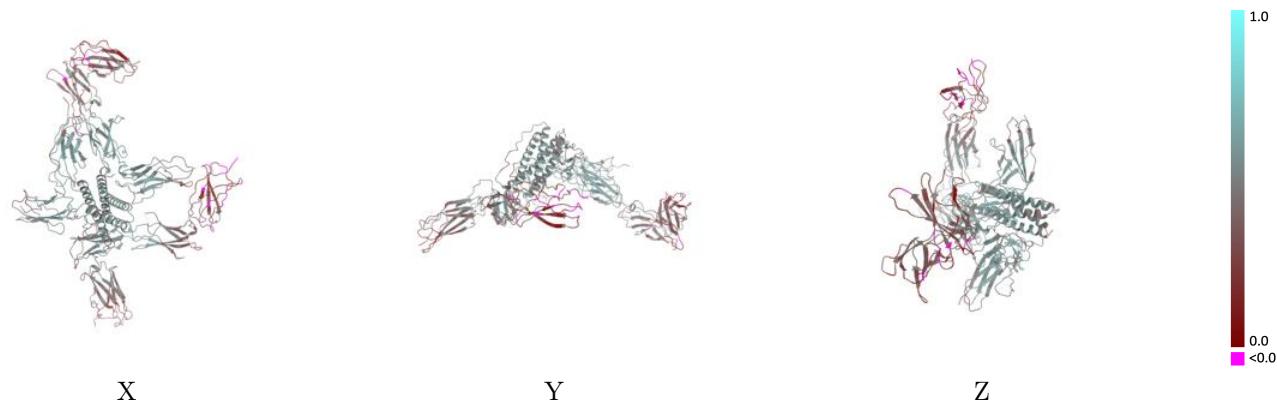
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
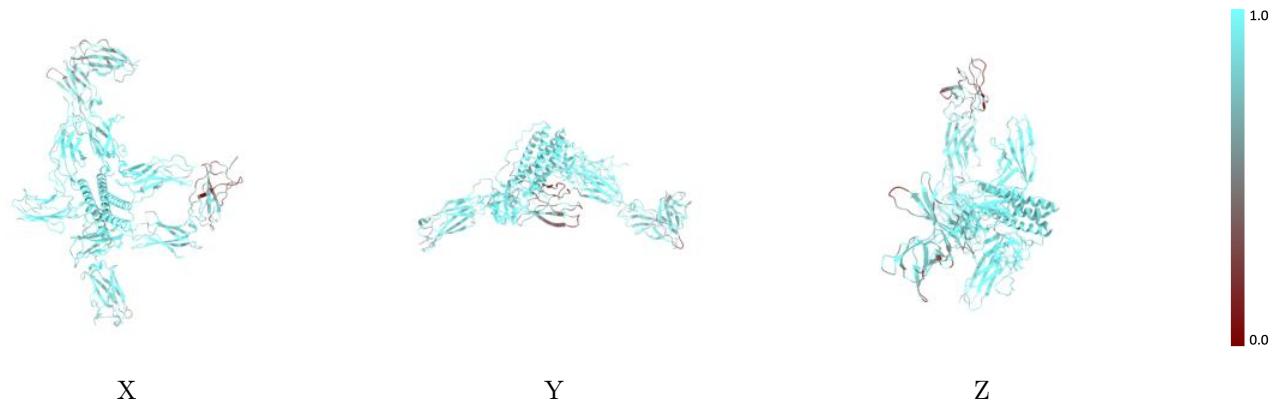
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion ⓘ
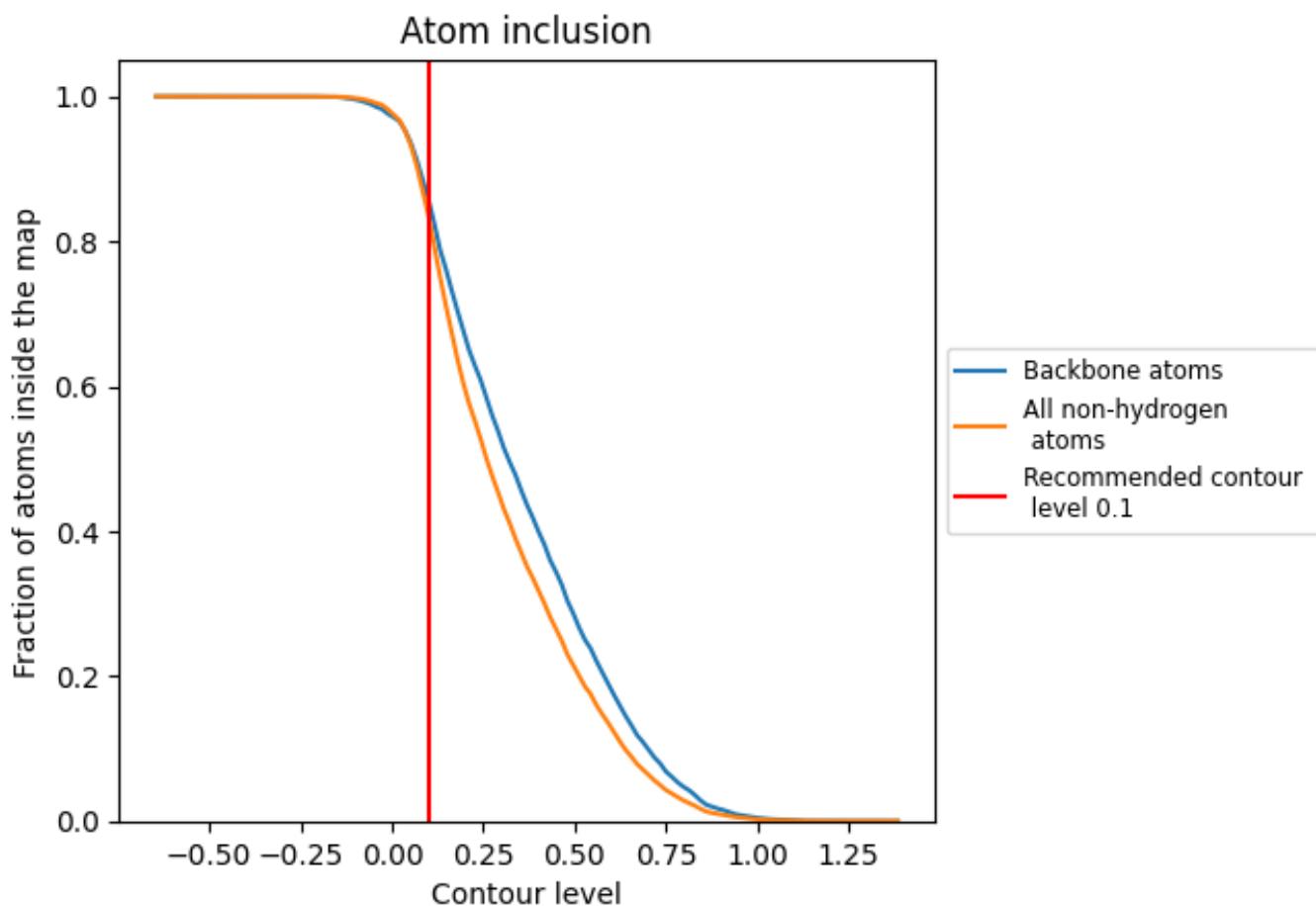
At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8362	0.4320
A	0.8274	0.4210
B	0.7799	0.3720
C	0.9225	0.5130
D	0.9040	0.5160
E	0.2143	0.1980
F	0.8929	0.3680
G	0.7143	0.2760
H	0.7500	0.3180
I	0.7143	0.3210
J	0.8214	0.2680

1.0

0.0
<0.0