wwPDB EM Validation Summary Report (i)

Dec 19, 2022 – 02:35 am GMT

PDB ID	:	7NVM
EMDB ID	:	EMD-12606
Title	:	Human TRiC complex in closed state with nanobody Nb18, actin and PhLP2A bound
Authors	:	Kelly, J.J.; Chi, G.; Bulawa, C.; Paavilainen, V.O.; Bountra, C.; Huiskonen, J.T.; Yue, W.; Structural Genomics Consortium (SGC)
Deposited on	:	2021-03-15
Resolution	:	3.10 Å(reported)

---

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 3.10 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
Ramachandran outliers		0.1%
Sidechain outliers		0.9%

Worse   *Better*

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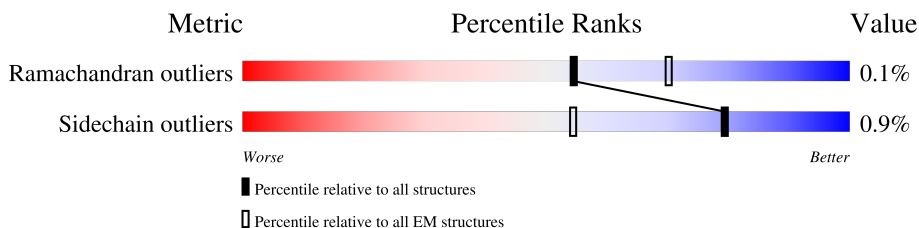
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	556	5% / 96% · ·
1	a	556	· / 95% · ·
2	B	535	5% / 97% · ·
2	b	535	6% / 97% · ·
3	D	539	5% / 96% · ·
3	d	539	6% / 96% ·
4	E	541	· / 98% · ·
4	e	541	· / 99% ·
5	G	545	· / 96% · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	g	545	5% / 98%
6	H	543	96%
6	h	543	96%
7	N	129	78% / 92% / 8%
7	n	129	79% / 92% / 8%
8	Q	548	97%
8	q	548	97%
9	Z	531	98%
9	z	531	99%
10	K	375	61% / 80% / 15%
11	P	239	71% / 77% / 21%

2 Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 71008 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	536	Total	C	N	O	S	0	0
			4069	2548	711	787	23		
1	a	532	Total	C	N	O	S	0	0
			4041	2533	707	778	23		

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			3952	2473	696	764	19		
2	b	525	Total	C	N	O	S	0	0
			3943	2467	694	763	19		

- Molecule 3 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	520	Total	C	N	O	S	0	0
			3923	2453	683	764	23		
3	d	520	Total	C	N	O	S	0	0
			3917	2450	680	764	23		

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	535	Total	C	N	O	S	1	0
			4132	2590	719	792	31		
4	e	540	Total	C	N	O	S	1	0
			4169	2610	724	804	31		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	526	Total 4089	C 2548	N 726	O 785	S 30	0	0
5	g	538	Total 4169	C 2590	N 740	O 809	S 30	0	0

- Molecule 6 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	528	Total 4054	C 2561	N 699	O 769	S 25	0	0
6	h	525	Total 4032	C 2548	N 696	O 763	S 25	0	0

- Molecule 7 is a protein called Nanobody Nb18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	119	Total 924	C 570	N 169	O 181	S 4	0	0
7	n	119	Total 924	C 570	N 169	O 181	S 4	0	0

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	538	Total 4086	C 2579	N 696	O 784	S 27	0	0
8	q	533	Total 4053	C 2558	N 690	O 778	S 27	0	0

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	525	Total 4022	C 2528	N 704	O 769	S 21	0	0
9	z	527	Total 4033	C 2534	N 706	O 772	S 21	0	0

- Molecule 10 is a protein called Actin, cytoplasmic 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	317	Total 2459	C 1563	N 409	O 469	S 18	0	0

- Molecule 11 is a protein called Phosducin-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	190	1486	955	239	287	5	0	0

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
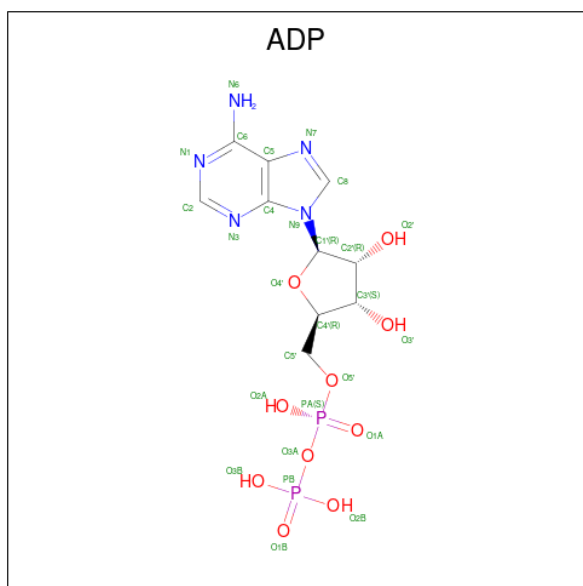
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	27	10	5	10	2	0
12	B	1	27	10	5	10	2	0
12	D	1	27	10	5	10	2	0
12	E	1	27	10	5	10	2	0
12	G	1	27	10	5	10	2	0
12	H	1	27	10	5	10	2	0
12	Q	1	27	10	5	10	2	0
12	Z	1	27	10	5	10	2	0
12	a	1	27	10	5	10	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
12	b	1	Total 27	C 10	N 5	O 10	P 2	0
12	d	1	Total 27	C 10	N 5	O 10	P 2	0
12	e	1	Total 27	C 10	N 5	O 10	P 2	0
12	g	1	Total 27	C 10	N 5	O 10	P 2	0
12	h	1	Total 27	C 10	N 5	O 10	P 2	0
12	q	1	Total 27	C 10	N 5	O 10	P 2	0
12	z	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 1	Mg 1	0
13	B	1	Total 1	Mg 1	0
13	D	1	Total 1	Mg 1	0
13	E	1	Total 1	Mg 1	0
13	G	1	Total 1	Mg 1	0
13	H	1	Total 1	Mg 1	0
13	Q	1	Total 1	Mg 1	0
13	Z	1	Total 1	Mg 1	0
13	a	1	Total 1	Mg 1	0
13	b	1	Total 1	Mg 1	0
13	d	1	Total 1	Mg 1	0
13	e	1	Total 1	Mg 1	0

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
13	g	1	Total 1	Mg 1	0
13	h	1	Total 1	Mg 1	0
13	q	1	Total 1	Mg 1	0
13	z	1	Total 1	Mg 1	0

- Molecule 14 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).
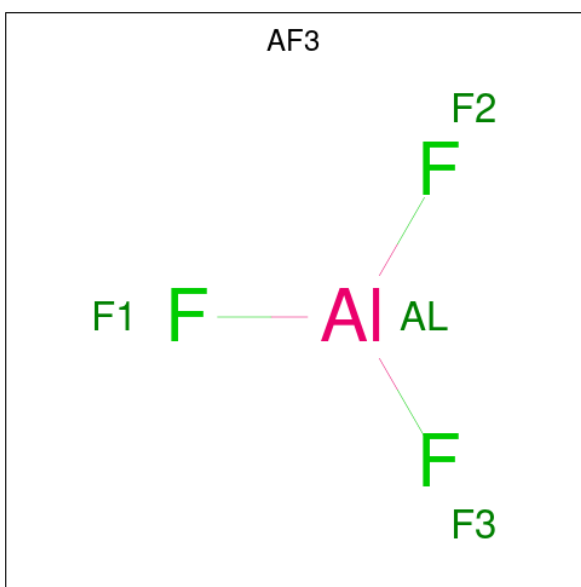
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total 4	Al 1	F 3	0
14	B	1	Total 4	Al 1	F 3	0
14	D	1	Total 4	Al 1	F 3	0
14	E	1	Total 4	Al 1	F 3	0
14	G	1	Total 4	Al 1	F 3	0
14	H	1	Total 4	Al 1	F 3	0
14	Q	1	Total 4	Al 1	F 3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
14	Z	1	Total 4	Al 1	F 3	0
14	a	1	Total 4	Al 1	F 3	0
14	b	1	Total 4	Al 1	F 3	0
14	d	1	Total 4	Al 1	F 3	0
14	e	1	Total 4	Al 1	F 3	0
14	g	1	Total 4	Al 1	F 3	0
14	h	1	Total 4	Al 1	F 3	0
14	q	1	Total 4	Al 1	F 3	0
14	z	1	Total 4	Al 1	F 3	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total 2	O 2	0
15	B	2	Total 2	O 2	0
15	D	1	Total 1	O 1	0
15	E	1	Total 1	O 1	0
15	G	1	Total 1	O 1	0
15	H	1	Total 1	O 1	0
15	Q	1	Total 1	O 1	0
15	Z	1	Total 1	O 1	0
15	a	2	Total 2	O 2	0
15	b	1	Total 1	O 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
15	d	1	Total 1	O 1	0
15	e	1	Total 1	O 1	0
15	g	1	Total 1	O 1	0
15	h	1	Total 1	O 1	0
15	q	1	Total 1	O 1	0
15	z	1	Total 1	O 1	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: T-complex protein 1 subunit alpha

Chain A:

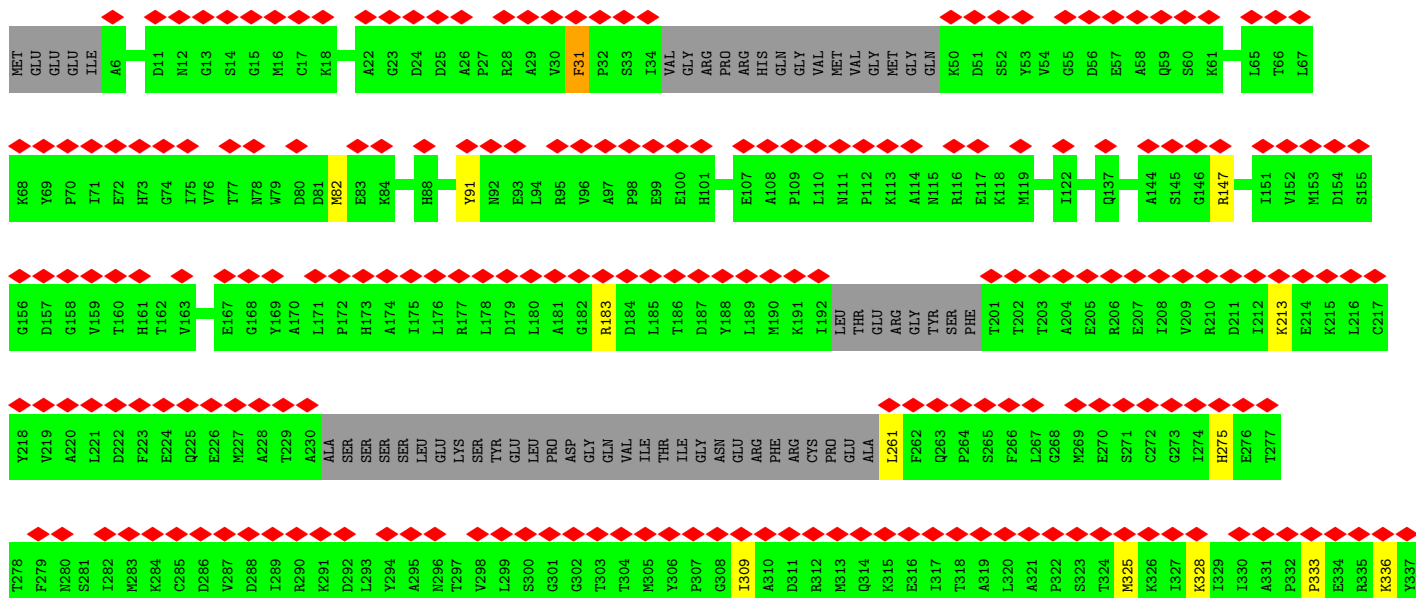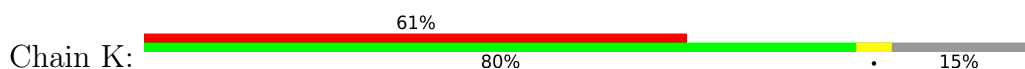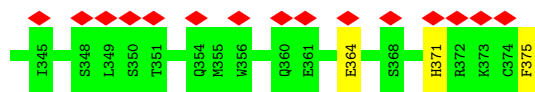- Molecule 1: T-complex protein 1 subunit alpha

Chain a:

- Molecule 2: T-complex protein 1 subunit beta

Chain B:

- Molecule 2: T-complex protein 1 subunit beta

Chain b:

R526 LYS ARG VAL PRO ASP HIS HIS PRO CYS

• Molecule 3: T-complex protein 1 subunit delta

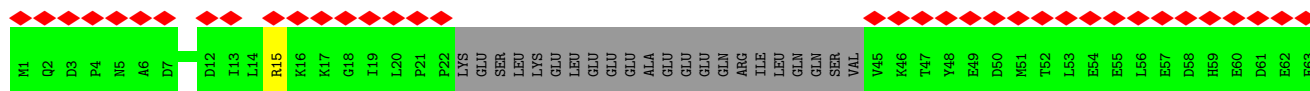Chain D:

5%

96%

MET PRO GLU ASN VAL ALA PRO ARG SER GLY ALA THR ALA GLY ALA ALA GLY GLY R19 G20 K21 G22 R27 D28 D46 D67 V83 D159 D196 S236 G237 D261 D273 G294 L305 D311 D327 D354 E364 G371 S381 P382

L432 D456 I461 K489 R496 E506 T538 ARG

• Molecule 3: T-complex protein 1 subunit delta

Chain d:

6%

96%

MET PRO GLU ASN VAL ALA PRO ARG SER GLY ALA THR ALA GLY ALA ALA GLY GLY R19 G20 K21 G22 A23 R27 D28 K65 G66 D67 Q82 D159 D196 T199 D204 L205 R206 S236 D259 M260 D261 L305 D311 D327 G369 T377 S381

P382 G383 K384 S404 S444 D456 N482 E524 T538 ARG

• Molecule 4: T-complex protein 1 subunit epsilon

Chain E:

98%

MET A2 S3 M4 G5 T6 L7 A8 F9 D10 E32 D65 D158 I159 K160 E163 D203 D231 D245 D307 Q316 K439 T442 K483 P536 GLY GLU SER GLU GLU

• Molecule 4: T-complex protein 1 subunit epsilon

Chain e:

99%

MET A2 S3 M4 G5 T6 L7 A8 F9 D10 D65 G66 D67 D158 D161 T162 E163 D203 D231 D308 Q316 K378 E436 A437 D438 T442 K483 K502 K535 P536 G537 E538 S539 E540 E541

• Molecule 5: T-complex protein 1 subunit gamma

Chain G:

96%

MET MET G3 H4 R5 P6 V7 L10 S11 Q12 N13 D145 E187 K234 R339 E358 D393 L403 D404 M429 T430 G431 Q442 I460 E473 N474 C475 E476 E483 T484 K528 LYS GLY ASP ASP GLN SER ARG GLN GLY GLY ALA PRO ASP ALA GLY

GLN GLU

• Molecule 5: T-complex protein 1 subunit gamma

Chain g:

• Molecule 6: T-complex protein 1 subunit eta

Chain H:

• Molecule 6: T-complex protein 1 subunit eta

Chain h:

• Molecule 7: Nanobody Nb18

Chain N:

• Molecule 7: Nanobody Nb18

Chain n:

• Molecule 8: T-complex protein 1 subunit theta

Chain Q:

97%

MET A2 E77 D193 S194 G195 D236 D299 N316 L341 E368 D369 D393 P431 L480 E485 E494 G532 P533 K534 P535 P536 S537 G538 K539 LYS ASP TRP ASP ASP GLN ASN ASP

• Molecule 8: T-complex protein 1 subunit theta

Chain q:

97%

MET A2 E17 D193 S194 G195 D236 D285 N316 R335 L341 E368 D369 E483 A484 E485 A530 G531 G532 P533 K534 PRO PRO SER GLY LYS LYS ASP TRP ASP ASP GLN ASN ASP

• Molecule 9: T-complex protein 1 subunit zeta

Chain Z:

98%

MET A2 A16 D86 D107 E146 D166 K181 Q182 D183 E184 D220 S246 G283 D284 S285 D286 D338 H346 E357 N367 D393 E415 M526 SER LEU LYS GLY

• Molecule 9: T-complex protein 1 subunit zeta

Chain z:

99%

M1 A2 R15 A16 E66 E142 M143 D144 K181 Q182 D183 D284 S285 D286 D337 D338 E357 N367 D403 D404 E415 M418 A419 Q475 E491 M526 S527 SER LEU LYS GLY

• Molecule 10: Actin, cytoplasmic 2

Chain K:

61%

80%

15%

MET GLU GLU GLU ILE A6 D11 N12 G13 S14 G15 M16 C17 K18 A22 G23 D24 D25 A26 P27 R28 A29 V30 F31 P32 S33 I34 VAL GLY ARG PRO ARG HIS GLN GLY VAL MET VAL GLY MET GLY GLN K50 D51 S52 Y53 V54 G55 D56 E57 A58 Q59 S60 K61 L65 T66 L67

K68 Y69 P70 I71 E72 H73 G74 I75 V76 T77 N78 W79 D80 D81 M82 E83 K84 H88 Y91 N92 E93 L94 R95 V96 A97 P98 E99 E100 H101 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 I122 Q137 A144 S145 G146 R147 I151 V152 M153 D154 S155

G156 D157 G158 V159 T160 H161 T162 V163 E167 G168 Y169 A170 L171 P172 H173 A174 I175 L176 R177 L178 D179 L180 A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190 K191 I192 LEU THR GLU ARG GLY TYR SER PHE T201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217

Y218 V219 A220 L221 D222 F223 E224 Q225 E226 M227 A228 T229 A230 ALA SER SER SER SER LEU GLU LYS SER TYR GLU LEU PRO ASP GLY GLN VAL ILE THR ILE GLY ASN GLU ARG PHE ARG CYS PRO GLU ALA L261 F262 Q263 P264 S265 F266 L267 G268 M269 E270 S271 C272 G273 I274 H275 E276 T277

T278 F279 N280 S281 I282 M283 K284 C285 D286 V287 D288 I289 R290 K291 D292 L293 Y294 A295 N296 T297 V298 L299 S300 G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313 Q314 K315 E316 I317 T318 A319 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337

I345 S348 L349 S350 T351 Q354 M355 W356 Q360 E361 E364 S368 H371 R372 K373 C374 F375

• Molecule 11: Phosducin-like protein 3

71%

Chain P:

77% · 21%

M1 Q2 D3 P4 N5 A6 D7 D12 I13 L14 R15 K16 K17 G18 I19 L20 P21 P22 LYS GLU SER LEU LYS GLU LEU GLU GLU GLU ALA GLU GLU GLU GLN ARG ILE LEU GLN GLN SER VAL V45 K46 T47 Y48 E49 D50 M51 T52 L53 E54 E55 L56 E57 D58 H59 E60 D61 E62 F63

N64 E65 E66 D67 E68 R69 A70 I71 E72 M73 Y74 R75 R76 L79 A80 E81 W82 K83 A84 T85 K86 L87 K88 N89 K90 F91 G92 E93 V94 L95 E96 I97 S98 G99 K100 D101 Y102 V103 Q104 E105 V106 T107 K108 A109 G110 E111 G112 L113 W114 V115 I116 L117 H118 L119 Y120 K121 Q122 G123 I124

P125 L126 C127 A128 L129 I130 N131 Q132 H133 L134 S135 A138 R139 K140 F141 P142 D143 V144 K145 F146 I147 K148 A149 I150 S151 T152 T153 C154 N157 Y158 P159 D160 R161 N162 L163 P164 T165 I166 F167 V168 Y169 L170 E171 G172 D173 I174 K175 A176 Q177 F178 I179 G180 P181 L182 V183 F184 G185 G186

M187 N188 L189 T190 R191 D192 E193 L194 E195 W196 K197 L198 S199 E200 S201 G202 A203 I204 M205 T206 D207 L208 E209 E210 N211 P212 LYS LYS PRO ILE GLU ASP VAL LEU LEU SER SER VAL ARG ARG SER VAL LEU MET LYS ARG ASP SER ASP SER GLU GLY GLY ASP

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63082	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: ADP, AF3, MG

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	0.31	0/4109	0.49	0/5548
1	a	0.31	0/4081	0.49	0/5510
2	B	0.30	0/3995	0.49	0/5386
2	b	0.31	0/3986	0.50	1/5375 (0.0%)
3	D	0.30	0/3955	0.48	0/5338
3	d	0.30	0/3949	0.50	0/5331
4	E	0.32	0/4183	0.51	0/5635
4	e	0.33	0/4220	0.51	0/5684
5	G	0.31	0/4136	0.50	0/5579
5	g	0.31	0/4215	0.49	0/5683
6	H	0.34	0/4111	0.49	0/5550
6	h	0.33	0/4089	0.48	0/5519
7	N	0.26	0/941	0.53	0/1270
7	n	0.28	0/941	0.54	0/1270
8	Q	0.33	0/4147	0.50	1/5606 (0.0%)
8	q	0.33	0/4112	0.49	0/5558
9	Z	0.31	0/4069	0.49	0/5486
9	z	0.31	0/4080	0.49	0/5501
10	K	0.29	0/2510	0.48	0/3401
11	P	0.26	0/1518	0.44	0/2062
All	All	0.31	0/71347	0.49	2/96292 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	e	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	316	ASP	CB-CG-OD2	5.20	122.98	118.30
8	Q	480	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	e	8	ALA	Mainchain

5.2   Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	534/556 (96%)	508 (95%)	26 (5%)	0	100	100
1	a	530/556 (95%)	502 (95%)	28 (5%)	0	100	100
2	B	524/535 (98%)	502 (96%)	21 (4%)	1 (0%)	47	79
2	b	523/535 (98%)	503 (96%)	19 (4%)	1 (0%)	47	79
3	D	518/539 (96%)	507 (98%)	11 (2%)	0	100	100
3	d	518/539 (96%)	487 (94%)	31 (6%)	0	100	100
4	E	534/541 (99%)	511 (96%)	20 (4%)	3 (1%)	25	59
4	e	539/541 (100%)	516 (96%)	22 (4%)	1 (0%)	47	79
5	G	524/545 (96%)	502 (96%)	22 (4%)	0	100	100
5	g	536/545 (98%)	519 (97%)	17 (3%)	0	100	100
6	H	526/543 (97%)	506 (96%)	20 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	h	523/543 (96%)	505 (97%)	18 (3%)	0	100	100
7	N	117/129 (91%)	110 (94%)	7 (6%)	0	100	100
7	n	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
8	Q	536/548 (98%)	516 (96%)	18 (3%)	2 (0%)	34	69
8	q	531/548 (97%)	512 (96%)	18 (3%)	1 (0%)	47	79
9	Z	523/531 (98%)	504 (96%)	18 (3%)	1 (0%)	47	79
9	z	525/531 (99%)	505 (96%)	19 (4%)	1 (0%)	47	79
10	K	309/375 (82%)	275 (89%)	32 (10%)	2 (1%)	25	59
11	P	186/239 (78%)	169 (91%)	17 (9%)	0	100	100
All	All	9173/9548 (96%)	8770 (96%)	390 (4%)	13 (0%)	54	83

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	10	ASP
9	Z	16	ALA
4	e	10	ASP
8	q	530	ALA
9	z	16	ALA

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	447/463 (96%)	442 (99%)	5 (1%)	73	89
1	a	444/463 (96%)	441 (99%)	3 (1%)	84	93
2	B	418/427 (98%)	414 (99%)	4 (1%)	76	90
2	b	417/427 (98%)	413 (99%)	4 (1%)	76	90
3	D	442/452 (98%)	439 (99%)	3 (1%)	84	93
3	d	441/452 (98%)	440 (100%)	1 (0%)	93	97
4	E	452/456 (99%)	449 (99%)	3 (1%)	84	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	e	456/456 (100%)	452 (99%)	4 (1%)	78	91
5	G	456/469 (97%)	453 (99%)	3 (1%)	84	93
5	g	463/469 (99%)	461 (100%)	2 (0%)	91	96
6	H	435/443 (98%)	430 (99%)	5 (1%)	73	89
6	h	432/443 (98%)	427 (99%)	5 (1%)	71	88
7	N	96/105 (91%)	96 (100%)	0	100	100
7	n	96/105 (91%)	96 (100%)	0	100	100
8	Q	442/452 (98%)	440 (100%)	2 (0%)	88	94
8	q	438/452 (97%)	437 (100%)	1 (0%)	93	97
9	Z	437/442 (99%)	436 (100%)	1 (0%)	93	97
9	z	438/442 (99%)	436 (100%)	2 (0%)	88	94
10	K	264/318 (83%)	249 (94%)	15 (6%)	20	52
11	P	155/215 (72%)	148 (96%)	7 (4%)	27	60
All	All	7669/7951 (96%)	7599 (99%)	70 (1%)	79	91

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	K	325	MET
10	K	336	LYS
11	P	96	GLU
8	Q	537	SER
8	Q	369	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
9	Z	438	GLN
9	z	17	GLN
2	b	285	HIS
9	z	8	ASN
10	K	111	ASN

5.3.3 RNA ⓘ

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 for Mogul analysis.

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	$\#|Z| > 2$
14	AF3	h	603	-	0,3,3	-	-	-		
12	ADP	D	601	13	24,29,29	0.93	1 (4%)	29,45,45	1.55	4 (13%)
14	AF3	Z	603	-	0,3,3	-	-	-		
14	AF3	E	603	-	0,3,3	-	-	-		
12	ADP	G	601	13	24,29,29	0.94	1 (4%)	29,45,45	1.19	3 (10%)
14	AF3	b	603	-	0,3,3	-	-	-		
12	ADP	H	601	13	24,29,29	0.97	1 (4%)	29,45,45	1.37	3 (10%)
12	ADP	Q	601	13	24,29,29	0.93	1 (4%)	29,45,45	1.39	3 (10%)
14	AF3	z	603	-	0,3,3	-	-	-		
14	AF3	Q	603	-	0,3,3	-	-	-		
12	ADP	q	601	13	24,29,29	0.95	1 (4%)	29,45,45	1.41	3 (10%)
12	ADP	a	601	13	24,29,29	0.97	1 (4%)	29,45,45	1.40	5 (17%)
14	AF3	q	603	-	0,3,3	-	-	-		
14	AF3	a	603	-	0,3,3	-	-	-		
12	ADP	Z	601	13	24,29,29	0.93	1 (4%)	29,45,45	1.53	5 (17%)
12	ADP	h	601	13	24,29,29	0.91	1 (4%)	29,45,45	1.33	4 (13%)
12	ADP	E	601	13	24,29,29	0.96	1 (4%)	29,45,45	1.41	6 (20%)
14	AF3	g	603	-	0,3,3	-	-	-		
12	ADP	e	601	13	24,29,29	0.93	1 (4%)	29,45,45	1.41	6 (20%)
12	ADP	b	601	13	24,29,29	0.92	1 (4%)	29,45,45	1.51	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	ADP	g	601	13	24,29,29	0.94	1 (4%)	29,45,45	1.33	3 (10%)
14	AF3	G	603	-	0,3,3	-	-	-		
14	AF3	d	603	-	0,3,3	-	-	-		
14	AF3	H	603	-	0,3,3	-	-	-		
14	AF3	e	603	-	0,3,3	-	-	-		
12	ADP	d	601	13	24,29,29	0.95	1 (4%)	29,45,45	1.61	5 (17%)
12	ADP	A	601	13	24,29,29	0.97	1 (4%)	29,45,45	1.44	5 (17%)
14	AF3	B	603	-	0,3,3	-	-	-		
14	AF3	A	603	-	0,3,3	-	-	-		
14	AF3	D	603	-	0,3,3	-	-	-		
12	ADP	B	601	13	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)
12	ADP	z	601	13	24,29,29	0.95	1 (4%)	29,45,45	1.53	5 (17%)

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
12	ADP	H	601	13	-	6/12/32/32	0/3/3/3
12	ADP	Q	601	13	-	3/12/32/32	0/3/3/3
12	ADP	D	601	13	-	2/12/32/32	0/3/3/3
12	ADP	b	601	13	-	2/12/32/32	0/3/3/3
12	ADP	G	601	13	-	6/12/32/32	0/3/3/3
12	ADP	a	601	13	-	1/12/32/32	0/3/3/3
12	ADP	d	601	13	-	0/12/32/32	0/3/3/3
12	ADP	g	601	13	-	6/12/32/32	0/3/3/3
12	ADP	A	601	13	-	0/12/32/32	0/3/3/3
12	ADP	q	601	13	-	3/12/32/32	0/3/3/3
12	ADP	Z	601	13	-	0/12/32/32	0/3/3/3
12	ADP	h	601	13	-	6/12/32/32	0/3/3/3
12	ADP	e	601	13	-	2/12/32/32	0/3/3/3
12	ADP	E	601	13	-	3/12/32/32	0/3/3/3
12	ADP	B	601	13	-	2/12/32/32	0/3/3/3
12	ADP	z	601	13	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	z	601	ADP	C5-C4	2.40	1.47	1.40
12	E	601	ADP	C5-C4	2.32	1.47	1.40
12	a	601	ADP	C5-C4	2.31	1.47	1.40
12	g	601	ADP	C5-C4	2.30	1.47	1.40
12	G	601	ADP	C5-C4	2.28	1.47	1.40

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Z	601	ADP	PA-O3A-PB	-4.32	118.00	132.83
12	z	601	ADP	PA-O3A-PB	-4.20	118.42	132.83
12	d	601	ADP	PA-O3A-PB	-3.73	120.03	132.83
12	Q	601	ADP	N3-C2-N1	-3.53	123.17	128.68
12	g	601	ADP	PA-O3A-PB	-3.51	120.77	132.83

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	601	ADP	PA-O3A-PB-O3B
12	G	601	ADP	C5'-O5'-PA-O2A
12	H	601	ADP	PA-O3A-PB-O2B
12	H	601	ADP	PB-O3A-PA-O5'
12	H	601	ADP	C3'-C4'-C5'-O5'

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP G 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP H 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP Q 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP q 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP a 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP Z 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP h 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP e 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP b 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP g 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP d 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP z 601

Bond lengths

Bond angles

Torsions

Rings

5.7　Other polymers ⓘ

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 ⓘ

This section contains visualisations of the EMDB entry EMD-12606. 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 ⓘ
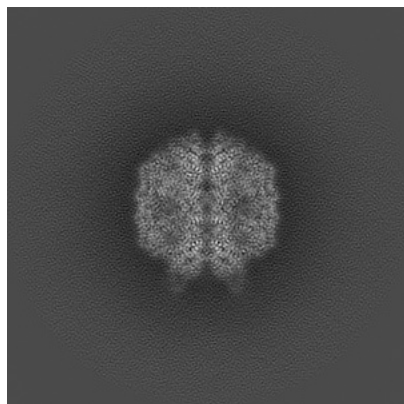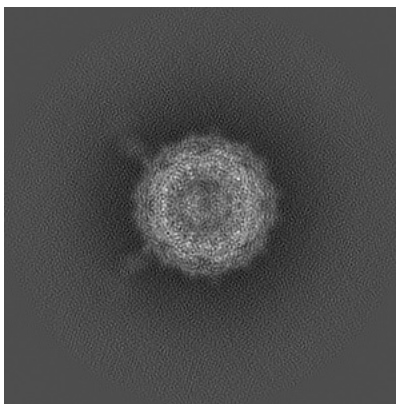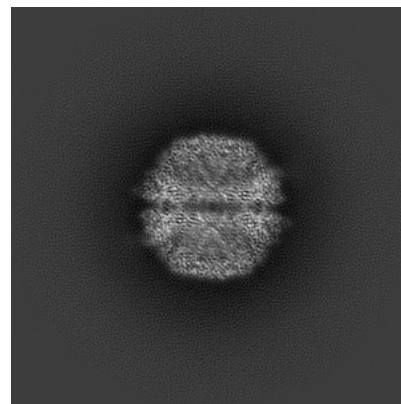
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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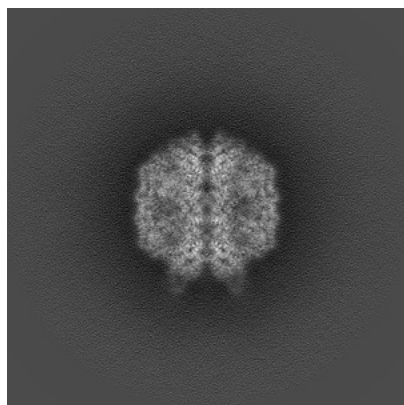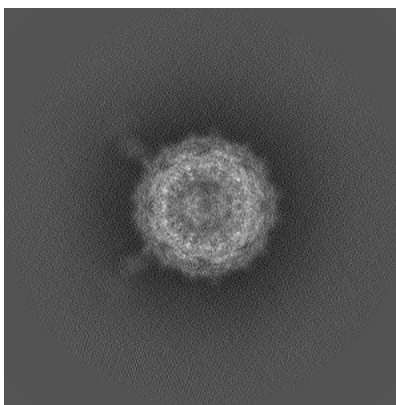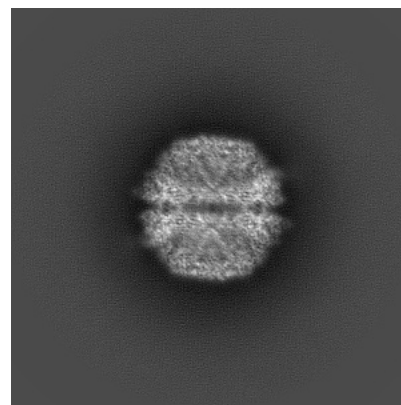
The images above show the map projected in three orthogonal directions.

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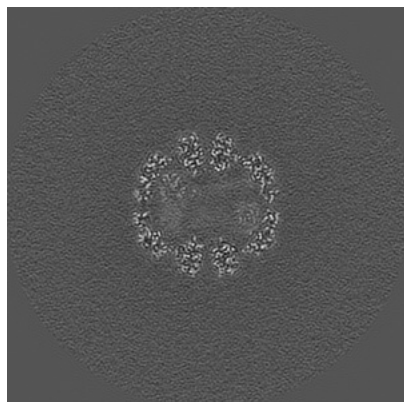
6.2.1   Primary map
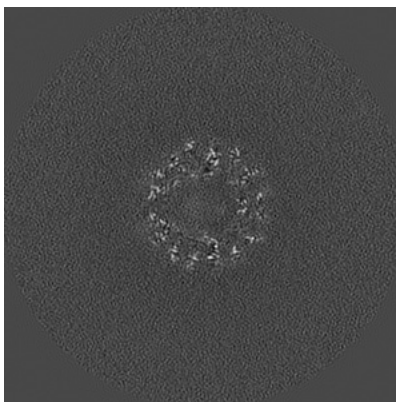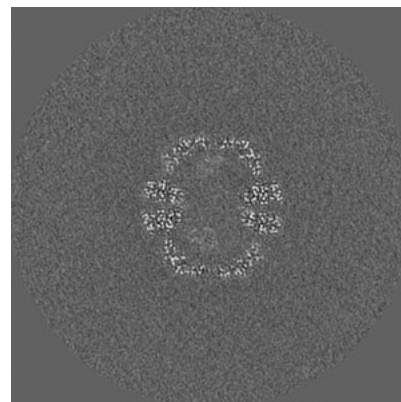
X Index: 200   Y Index: 200   Z Index: 200

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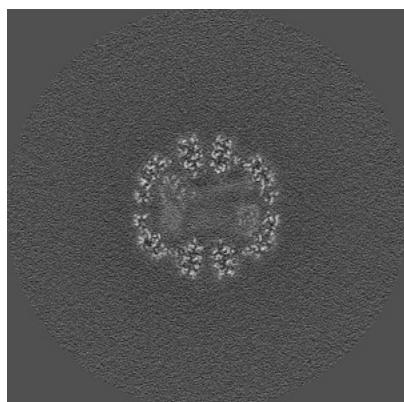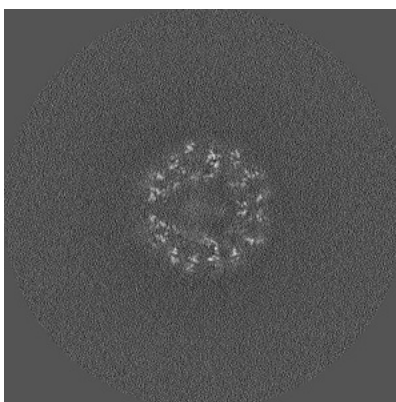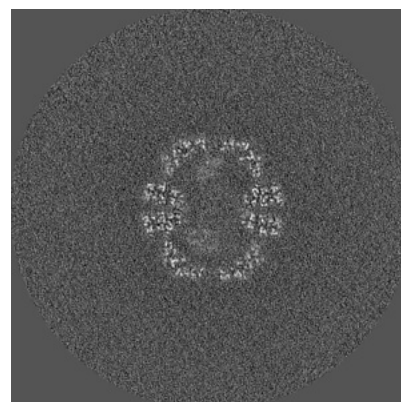
X Index: 200   Y Index: 200   Z Index: 200

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

6.3   Largest variance slices   ⓘ
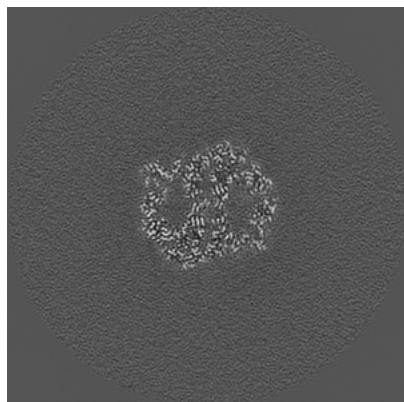
6.3.1   Primary map
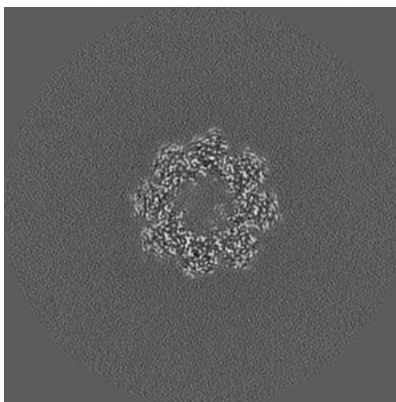
X Index: 169   Y Index: 186   Z Index: 166
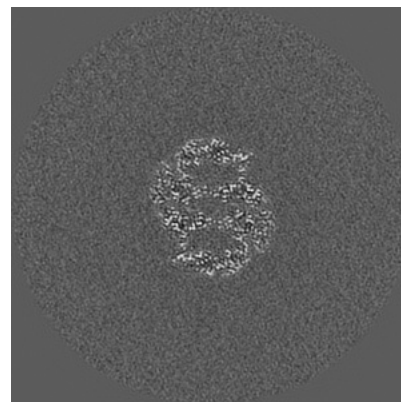
6.3.2   Raw map
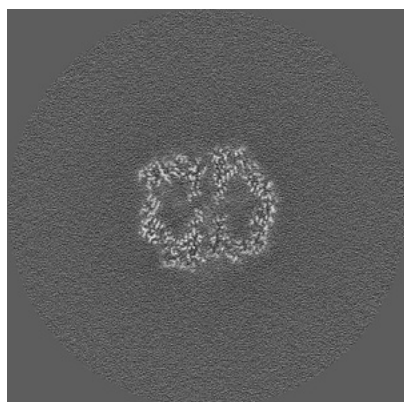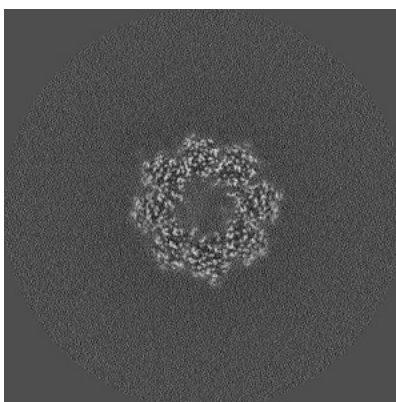
X Index: 173   Y Index: 212   Z Index: 231
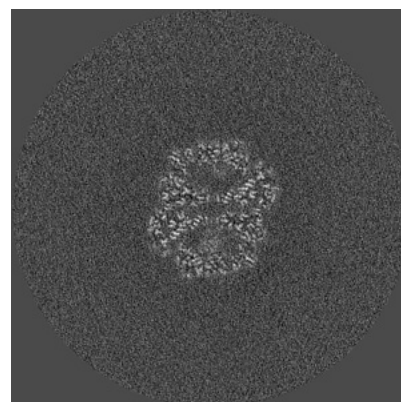
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X	Y	Z
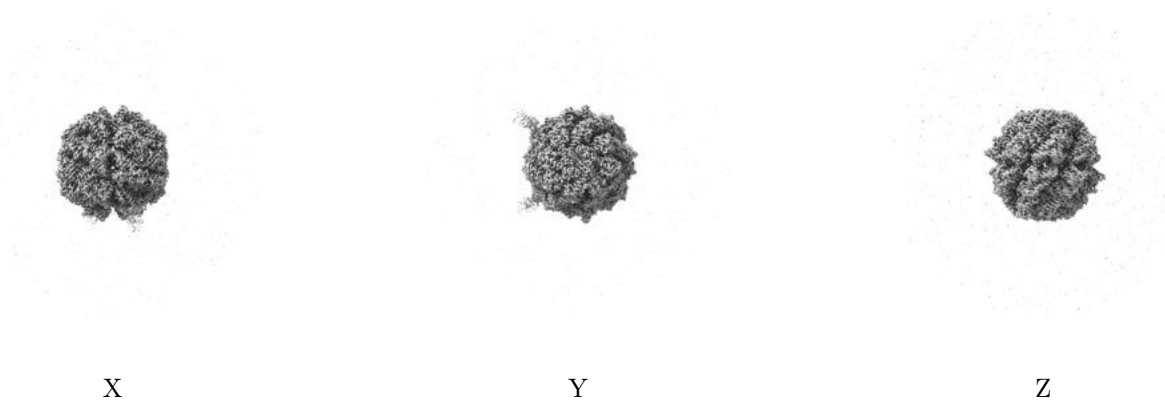
The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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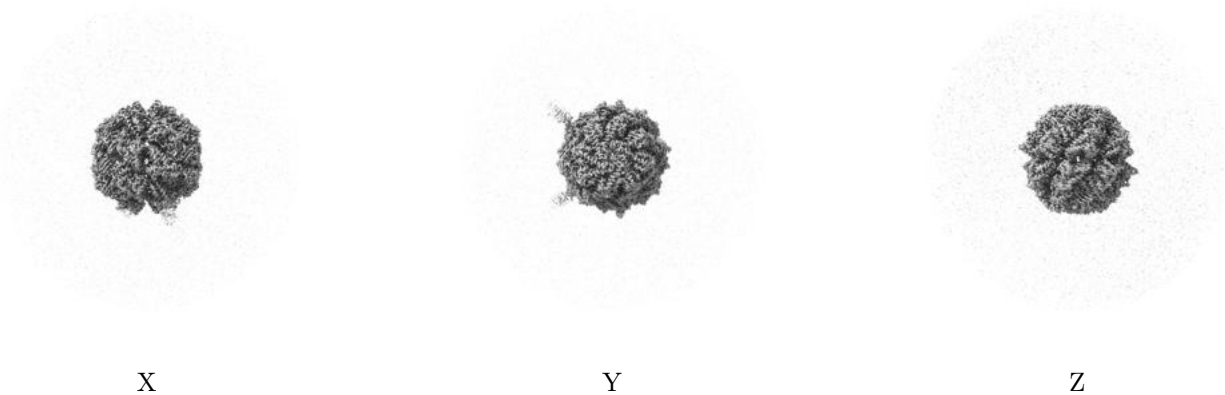
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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

A mask typically either:

- Encompasses the whole structure

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

6.5.1 emd_12606_msk_1.map ⓘ

X   Y   Z
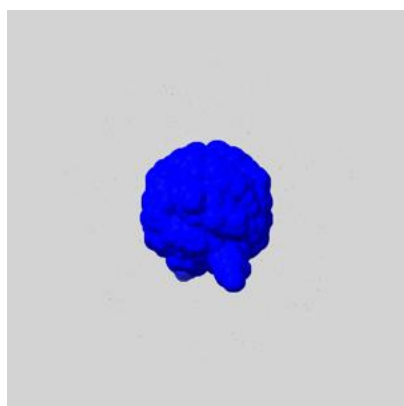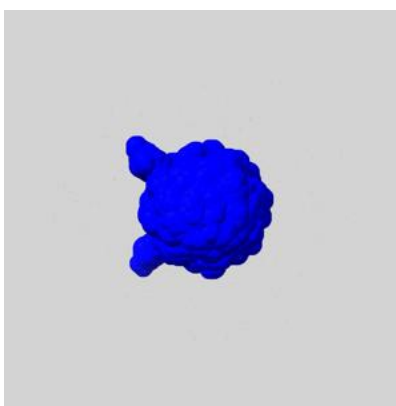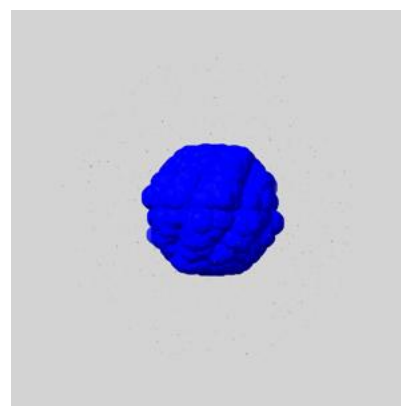
7 Map analysis ⓘ

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 ⓘ
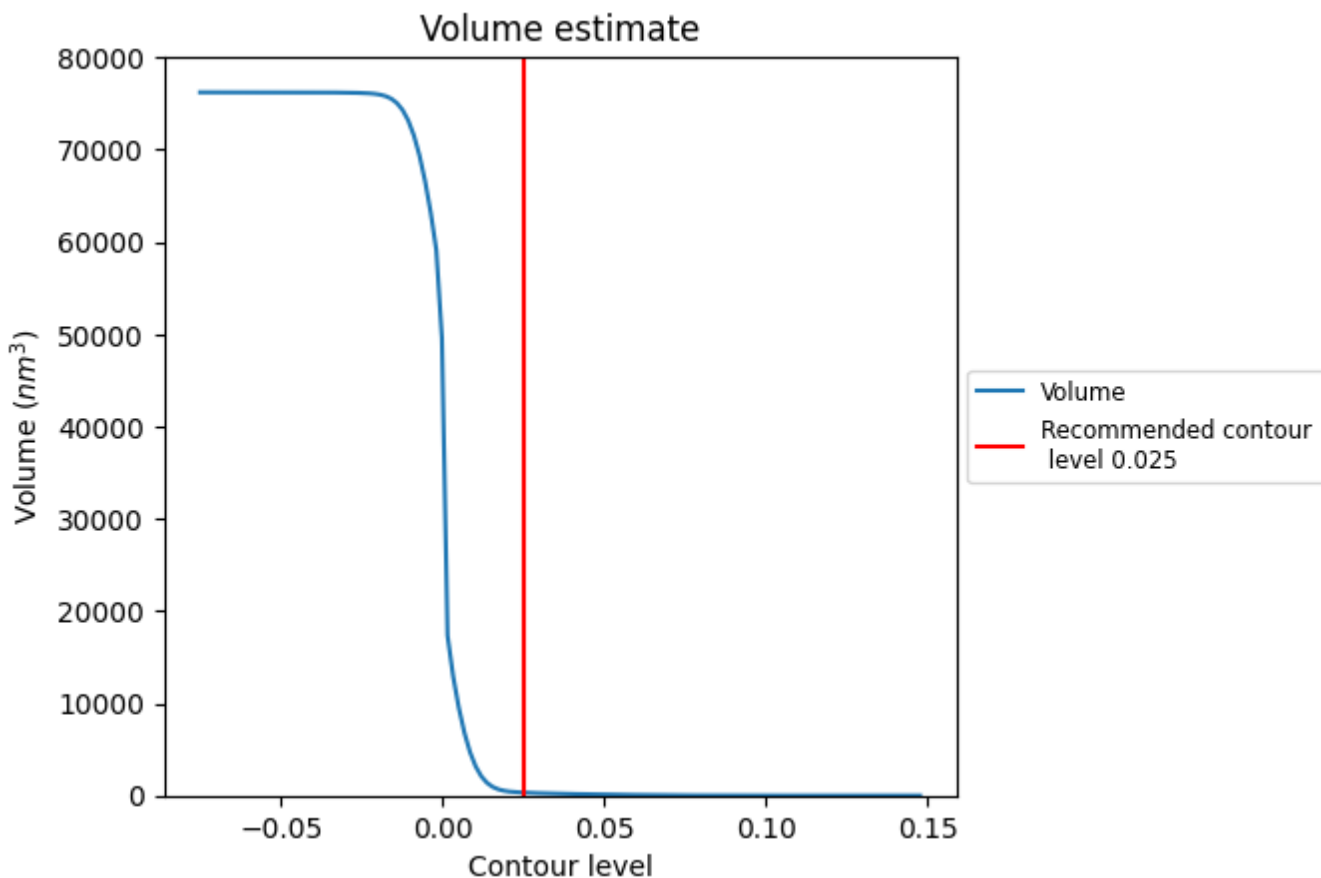
The volume at the recommended contour level is 321 nm^3; this corresponds to an approximate mass of 290 kDa.

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 ⓘ
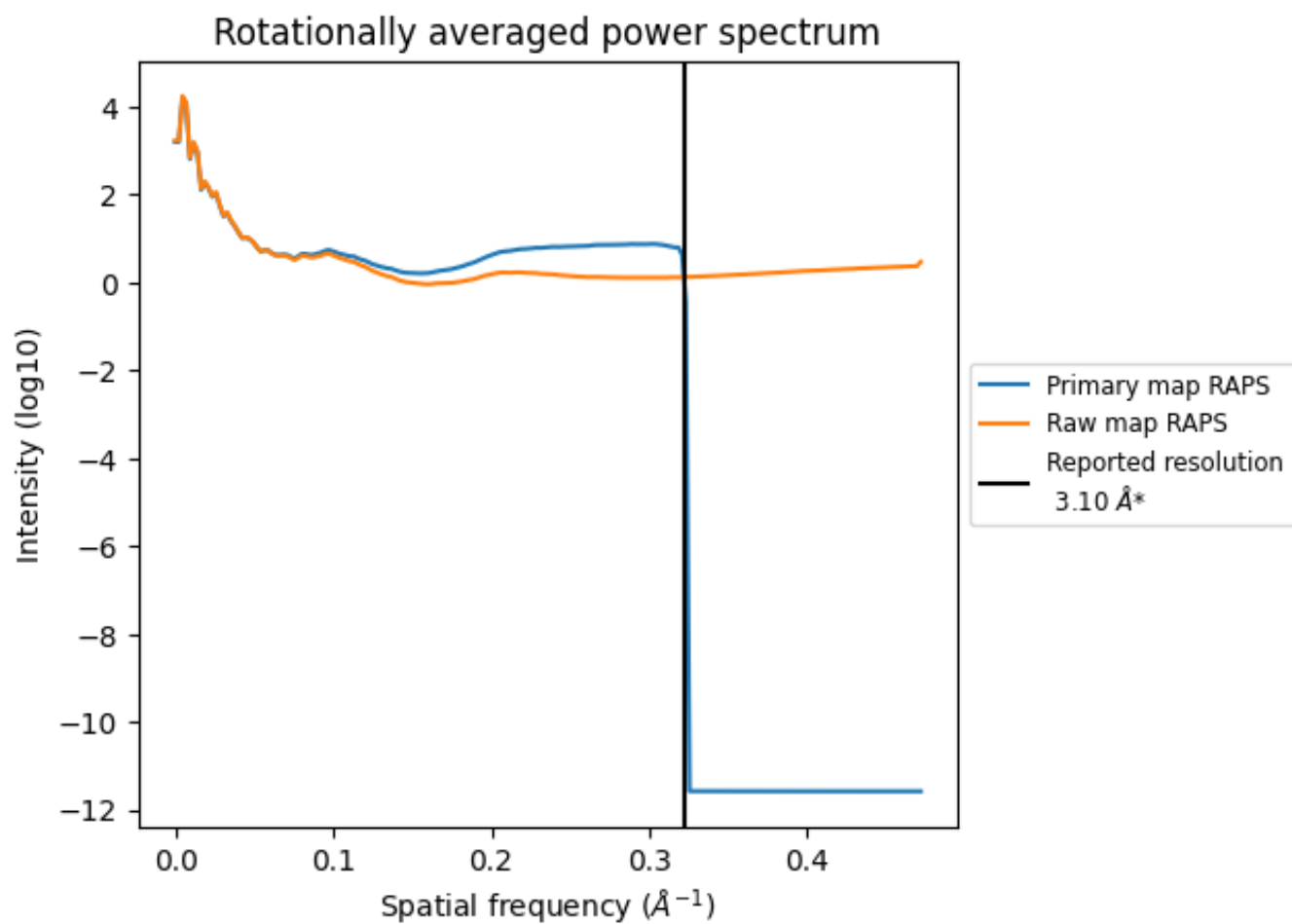
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ
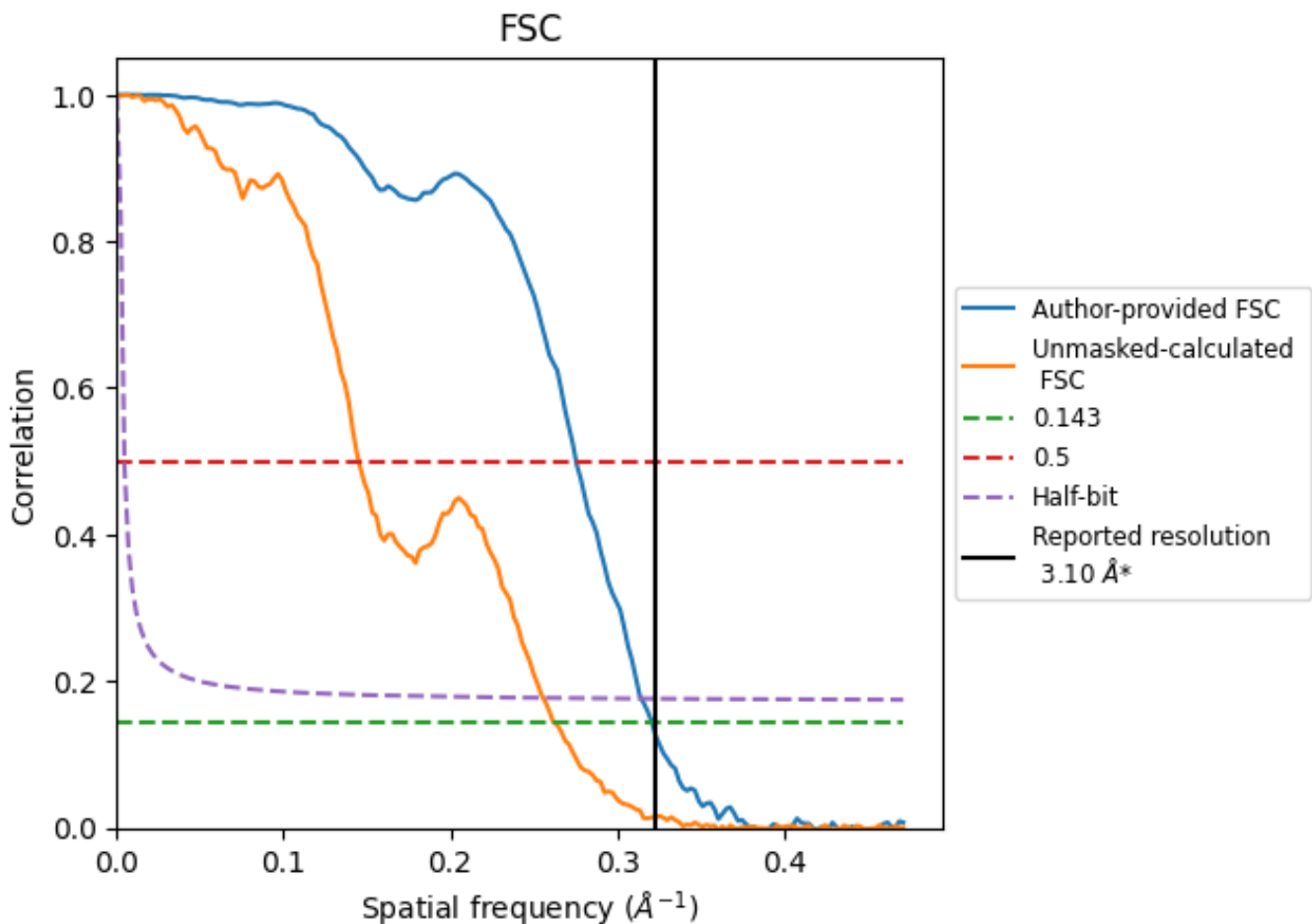
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.63	3.18
Unmasked-calculated*	3.81	6.89	3.91

*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 3.81 differs from the reported value 3.1 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-12606 and PDB model 7NVM. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ

| X | Y | Z |
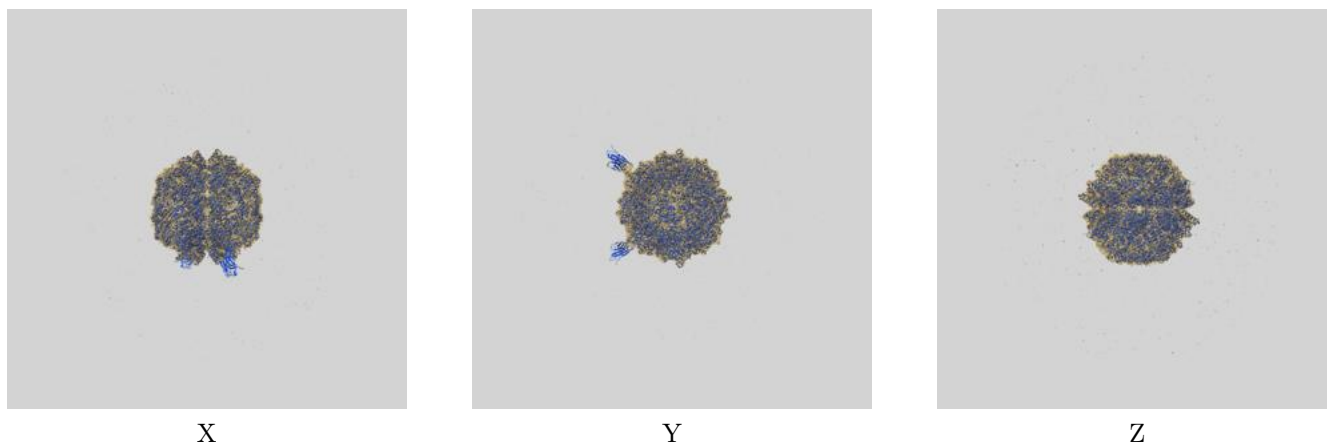
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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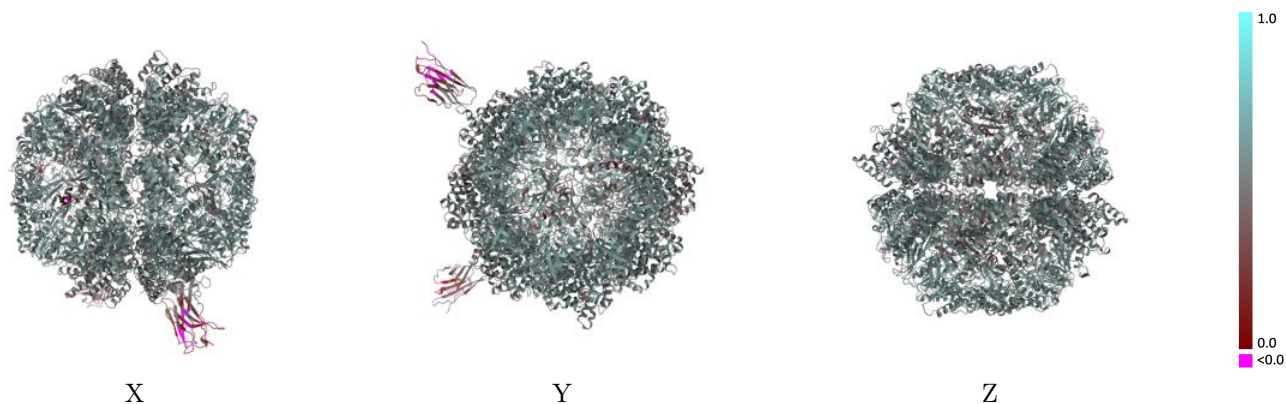
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model (i)
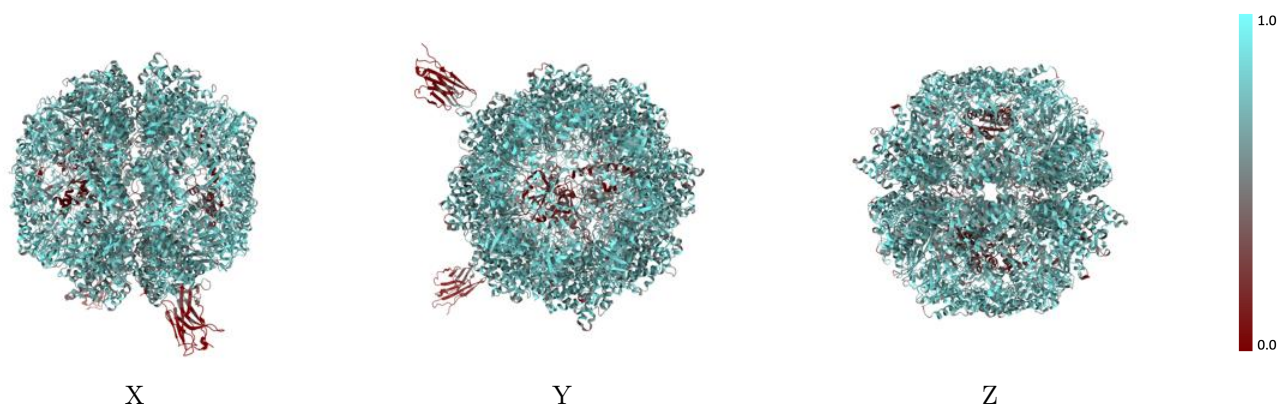
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

WORLDWIDE
wwPDB
PROTEIN DATA BANK
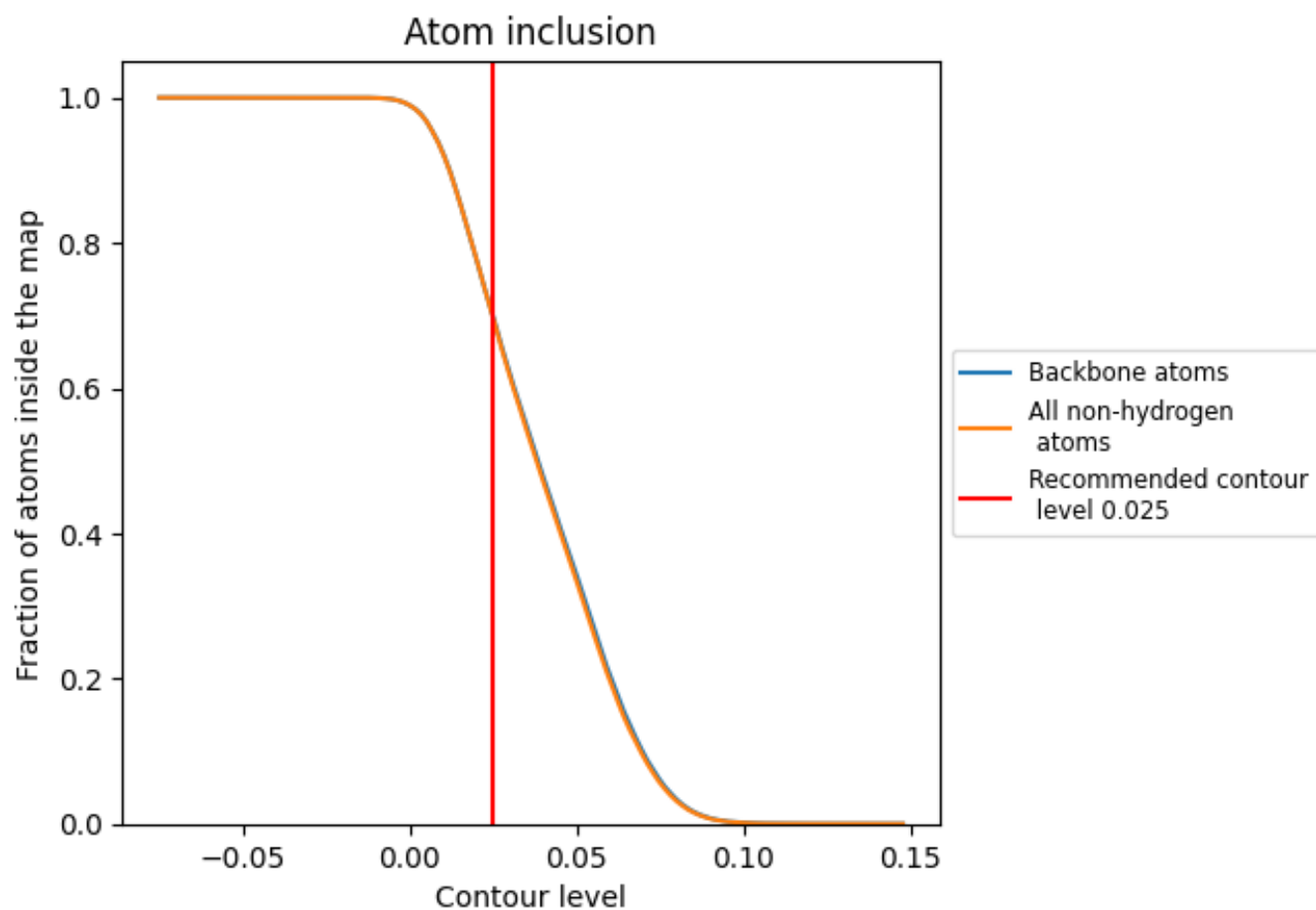
9.4 Atom inclusion ⓘ

At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6949	0.5290
A	0.7382	0.5380
B	0.7219	0.5310
D	0.7330	0.5420
E	0.7547	0.5440
G	0.7389	0.5360
H	0.7797	0.5680
K	0.2582	0.4280
N	0.1696	0.2840
P	0.1826	0.4180
Q	0.7485	0.5530
Z	0.7352	0.5380
a	0.7466	0.5420
b	0.7289	0.5270
d	0.7340	0.5380
e	0.7381	0.5420
g	0.7282	0.5360
h	0.7747	0.5630
n	0.1529	0.2660
q	0.7667	0.5560
z	0.7322	0.5320

1.0

0.0
<0.0