wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 07:08 PM EST

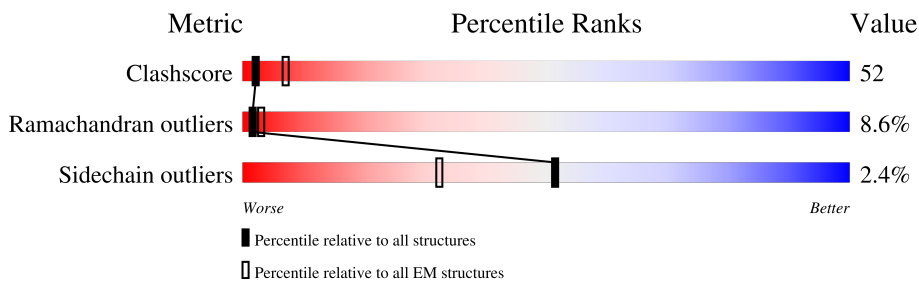|		
PDB ID	:	3J8F
EMDB ID	:	EMD-6147
Title	:	Cryo-EM reconstruction of poliovirus-receptor complex
Authors	:	Strauss, M.; Filman, D.J.; Belnap, D.M.; Cheng, N.; Noel, R.T.; Hogle, J.M.
Deposited on	:	2014-10-20
Resolution	:	3.70 Å(reported)
Based on initial models	:	1HXS, 4FQP

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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 3.70 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		52
Ramachandran outliers		8.6%
Sidechain outliers		2.4%

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	1	302	42% 47% 5% 6%
2	2	272	44% 47% 7% •
3	3	238	46% 45% 7% ••
4	4	69	41% 48% 10% •
5	7	423	55% 27% 38% 7% 28%
6	A	3	100% 67% 33%
6	E	3	100% 33% 33% 33%
7	B	5	80% 80% 20%

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Mol	Chain	Length	Quality of chain
8	C	2	100% / 100%
8	D	2	100% / 50% 50%
9	F	4	100% / 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	F	1	-	-	X	-

2   Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 9263 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	283	Total	C	N	O	S	0	0
			2221	1416	378	422	5		

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	267	Total	C	N	O	S	0	0
			2075	1312	357	392	14		

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	235	Total	C	N	O	S	0	0
			1834	1169	299	349	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	69	Total	C	N	O	S	0	0
			534	333	91	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	MYR	-	modified residue	UNP P03300

- Molecule 5 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	7	306	2342	1478	403	449	12	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	418	HIS	-	expression tag	UNP P15151
7	419	HIS	-	expression tag	UNP P15151
7	420	HIS	-	expression tag	UNP P15151
7	421	HIS	-	expression tag	UNP P15151
7	422	HIS	-	expression tag	UNP P15151
7	423	HIS	-	expression tag	UNP P15151

- Molecule 6 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.
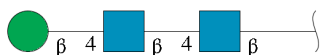
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	A	3	39	22	2	15	0	0
6	E	3	39	22	2	15	0	0

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
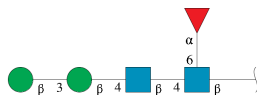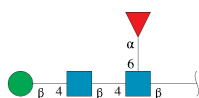

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	B	5	60	34	2	24	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
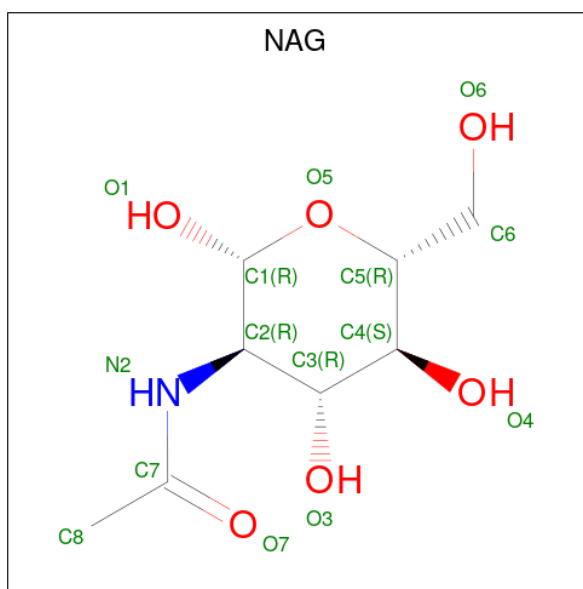
Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	2	Total 28	C 16	N 2	O 10	0	0
8	D	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	F	4	Total 49	C 28	N 2	O 19	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

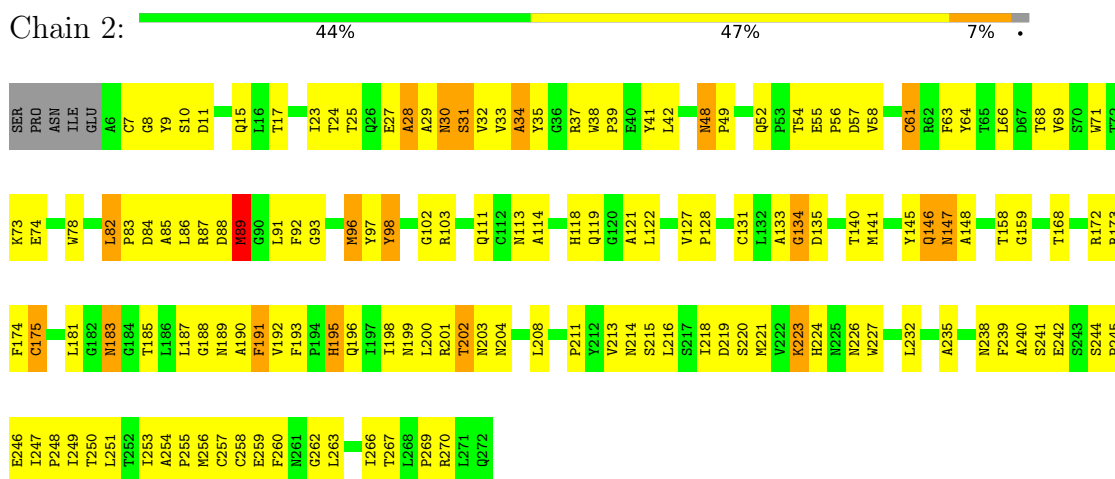| Mol	Chain	Residues	Atoms				AltConf
10	7	1	Total 14	C 8	N 1	O 5	0

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.
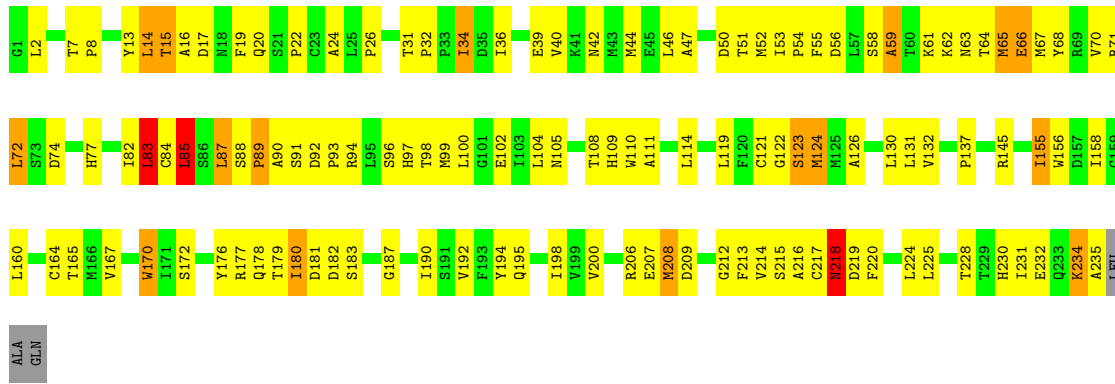
• Molecule 1: Capsid protein VP1
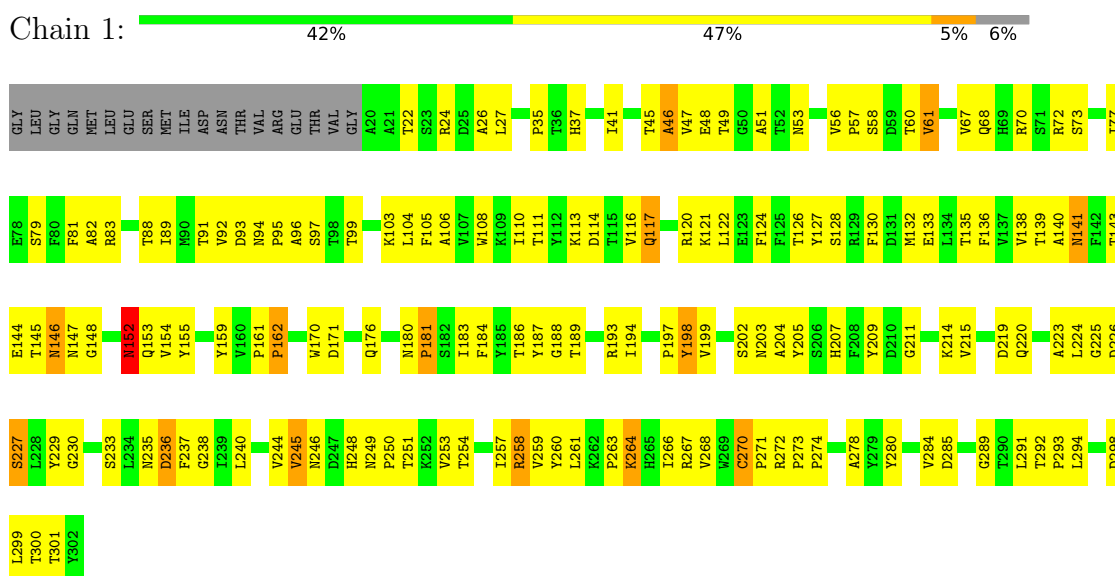
• Molecule 2: Capsid protein VP2

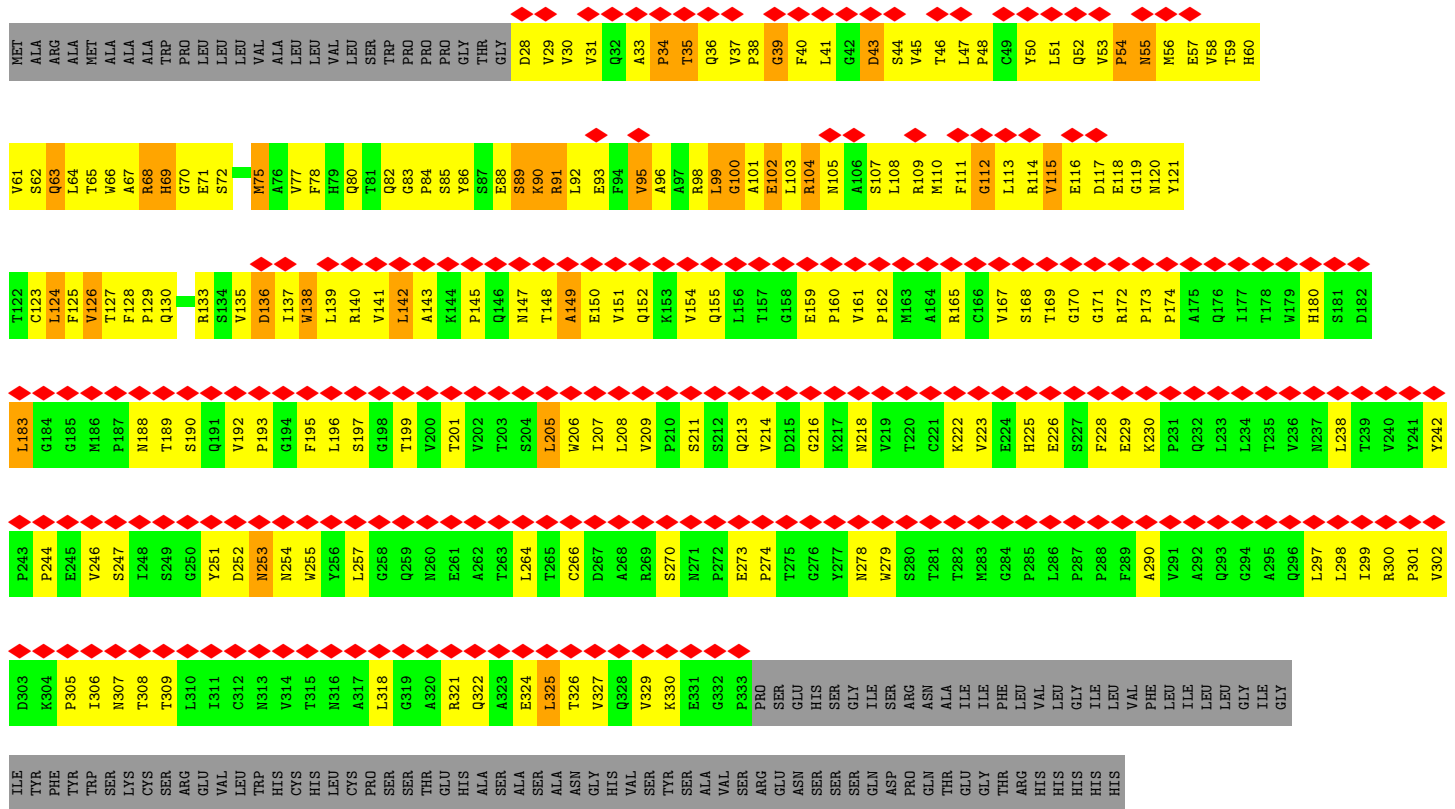• Molecule 3: Capsid protein VP3

Chain 3:

46%　　　　45%　　　　7%

G1 L2 T7 P8 Y13 L14 T15 A16 D17 N18 F19 Q20 S21 P22 C23 A24 L25 P26 T31 P32 P33 I34 D35 I36 E39 V40 K41 N42 M43 M44 E45 L46 A47 D50 T51 M52 I53 P54 F55 D56 L57 S58 A59 T60 K61 K62 N63 T64 M65 E66 M67 Y68 R69 V70 R71

L72 S73 D74 H77 I82 L83 C84 L85 S86 L87 S88 P89 A90 S91 D92 P93 R94 L95 S96 H97 T98 M99 L100 G101 E102 I103 L104 N105 T108 H109 W110 A111 L114 L119 F120 C121 G122 S123 M124 M125 A126 L130 L131 V132 P137 R145 I155 W156 D157 I158 G159

L160 C164 T165 M166 V167 W170 I171 S172 Y176 R177 Q178 T179 I180 D181 D182 S183 G187 I190 S191 V192 F193 Y194 Q195 I198 V199 V200 R206 E207 M208 D209 G212 F213 V214 S215 A216 C217 N218 D219 F220 L224 L225 T228 T229 I231 E232 Q233 K234 A235 LEU

ALA
GLN

• Molecule 4: Capsid protein VP4

Chain 4:

41%　　　　48%　　　　10%

MYR1 Q4 Q8 K9 A12 N15 S16 N17 R18 A19 Y20 G21 G22 S23 T24 I25 N26 Y27 T28 T29 Y32 Y33 R34 D35 S36 A37 S38 N39 A40 A41 S42 K43 Q44 D45 F46 D49 P50 S51 K52 F53 T54 E55 P56 I57 K58 D59 V60 L61 P66 M67 L68 N69

• Molecule 5: Poliovirus receptor

Chain 7:

55%

27%　　　　38%　　　　7%　　　　28%

MET ALA ARG ALA MET ALA ALA TRP PRO LEU LEU LEU VAL ALA LEU LEU VAL LEU SER TRP PRO PRO PRO GLY THR GLY D28 V29 V30 V31 Q32 A33 P34 T35 Q36 V37 P38 G39 F40 L41 G42 D43 S44 V45 T46 L47 P48 C49 Y50 L51 Q52 V53 P54 N55 M56 E57 V58 T59 H60

V61 S62 Q63 L64 T65 W66 A67 R68 H69 G70 E71 S72 M75 A76 V77 F78 H79 Q80 T81 Q82 G83 P84 S85 Y86 S87 E88 S89 K90 R91 L92 E93 F94 V95 A96 A97 R98 L99 G100 A101 E102 L103 R104 N105 A106 S107 L108 R109 M110 F111 G112 L113 R114 V115 E116 D117 E118 G119 N120 Y121

T122 C123 L124 F125 V126 T127 F128 P129 Q130 R133 S134 V135 D136 I137 W138 L139 R140 V141 L142 A143 K144 P145 Q146 N147 T148 A149 E150 V151 Q152 K153 V154 Q155 L156 T157 G158 E159 P160 V161 P162 M163 A164 R165 C166 V167 S168 T169 G170 G171 R172 P173 P174 A175 Q176 I177 I178 W179 H180 S181 D182

L183 G184 G185 M186 P187 N188 T189 S190 Q191 V192 P193 G194 F195 L196 S197 G198 T199 V200 T201 V202 T203 S204 L205 W206 I207 L208 V209 P210 S211 S212 Q213 V214 D215 G216 K217 N218 V219 T220 C221 K222 V223 E224 H225 E226 S227 F228 E229 K230 P231 Q232 L233 L234 T235 V236 N237 L238 T239 V240 Y241 Y242

P243 P244 E245 V246 S247 I248 S249 G250 Y251 D252 N253 N254 W255 Y256 L257 G258 Q259 N260 E261 A262 T263 L264 T265 C266 D267 A268 R269 S270 N271 P272 E273 P274 T275 Q276 Y277 N278 W279 S280 T281 T282 M283 G284 P285 L286 P287 P288 F289 A290 V291 A292 Q293 G294 A295 Q296 L297 L298 I299 R300 P301 V302

D303 K304 P305 I306 N307 T308 T309 L310 I311 C312 N313 V314 T315 N316 A317 L318 G319 A320 R321 Q322 A323 E324 L325 T326 V327 Q328 V329 K330 E331 G332 P333 PRO SER GLU HIS SER GLY ILE SER ARG ASN ALA ILE ILE PHE LEU VAL LEU GLY ILE LEU VAL PHE LEU LEU LEU GLY ILE GLY

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

HIS

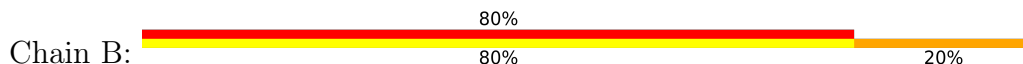• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

100%

67%   33%

NAG1 NAG2 BMA3

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

Chain E:

100%

33%   33%   33%

NAG1 NAG2 BMA3

• Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

80%

80%   20%

NAG1 NAG2 BMA3 BMA4 FUC5

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

Chain C:

100%

100%

NAG1 NAG2

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

Chain D:

100%

50%   50%

NAG1 NAG2

• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

100%

NAG1 NAG2 BMA3 FUC4
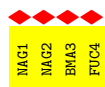
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9248	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	25355	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.00688	Depositor
Map size (Å)	631.04, 631.04, 631.04	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98599994, 0.98599994, 0.98599994	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: BMA, NAG, FUC, MYR

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	1	0.56	0/2284	0.94	0/3124
2	2	0.56	0/2132	0.99	4/2916 (0.1%)
3	3	0.53	0/1881	1.00	6/2562 (0.2%)
4	4	0.61	0/528	0.97	1/714 (0.1%)
5	7	0.54	1/2400 (0.0%)	1.06	4/3286 (0.1%)
All	All	0.55	1/9225 (0.0%)	1.00	15/12602 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	7	136	ASP	C-N	21.37	1.83	1.34

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	7	136	ASP	O-C-N	-40.95	57.18	122.70
5	7	136	ASP	C-N-CA	11.70	150.96	121.70
5	7	136	ASP	CA-C-N	9.80	138.76	117.20
3	3	14	LEU	CA-CB-CG	7.38	132.27	115.30
5	7	138	TRP	CB-CA-C	-6.46	97.47	110.40

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	1	2221	0	2173	205	0
2	2	2075	0	1994	155	0
3	3	1834	0	1816	169	0
4	4	534	0	523	59	0
5	7	2342	0	2292	422	0
6	A	39	0	34	0	0
6	E	39	0	34	2	0
7	B	60	0	52	11	0
8	C	28	0	25	2	0
8	D	28	0	25	1	0
9	F	49	0	43	10	0
10	7	14	0	13	0	0
All	All	9263	0	9024	948	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 52.

The worst 5 of 948 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)
5:7:29:VAL:CG1	5:7:53:VAL:HA	1.26	1.61
5:7:31:VAL:CG1	5:7:135:VAL:CG2	1.76	1.58
5:7:31:VAL:HG13	5:7:135:VAL:CG2	1.35	1.51
5:7:64:LEU:CD2	5:7:103:LEU:HD13	1.44	1.47
5:7:29:VAL:HG11	5:7:53:VAL:CA	1.47	1.45

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	1	281/302 (93%)	206 (73%)	52 (18%)	23 (8%)	1	11
2	2	265/272 (97%)	192 (72%)	51 (19%)	22 (8%)	1	10
3	3	233/238 (98%)	180 (77%)	37 (16%)	16 (7%)	1	15
4	4	66/69 (96%)	42 (64%)	14 (21%)	10 (15%)	0	3
5	7	304/423 (72%)	235 (77%)	41 (14%)	28 (9%)	1	9
All	All	1149/1304 (88%)	855 (74%)	195 (17%)	99 (9%)	2	10

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	37	HIS
1	1	46	ALA
1	1	61	VAL
1	1	113	LYS
1	1	224	LEU

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	1	245/261 (94%)	241 (98%)	4 (2%)	62	80
2	2	227/232 (98%)	222 (98%)	5 (2%)	52	72
3	3	210/212 (99%)	204 (97%)	6 (3%)	42	66
4	4	57/57 (100%)	55 (96%)	2 (4%)	36	63
5	7	263/361 (73%)	256 (97%)	7 (3%)	44	68
All	All	1002/1123 (89%)	978 (98%)	24 (2%)	51	71

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	234	LYS
5	7	63	GLN
4	4	69	ASN

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type
5	7	90	LYS
2	2	146	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
4	4	69	ASN
5	7	52	GLN
5	7	180	HIS
2	2	137	ASN
2	2	95	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 ⓘ

19 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	A	1	6,5	14,14,15	0.59	0	17,19,21	0.91	1 (5%)
6	NAG	A	2	6	14,14,15	0.55	0	17,19,21	0.92	0
6	BMA	A	3	6	11,11,12	0.23	0	15,15,17	0.68	0
7	NAG	B	1	7,5	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
7	NAG	B	2	7	14,14,15	0.55	0	17,19,21	0.79	0
7	BMA	B	3	7	11,11,12	0.33	0	15,15,17	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	BMA	B	4	7	11,11,12	0.66	0	15,15,17	0.75	0
7	FUC	B	5	7	10,10,11	0.72	0	14,14,16	0.62	0
8	NAG	C	1	8,5	14,14,15	0.66	0	17,19,21	0.74	0
8	NAG	C	2	8	14,14,15	0.60	0	17,19,21	0.62	0
8	NAG	D	1	8,5	14,14,15	0.55	0	17,19,21	0.88	1 (5%)
8	NAG	D	2	8	14,14,15	0.56	0	17,19,21	0.67	0
6	NAG	E	1	6,5	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
6	NAG	E	2	6	14,14,15	0.58	0	17,19,21	0.99	1 (5%)
6	BMA	E	3	6	11,11,12	0.33	0	15,15,17	0.66	0
9	NAG	F	1	9,5	14,14,15	0.61	0	17,19,21	0.63	0
9	NAG	F	2	9	14,14,15	0.54	0	17,19,21	0.66	0
9	BMA	F	3	9	11,11,12	0.27	0	15,15,17	0.59	0
9	FUC	F	4	9	10,10,11	0.68	0	14,14,16	0.55	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	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	A	2	6	-	0/6/23/26	0/1/1/1
6	BMA	A	3	6	-	2/2/19/22	1/1/1/1
7	NAG	B	1	7,5	-	0/6/23/26	0/1/1/1
7	NAG	B	2	7	-	2/6/23/26	0/1/1/1
7	BMA	B	3	7	-	2/2/19/22	0/1/1/1
7	BMA	B	4	7	-	1/2/19/22	0/1/1/1
7	FUC	B	5	7	-	-	0/1/1/1
8	NAG	C	1	8,5	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
8	NAG	D	1	8,5	-	0/6/23/26	0/1/1/1
8	NAG	D	2	8	-	2/6/23/26	0/1/1/1
6	NAG	E	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	BMA	E	3	6	-	2/2/19/22	0/1/1/1
9	NAG	F	1	9,5	-	4/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	1/2/19/22	0/1/1/1
9	FUC	F	4	9	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1	NAG	O5-C1-C2	-2.32	107.63	111.29
8	D	1	NAG	C1-O5-C5	2.30	115.31	112.19
6	E	2	NAG	O5-C1-C2	-2.27	107.70	111.29
6	E	1	NAG	O5-C1-C2	-2.18	107.85	111.29
7	B	1	NAG	O5-C5-C6	2.17	110.61	107.20

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	3	BMA	O5-C5-C6-O6
6	A	1	NAG	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
6	A	3	BMA	O5-C5-C6-O6
6	E	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	3	BMA	C1-C2-C3-C4-C5-O5

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1	NAG	5	0
8	C	1	NAG	2	0
9	F	4	FUC	3	0
9	F	2	NAG	5	0
8	C	2	NAG	2	0
7	B	2	NAG	1	0
7	B	3	BMA	4	0
7	B	5	FUC	5	0
9	F	1	NAG	9	0
7	B	4	BMA	3	0
9	F	3	BMA	1	0
6	E	1	NAG	2	0
8	D	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 A

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths — Bond angles — Torsions — Rings

5.6 Ligand geometry ⓘ

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
10	NAG	7	520	5	14,14,15	0.56	0	17,19,21	0.69	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
10	NAG	7	520	5	-	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
10	7	520	NAG	C4-C5-C6-O6
10	7	520	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	136:ASP	C	137:ILE	N	1.83

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-6147. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

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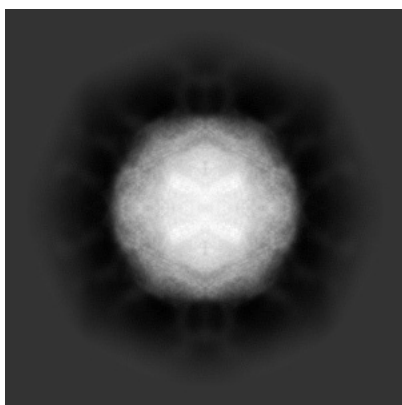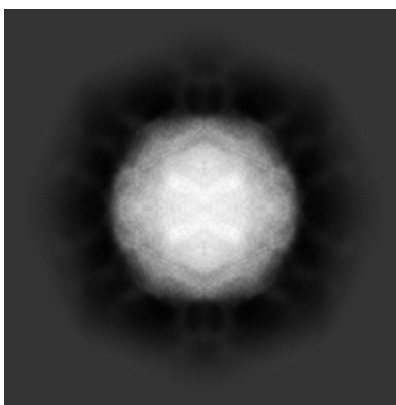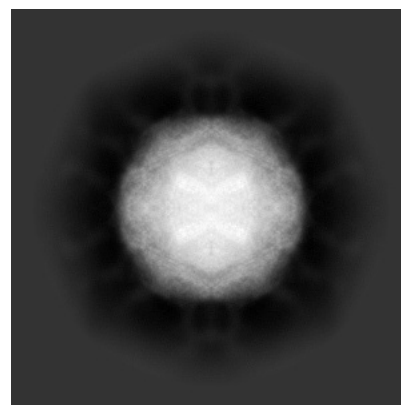
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
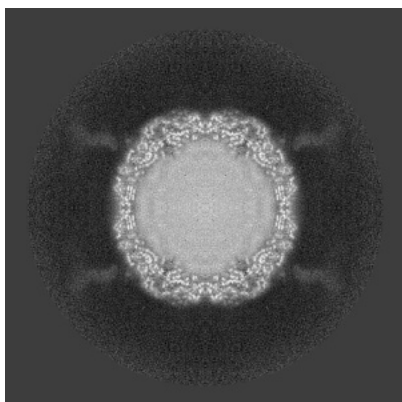
6.2.1 Primary map
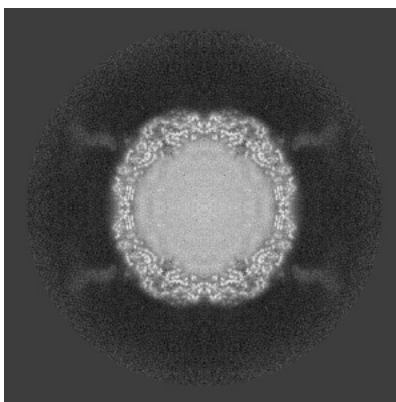
| X Index: 320 | Y Index: 320 | Z Index: 320 |
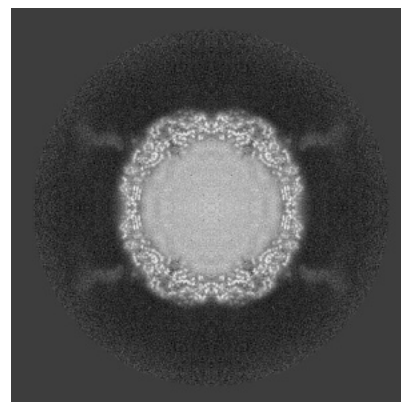
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
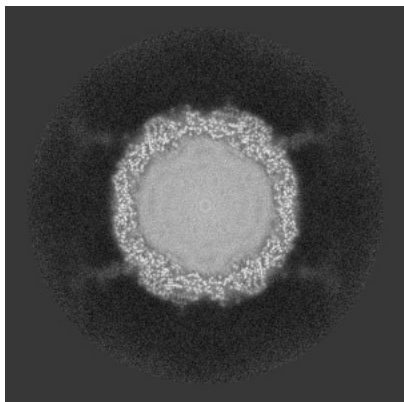
6.3.1 Primary map
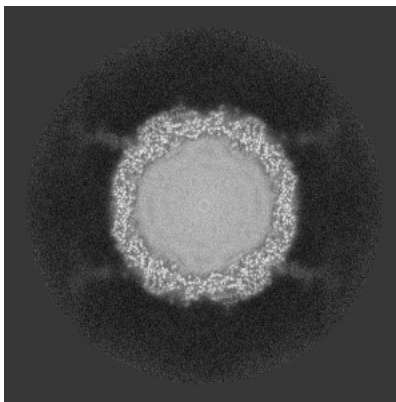
| X Index: 327 | Y Index: 313 | Z Index: 313 |
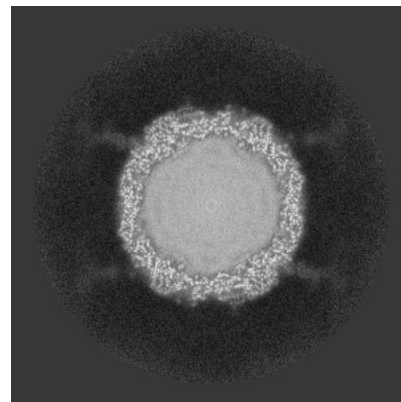
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.00688. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5   Mask visualisation ⓘ

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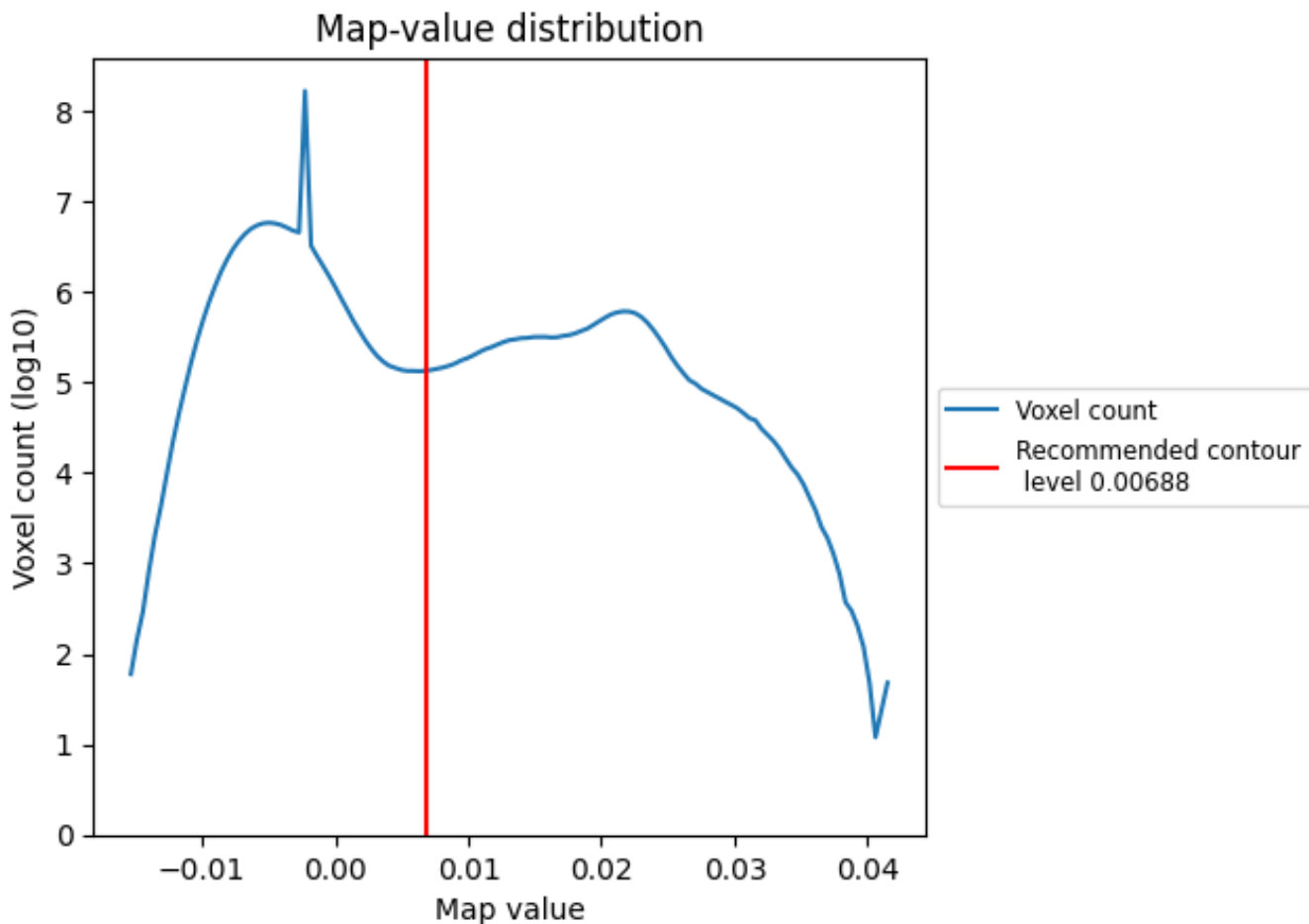
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
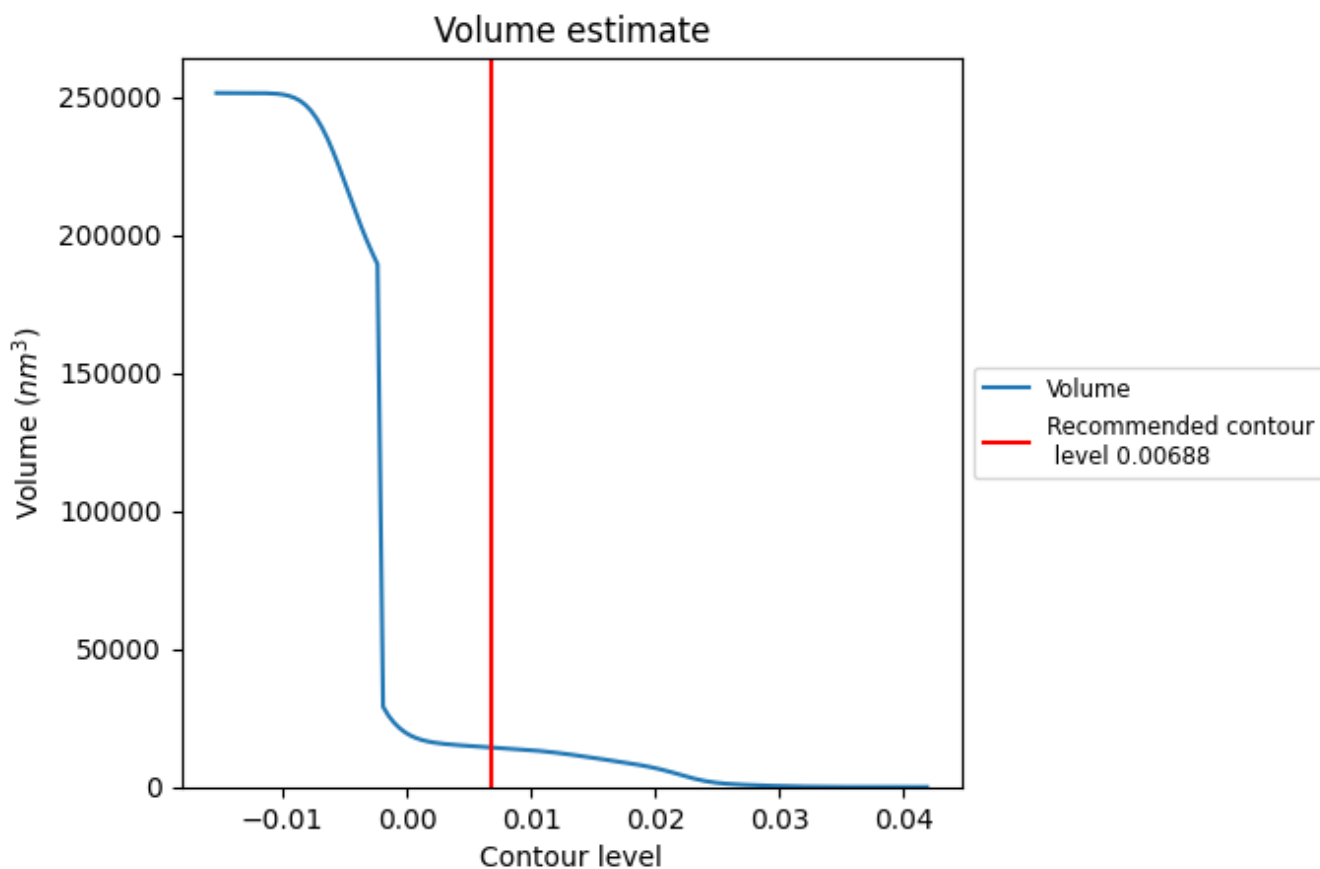
The volume at the recommended contour level is 14336 nm^3; this corresponds to an approximate mass of 12950 kDa.

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)
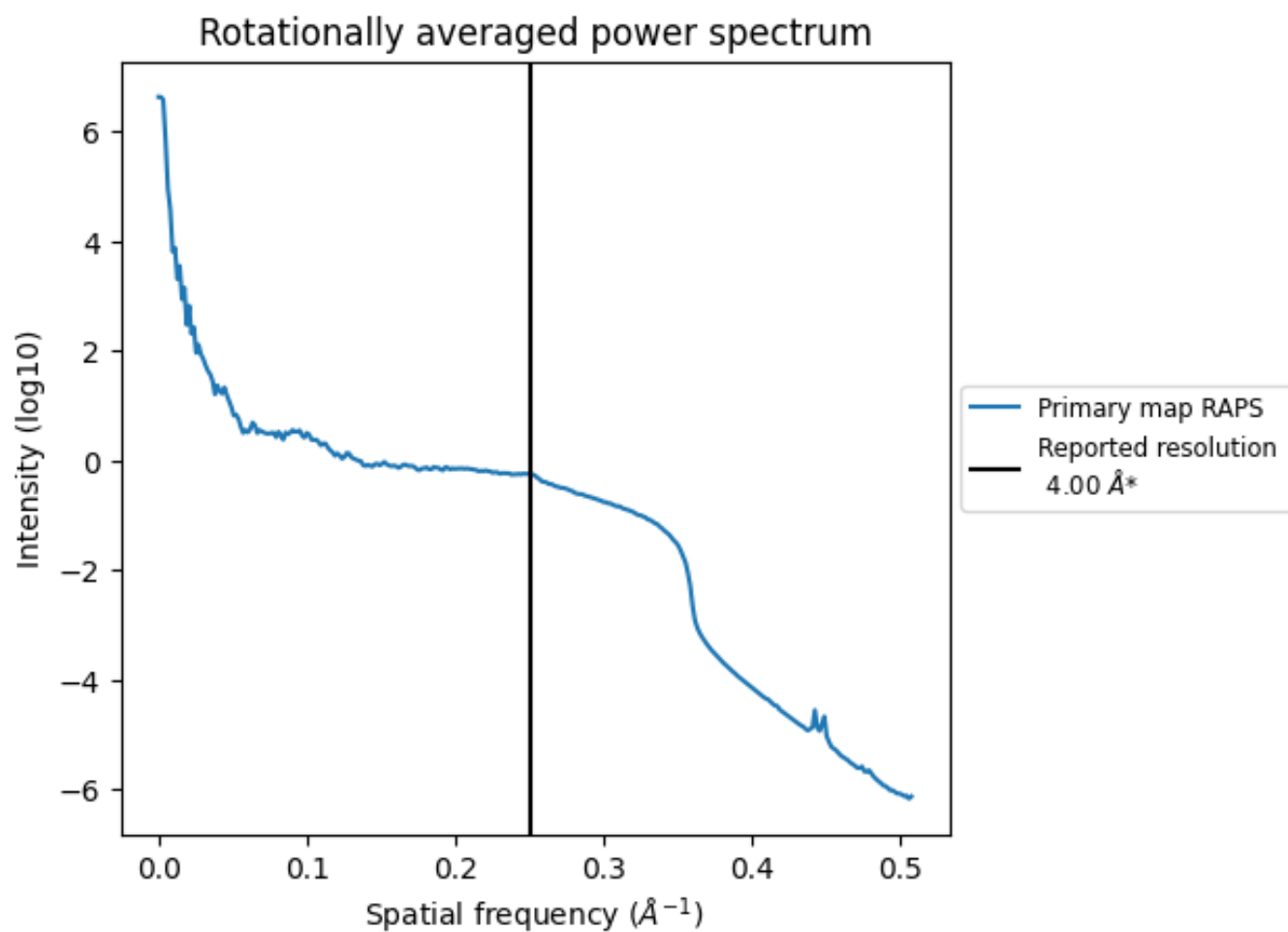
*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-6147 and PDB model 3J8F. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ

| X | Y | Z |

9.1.2 Map-model assembly overlay ⓘ
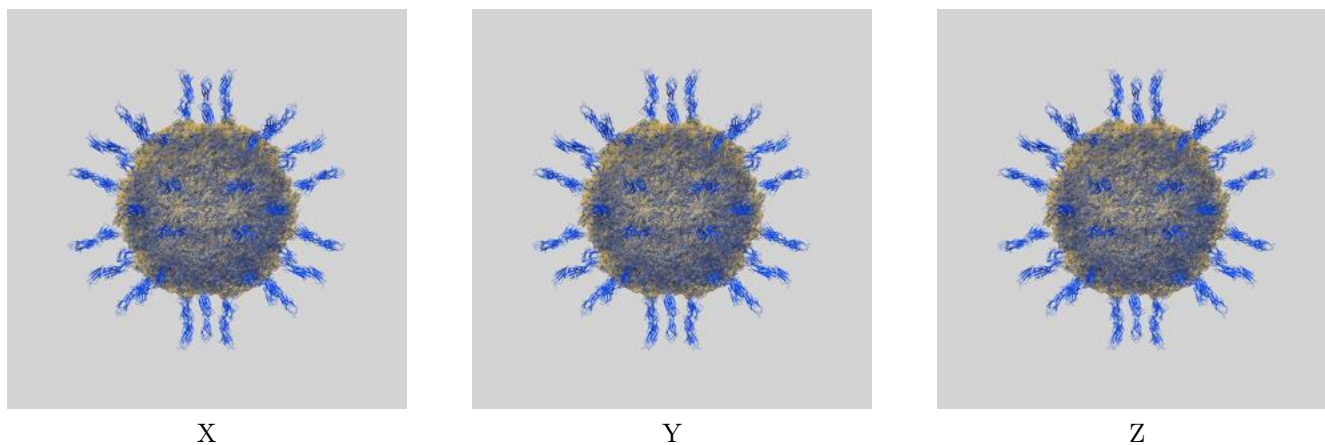
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.00688 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
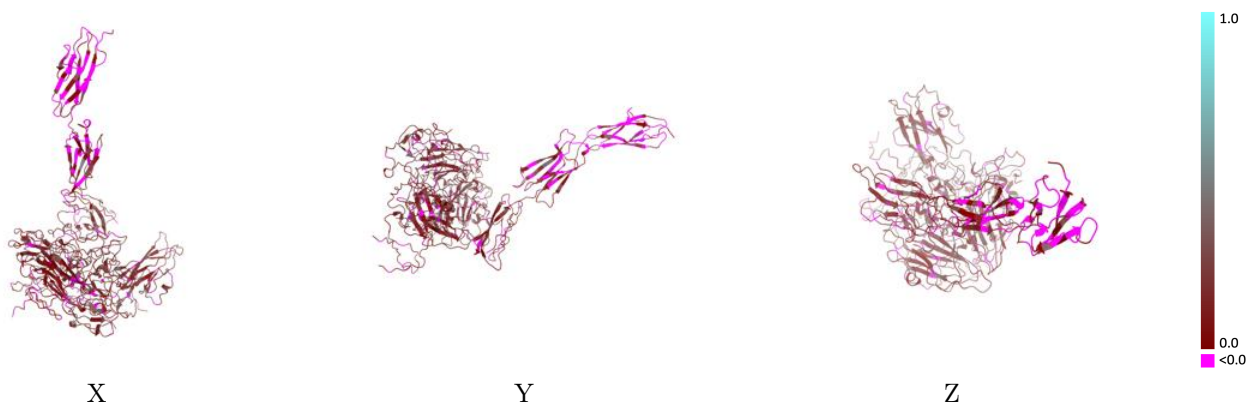
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
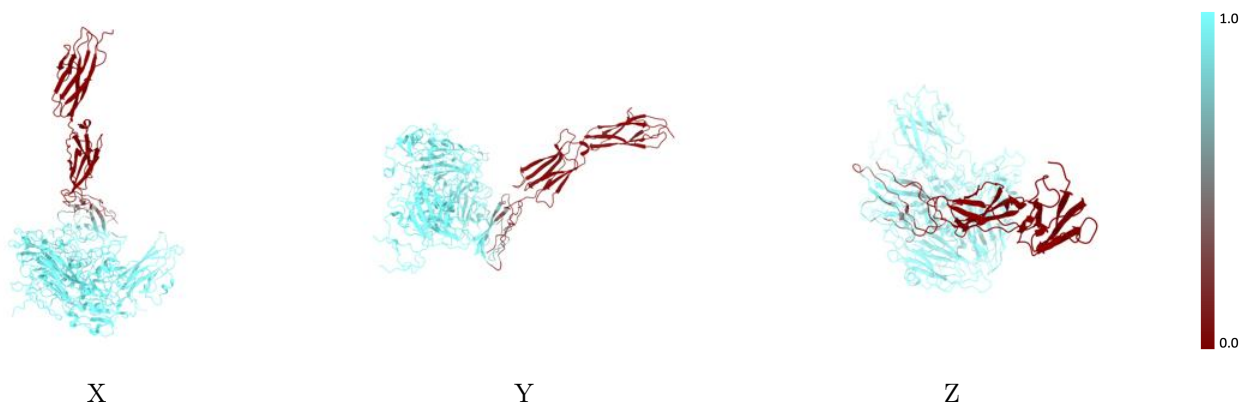
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00688).

9.4　Atom inclusion ⓘ
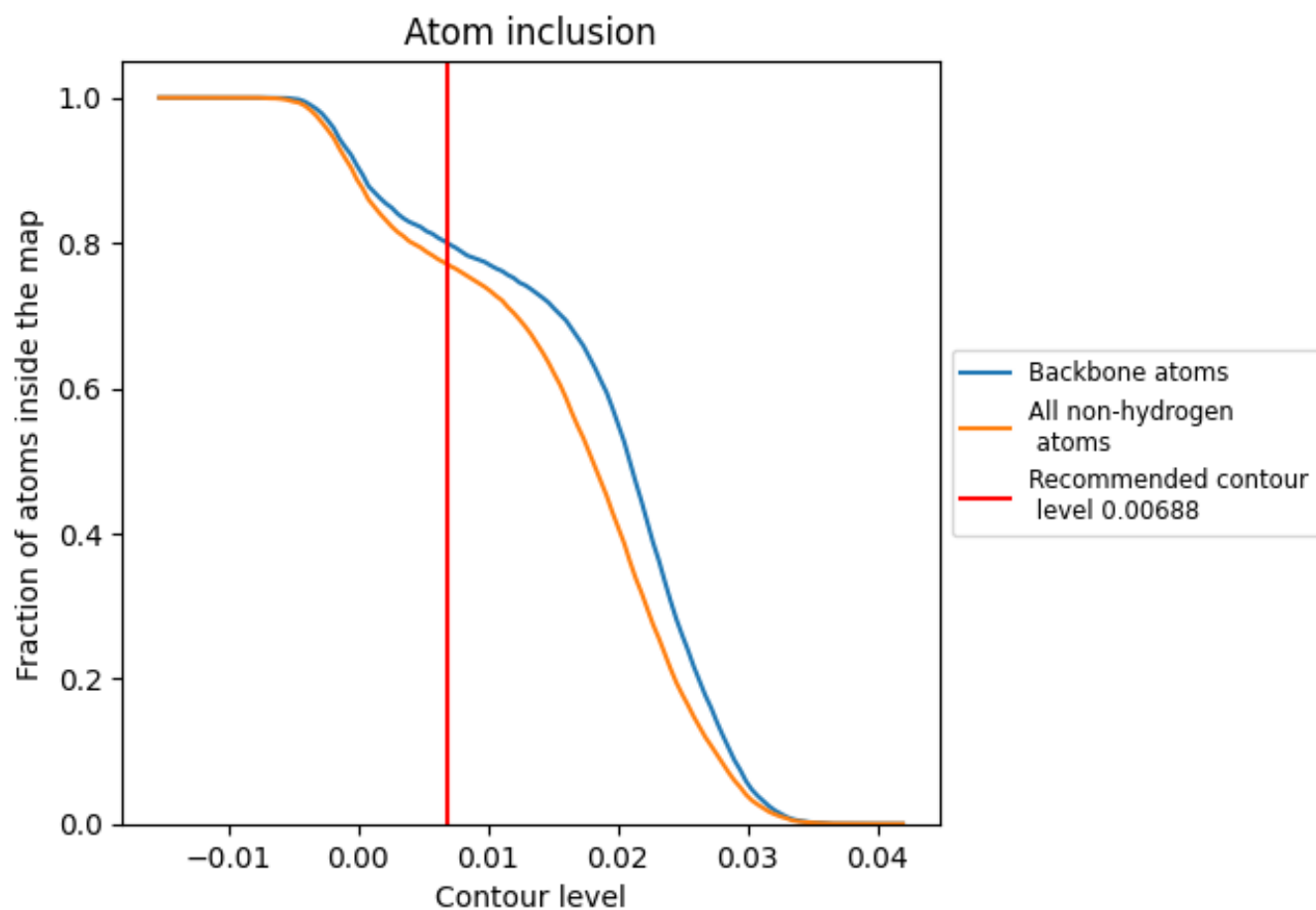
At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00688) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7704	0.1350
1	0.9959	0.1760
2	0.9926	0.1550
3	0.9994	0.1620
4	1.0000	0.1540
7	0.2103	0.0630
A	0.0256	0.0820
B	0.1167	0.2220
C	0.0000	0.0450
D	0.0000	-0.0510
E	0.0000	0.0030
F	0.0000	-0.0290

1.0

0.0
<0.0