Full wwPDB EM Validation Report (i)

Mar 10, 2024 – 11:08 PM EDT

PDB ID	:	6U5B
EMDB ID	:	EMD-20643
Title	:	CryoEM Structure of Pyocin R2 - precontracted - baseplate
Authors	:	Ge, P.; Avaylon, J.; Scholl, D.; Shneider, M.M.; Browning, C.; Buth, S.A.; Plattner, M.; Ding, K.; Leiman, P.G.; Miller, J.F.; Zhou, Z.H.
Deposited on	:	2019-08-27
Resolution	:	3.50 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:

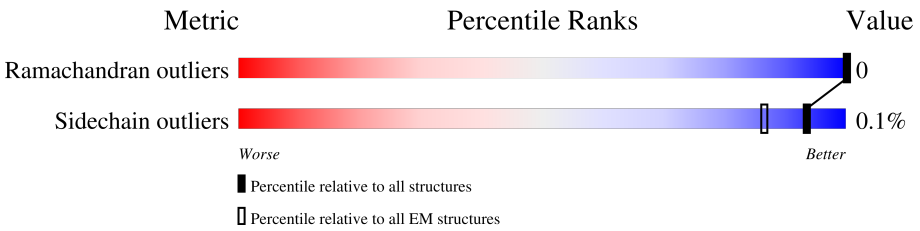
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	m	295	67% 99% .
1	n	295	67% 99% .
1	o	295	66% 99% .
1	p	295	66% 99% .
1	q	295	67% 99% .
1	r	295	65% 99% .
1	s	295	54% 99% .
1	t	295	54% 99% .
1	u	295	53% 99% .

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Mol	Chain	Length	Quality of chain
1	v	295	53% 99%
1	w	295	54% 99%
1	x	295	54% 99%
2	A	386	15% 99%
2	B	386	15% 99%
2	C	386	14% 99%
2	D	386	16% 99%
2	E	386	16% 99%
2	F	386	15% 99%
2	M	386	17% 99%
2	N	386	17% 99%
2	O	386	17% 99%
2	P	386	16% 99%
2	Q	386	17% 99%
2	R	386	17% 99%
3	G	167	5% 99%
3	H	167	7% 99%
3	I	167	7% 99%
3	J	167	5% 99%
3	K	167	7% 99%
3	L	167	7% 99%
3	S	167	7% 98%
3	T	167	8% 98%
3	U	167	8% 98%
3	V	167	7% 98%

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Mol	Chain	Length	Quality of chain
3	W	167	8% 98%
3	X	167	7% 98%
4	0	177	48% 85% 15%
4	1	177	47% 85% 15%
4	2	177	47% 85% 15%
4	3	177	47% 85% 15%
4	4	177	47% 85% 15%
4	5	177	47% 85% 15%
5	a	108	8% 92% 8%
5	b	108	6% 92% 8%
5	c	108	7% 92% 8%
5	d	108	8% 92% 8%
5	e	108	7% 92% 8%
5	f	108	6% 92% 8%
6	6	68	9% 81% 19%
6	7	68	10% 81% 19%
6	8	68	9% 81% 19%
6	9	68	12% 81% 19%
6	Y	68	10% 81% 19%
6	Z	68	9% 81% 19%
7	g	290	20% 98%
7	h	290	20% 98%
7	i	290	19% 98%
7	j	290	20% 98%
7	k	290	20% 98%

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Mol	Chain	Length	Quality of chain
7	l	290	19% 98%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 103392 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 Tri1a PA0618.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	m	291	2218	1394	392	428	4	0	0
1	n	291	2218	1394	392	428	4	0	0
1	q	291	2218	1394	392	428	4	0	0
1	r	291	2218	1394	392	428	4	0	0
1	o	291	2218	1394	392	428	4	0	0
1	p	291	2218	1394	392	428	4	0	0
1	s	292	2223	1397	393	429	4	0	0
1	t	292	2223	1397	393	429	4	0	0
1	w	292	2223	1397	393	429	4	0	0
1	x	292	2223	1397	393	429	4	0	0
1	u	292	2223	1397	393	429	4	0	0
1	v	292	2223	1397	393	429	4	0	0

- Molecule 2 is a protein called Sheath PA0622.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	382	2876	1813	503	552	8	0	0
2	N	382	2876	1813	503	552	8	0	0
2	Q	382	2876	1813	503	552	8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	382	2876	1813	503	552	8	0	0
2	O	382	2876	1813	503	552	8	0	0
2	P	382	2876	1813	503	552	8	0	0
2	A	382	2876	1813	503	552	8	0	0
2	B	382	2876	1813	503	552	8	0	0
2	E	382	2876	1813	503	552	8	0	0
2	F	382	2876	1813	503	552	8	0	0
2	C	382	2876	1813	503	552	8	0	0
2	D	382	2876	1813	503	552	8	0	0

- Molecule 3 is a protein called Tube PA0623.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S	165	1250	792	213	240	5	0	0
3	T	165	1250	792	213	240	5	0	0
3	W	165	1250	792	213	240	5	0	0
3	X	165	1250	792	213	240	5	0	0
3	U	165	1250	792	213	240	5	0	0
3	V	165	1250	792	213	240	5	0	0
3	G	166	1255	795	214	242	4	0	0
3	H	166	1255	795	214	242	4	0	0
3	K	166	1255	795	214	242	4	0	0
3	L	166	1255	795	214	242	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	166	1255	795	214	242	4	0	0
3	J	166	1255	795	214	242	4	0	0

- Molecule 4 is a protein called Tri2 PA0619.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	0	151	1202	754	220	227	1	0	0
4	1	151	1202	754	220	227	1	0	0
4	4	151	1202	754	220	227	1	0	0
4	5	151	1202	754	220	227	1	0	0
4	2	151	1202	754	220	227	1	0	0
4	3	151	1202	754	220	227	1	0	0

- Molecule 5 is a protein called Sheath Initiator PA0617.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	a	99	759	474	144	136	5	0	0
5	b	99	759	474	144	136	5	0	0
5	e	99	759	474	144	136	5	0	0
5	f	99	759	474	144	136	5	0	0
5	c	99	759	474	144	136	5	0	0
5	d	99	759	474	144	136	5	0	0

- Molecule 6 is a protein called Glue PA0627.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	55	413	258	68	82	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	55	413	258	68	82	5	0	0
6	Y	55	413	258	68	82	5	0	0
6	Z	55	413	258	68	82	5	0	0
6	8	55	413	258	68	82	5	0	0
6	9	55	413	258	68	82	5	0	0

- Molecule 7 is a protein called Ripcord PA0626.

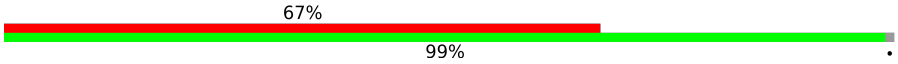
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	h	285	2160	1352	401	402	5	0	0
7	g	285	2160	1352	401	402	5	0	0
7	l	285	2160	1352	401	402	5	0	0
7	k	285	2160	1352	401	402	5	0	0
7	j	285	2160	1352	401	402	5	0	0
7	i	285	2160	1352	401	402	5	0	0

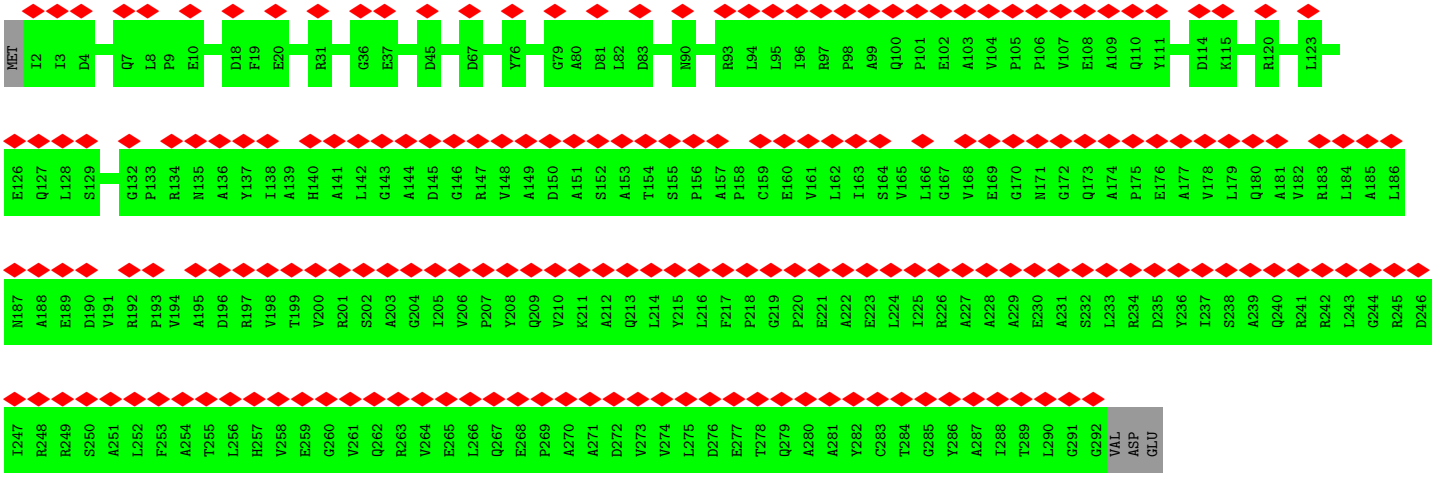
3 Residue-property plots (i)

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

- Molecule 1: Tri1a PA0618

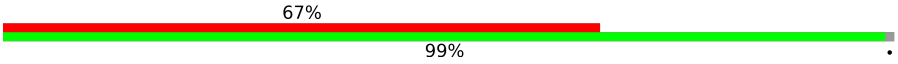
Chain m:

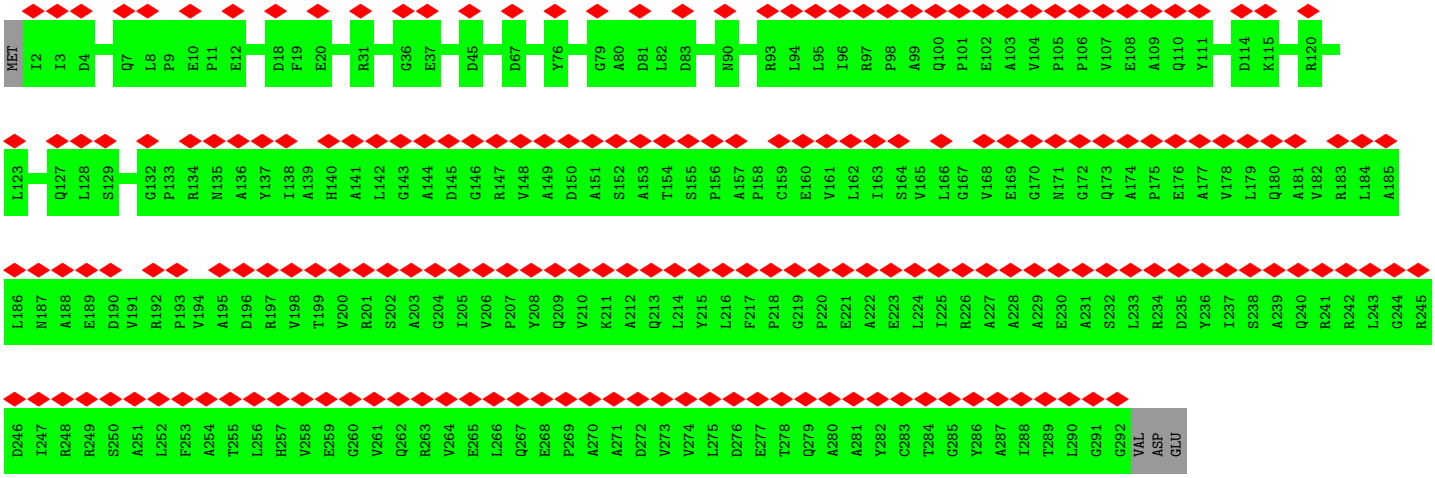




- Molecule 1: Tri1a PA0618

Chain n:





- Molecule 1: Tri1a PA0618

Chain q: 67% 99%

MET I2 I3 D4 L5 S6 Q7 L8 P9 E10 P11 E12 D18 F19 E20 R31 G36 E37 D45 D67 Y76 G79 A80 D81 L82 D83 N90 R93 L94 L95 I96 R97 P98 A99 Q100 P101 E102 A103 V104 P105 P106 V107 E108 A109 Q110 Y111 D114 K115 R120

L123 Q127 L128 S129 G132 P133 R134 N135 A136 Y137 I138 A139 H140 A141 L142 G143 A144 D145 G146 R147 V148 A149 D150 A151 S152 A153 T154 S155 P156 A157 P158 C159 E160 V161 L162 I163 S164 V165 L166 G167 V168 E169 G170 N171 G172 Q173 A174 P175 E176 A177 V178 L179 Q180 A181 V182 R183 L184

A185 L186 N187 A188 E189 D190 V191 R192 P193 V194 A195 D196 R197 V198 T199 V200 R201 S202 A203 G204 I205 V206 P207 Y208 Q209 V210 K211 A212 Q213 L214 Y215 L216 F217 P218 G219 P220 E221 A222 E223 L224 I225 R226 A227 A228 A229 E230 A231 S232 L233 R234 D235 Y236 I237 S238 A239 Q240 R241 R242 L243 G244

R245 D246 I247 R248 R249 S250 A251 L252 F253 A254 T255 L256 H257 V258 E259 G260 V261 Q262 R263 V264 E265 L266 Q267 E268 P269 A270 A271 D272 V273 V274 L275 D276 E277 T278 Q279 A280 A281 Y282 C283 T284 G285 Y286 A287 I288 T289 L290 G291 G292 VAL ASP GLU

- Molecule 1: Tri1a PA0618

Chain r: 65% 99%

MET I2 I3 D4 L5 S6 Q7 L8 P9 E10 D18 F19 E20 G36 E37 D45 D67 Y76 G79 A80 D81 L82 D83 N90 R93 L94 L95 I96 R97 P98 A99 Q100 P101 E102 A103 V104 P105 P106 V107 E108 A109 Q110 Y111 D114 K115 R120 L123 Q127

G132 P133 R134 N135 A136 Y137 I138 A139 H140 A141 L142 G143 A144 D145 G146 R147 V148 A149 D150 A151 S152 A153 T154 S155 P156 A157 P158 C159 E160 V161 L162 I163 S164 V165 L166 G167 V168 E169 G170 N171 G172 Q173 A174 P175 E176 A177 V178 L179 Q180 A181 V182 R183 L184 A185 L186 N187 A188 E189 D190

V191 R192 P193 V194 A195 D196 R197 V198 T199 V200 R201 S202 A203 G204 I205 V206 P207 Y208 Q209 V210 K211 A212 Q213 L214 Y215 L216 F217 P218 G219 P220 E221 A222 E223 L224 I225 R226 A227 A228 A229 E230 A231 S232 L233 R234 D235 Y236 I237 S238 A239 Q240 R241 R242 L243 G244 R245 D246 I247 R248 R249 S250

A251 L252 F253 A254 T255 L256 H257 V258 E259 G260 V261 Q262 R263 V264 E265 L266 Q267 E268 P269 A270 A271 D272 V273 V274 L275 D276 E277 T278 Q279 A280 A281 Y282 C283 T284 G285 Y286 A287 I288 T289 L290 G291 G292 VAL ASP GLU

- Molecule 1: Tri1a PA0618

Chain o: 66% 99%

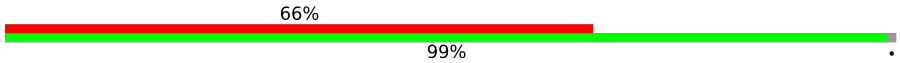
MET I2 I3 D4 L5 S6 Q7 L8 P9 E10 D18 F19 E20 G36 E37 D45 D67 Y76 G79 A80 D81 L82 D83 N90 R93 L94 L95 I96 R97 P98 A99 Q100 P101 E102 A103 V104 P105 P106 V107 E108 A109 Q110 Y111 D114 K115 S116 R120 L123

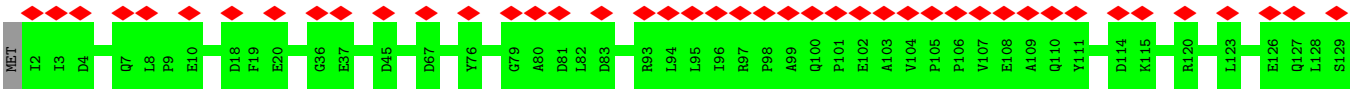
Q127 G132 P133 R134 N135 A136 Y137 I138 A139 H140 A141 L142 G143 A144 D145 G146 R147 V148 A149 D150 A151 S152 A153 T154 S155 P156 A157 P158 C159 E160 V161 L162 I163 S164 V165 L166 G167 V168 E169 G170 N171 G172 Q173 A174 P175 E176 A177 V178 L179 Q180 A181 V182 R183 L184 A185 L186 N187 A188 E189

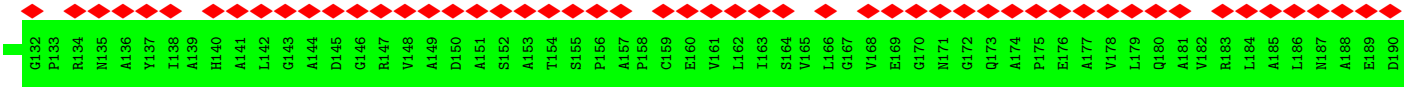
D190 V191 R192 P193 V194 A195 D196 R197 V198 T199 V200 R201 S202 A203 G204 I205 V206 P207 Y208 Q209 V210 K211 A212 Q213 L214 Y215 L216 F217 P218 G219 P220 E221 A222 E223 L224 I225 R226 A227 A228 A229 E230 A231 S232 L233 R234 D235 Y236 I237 S238 A239 Q240 R241 R242 L243 G244 R245 D246 I247 R248 R249

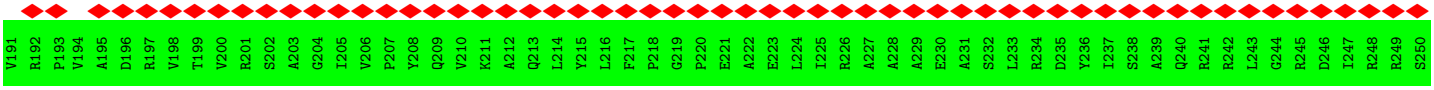
- Molecule 1: Tri1a PA0618

Chain p:



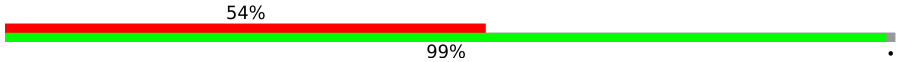


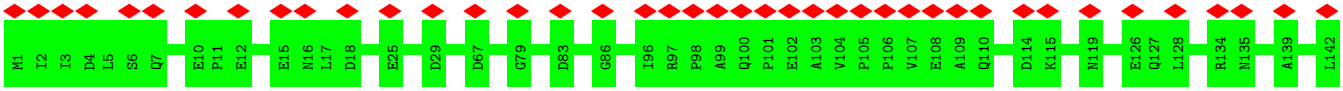


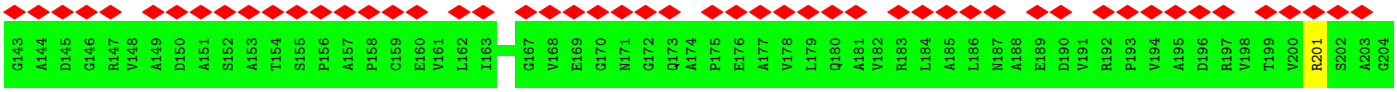


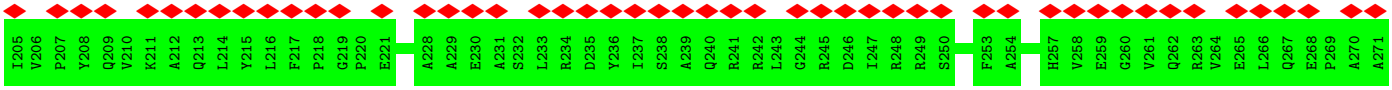
- Molecule 1: Tri1a PA0618

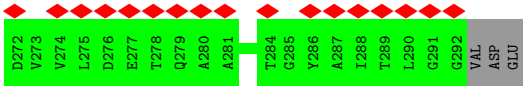
Chain s:





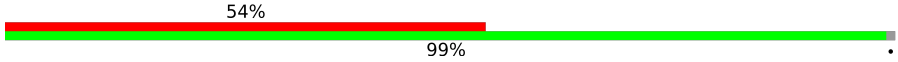


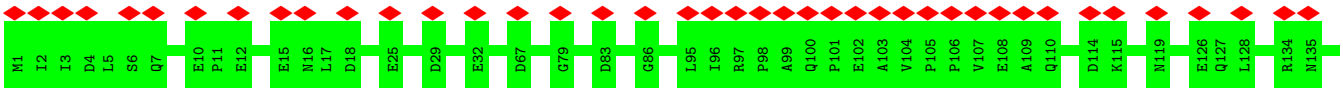


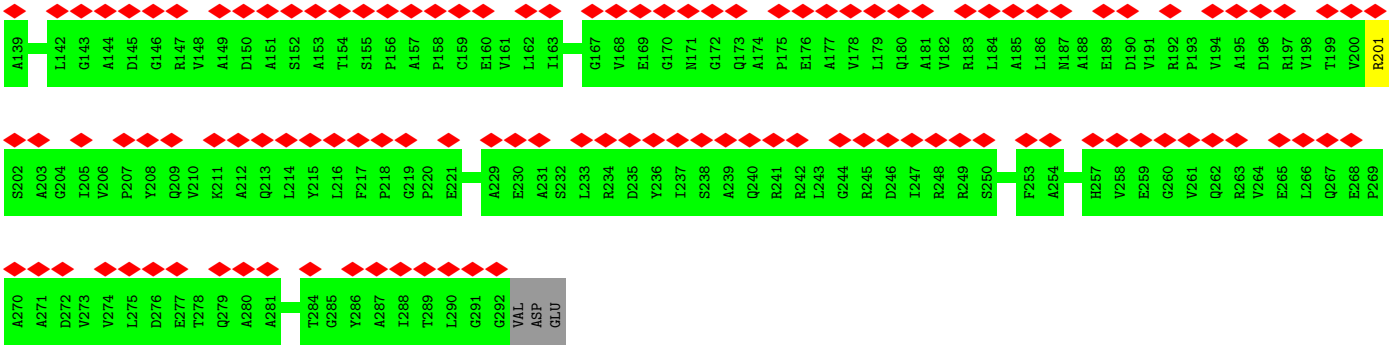


- Molecule 1: Tri1a PA0618

Chain t:

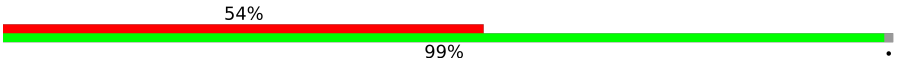


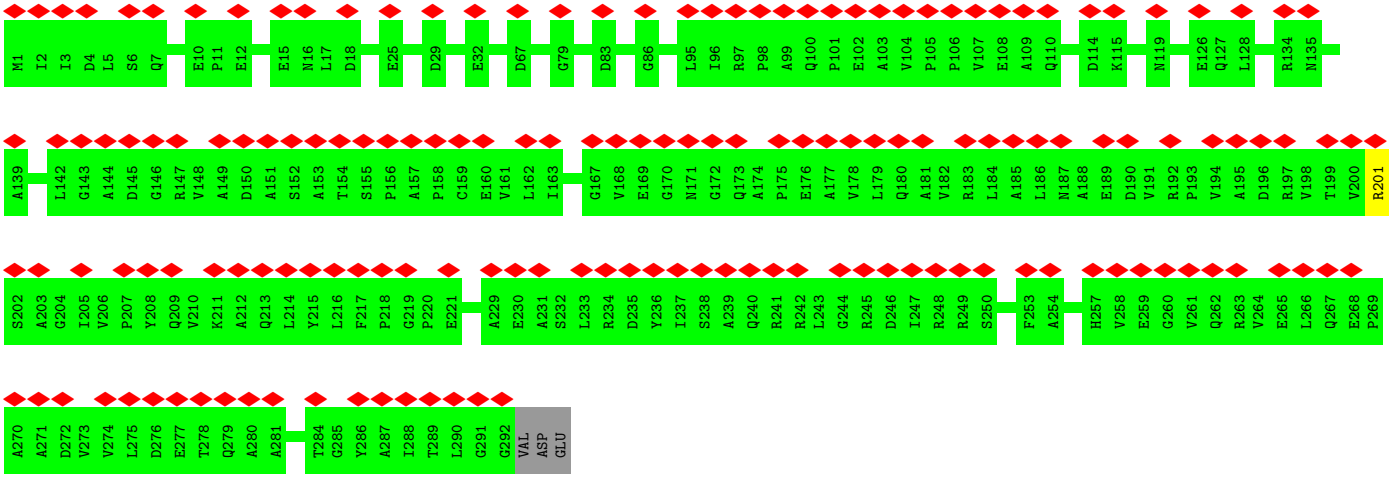




- Molecule 1: Tri1a PA0618

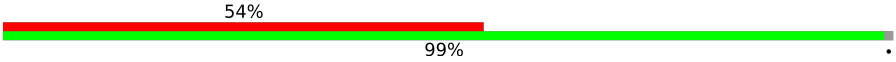
Chain w:

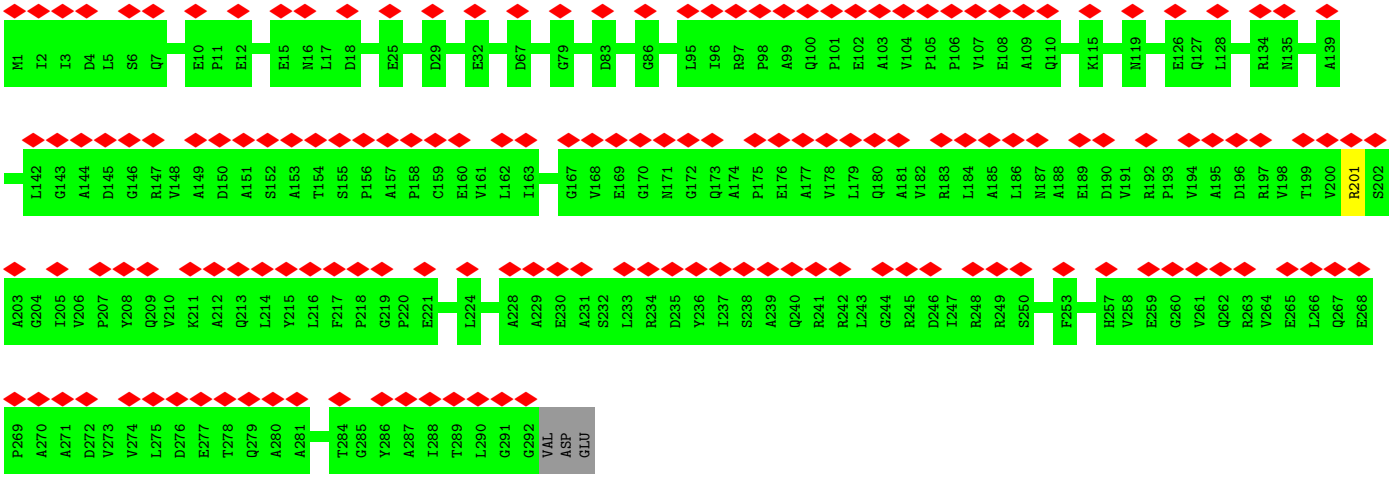




- Molecule 1: Tri1a PA0618

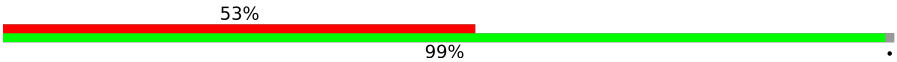
Chain x:

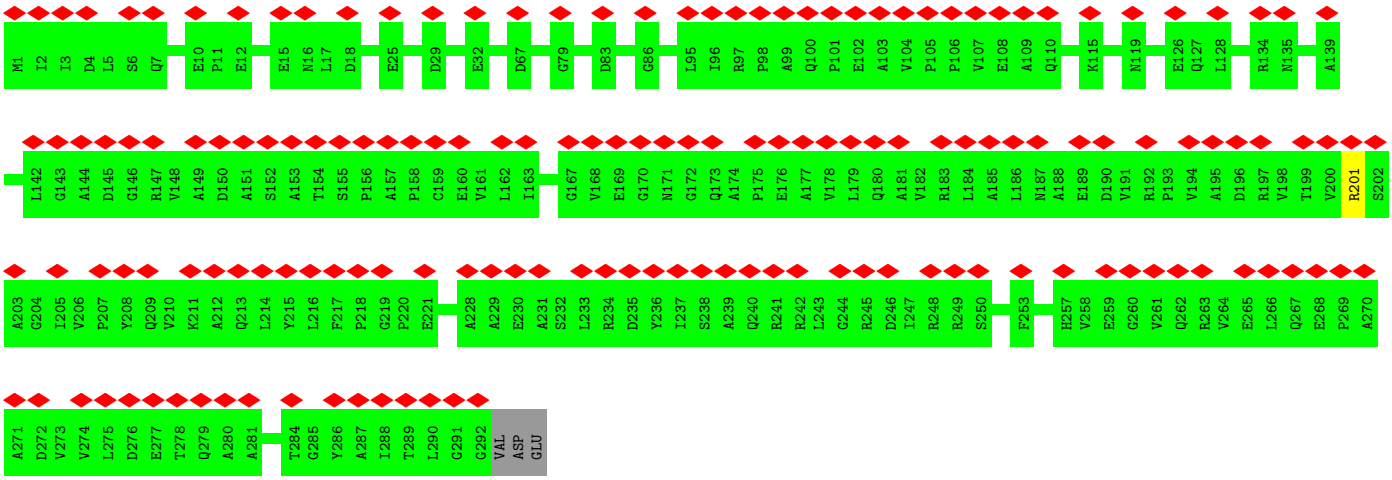




- Molecule 1: Tri1a PA0618

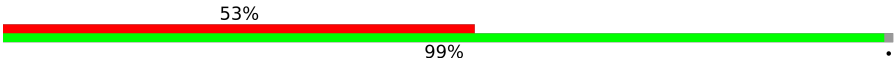
Chain u:

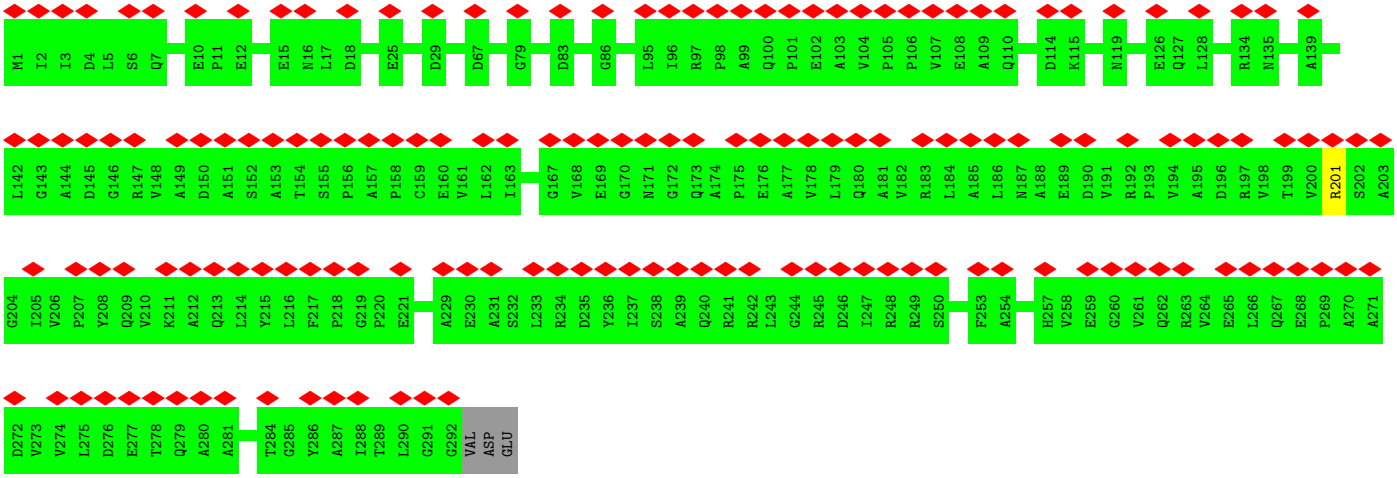




- Molecule 1: Tri1a PA0618

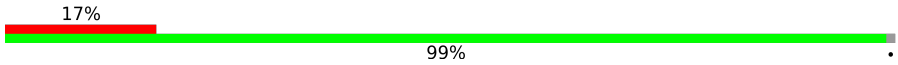
Chain v:

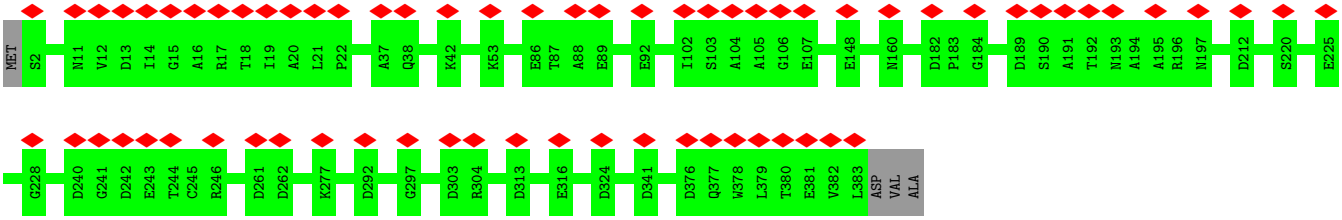




- Molecule 2: Sheath PA0622

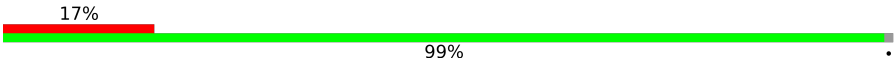
Chain M:

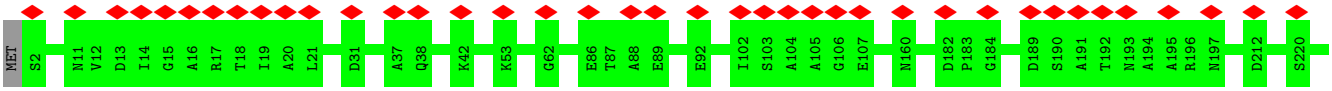


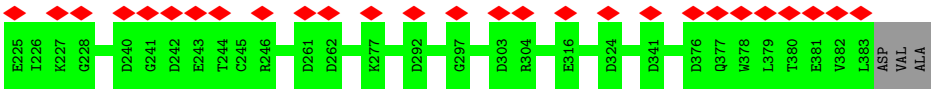


- Molecule 2: Sheath PA0622

Chain N:

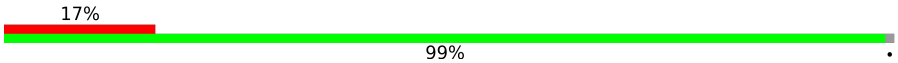


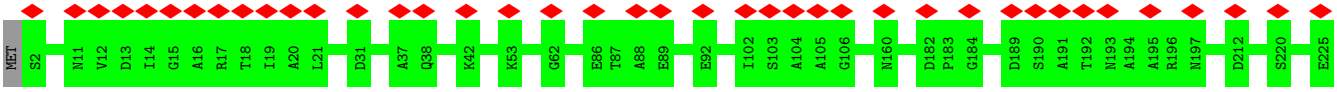


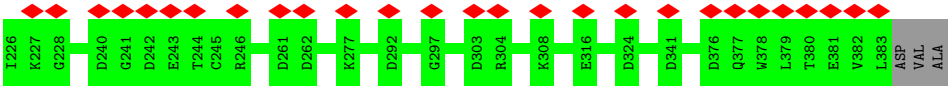


• Molecule 2: Sheath PA0622

Chain Q:

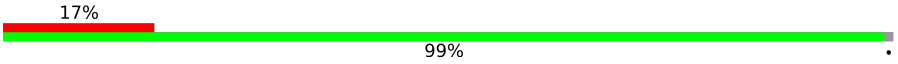


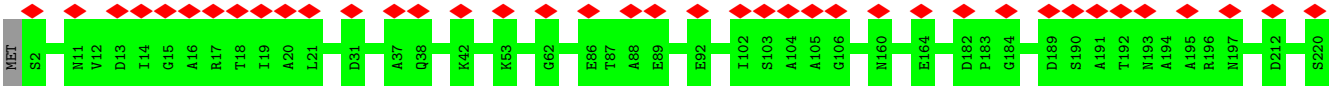


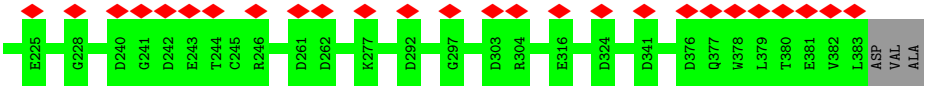


• Molecule 2: Sheath PA0622

Chain R:

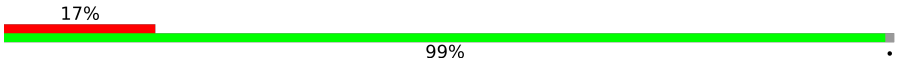


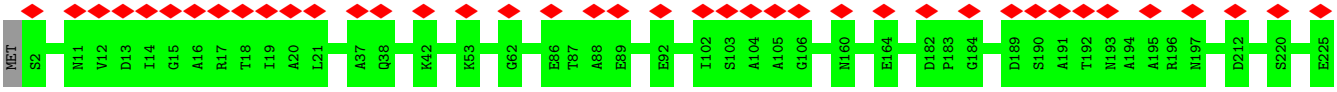


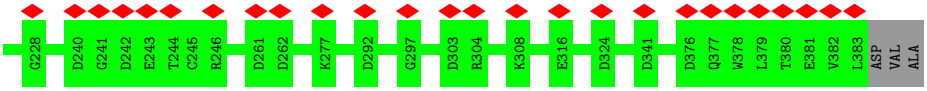


• Molecule 2: Sheath PA0622

Chain O:

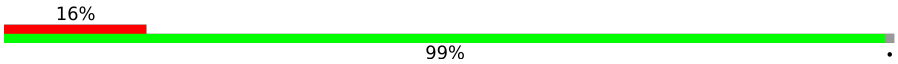


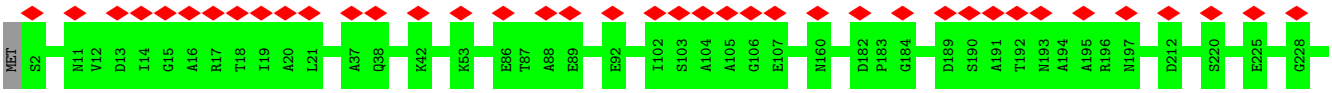


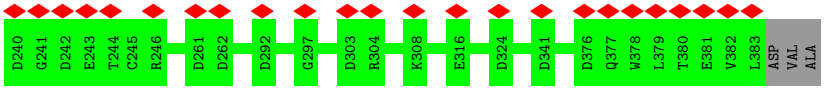


• Molecule 2: Sheath PA0622

Chain P:







• Molecule 2: Sheath PA0622

Chain A: 15% 99%

MET S2 D13 R17 T18 I19 A20 L21 P22 A23 S24 D31 A37 Q38 K42 K53 D54 E70 E86 T87 A88 E89 E92 I102 S103 A104 A105 G106 S119 G145 N160 D163 D182 P183 G184 W188 D189 S190 A191 T192 N193 A194 D212

A213 E214 S220 E225 G228 G241 D242 D261 D262 D275 S276 D292 D303 D313 D324 N333 D341 E381 V382 L383 ASP VAL ALA

- Molecule 2: Sheath PA0622

Chain B: 15% 99%

MET S2 D13 R17 T18 I19 A20 L21 P22 A23 S24 A37 Q38 K42 P43 N44 K53 D54 E70 E86 T87 A88 E89 E92 I102 S103 A104 A105 G106 S119 G145 N160 D163 D182 P183 G184 D189 S190 A191 T192 N193 A194 D212 A213

E214 S220 E225 G228 G241 D242 D261 D262 S276 D292 D303 D313 F321 D324 N333 D341 E381 V382 L383 ASP VAL ALA

- Molecule 2: Sheath PA0622

Chain E: 16% 99%

MET S2 D13 R17 T18 I19 A20 L21 P22 A23 S24 G36 A37 Q38 A39 K42 P43 N44 K53 D54 E70 E86 T87 A88 E89 E92 I102 S103 A104 A105 G106 S119 G145 N160 D163 D182 P183 G184 D189 S190 A191 T192 N193 A194

D212 A213 E214 S220 E225 G228 G241 D242 D261 D262 S276 D292 D303 K312 D313 F321 D324 N333 D341 E381 V382 L383 ASP VAL ALA

- Molecule 2: Sheath PA0622

Chain F: 15% 99%

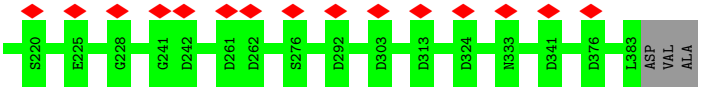
MET S2 D13 R17 T18 I19 A20 L21 P22 A23 S24 T34 A37 Q38 N44 K52 K53 D54 E70 E86 T87 A88 E89 E92 I102 S103 A104 A105 G106 S119 G145 N160 D163 D182 P183 G184 D189 S190 A191 T192 N193 A194 D212

A213 E214 S220 E225 I226 K227 G228 G241 D242 D261 D262 S276 D292 D303 D313 D324 D341 E381 V382 L383 ASP VAL ALA

- Molecule 2: Sheath PA0622

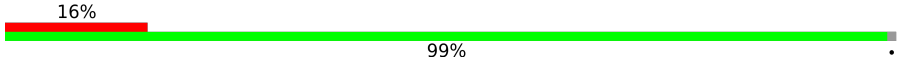
Chain C: 14% 99%

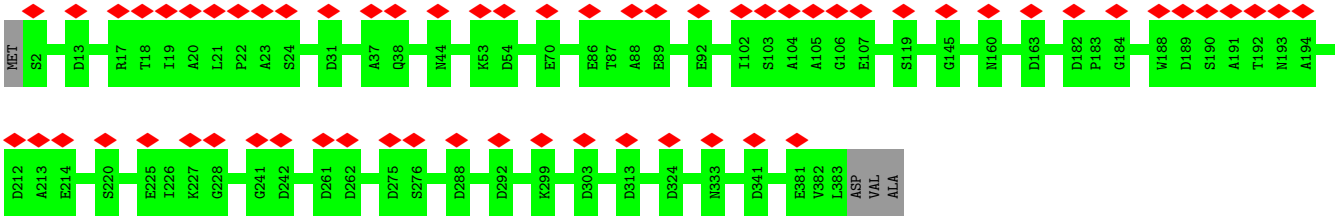
MET S2 D13 R17 T18 I19 A20 L21 P22 A23 S24 T34 A37 Q38 K42 K53 D54 E70 E86 T87 A88 E89 E92 I102 S103 A104 A105 G106 S119 N160 D163 D182 P183 G184 W188 D189 S190 A191 T192 N193 A194 D212 A213 E214



• Molecule 2: Sheath PA0622

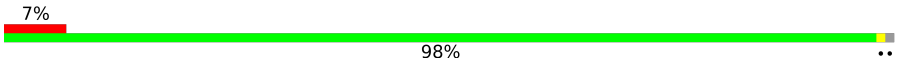
Chain D:

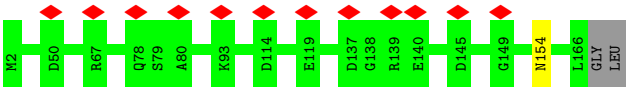




• Molecule 3: Tube PA0623

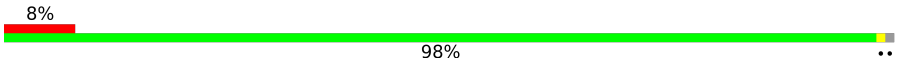
Chain S:

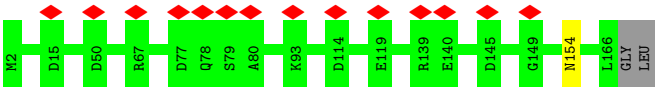




• Molecule 3: Tube PA0623

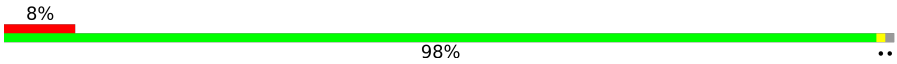
Chain T:

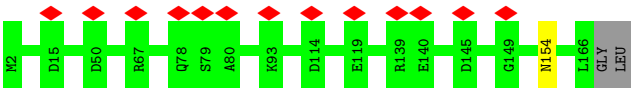




• Molecule 3: Tube PA0623

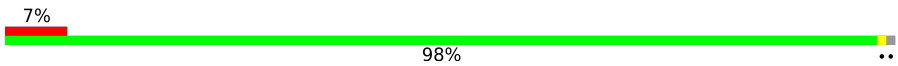
Chain W:

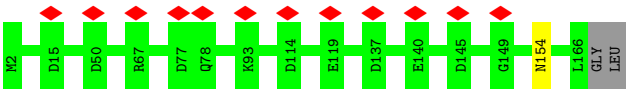




• Molecule 3: Tube PA0623

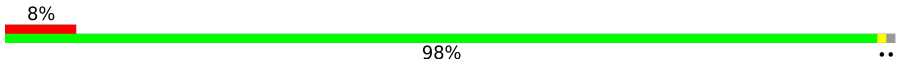
Chain X:

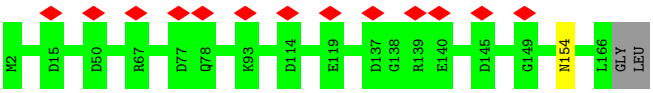




• Molecule 3: Tube PA0623

Chain U:





• Molecule 3: Tube PA0623

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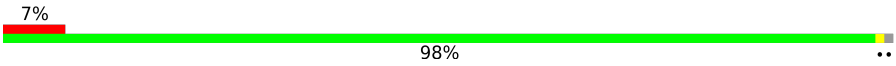
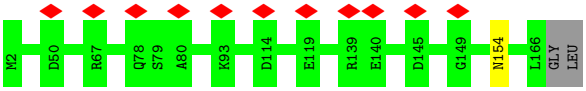
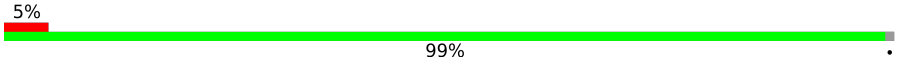
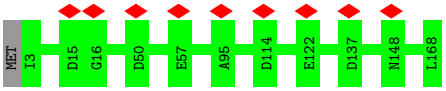




• Molecule 3: Tube PA0623

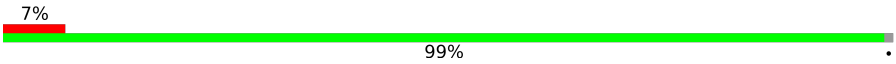
Chain G:

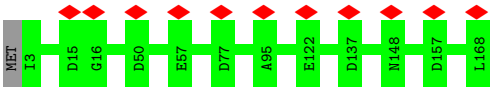




• Molecule 3: Tube PA0623

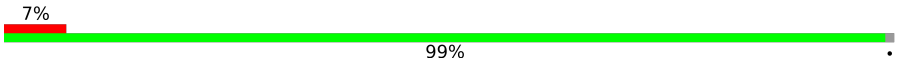
Chain H:

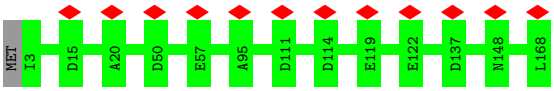




• Molecule 3: Tube PA0623

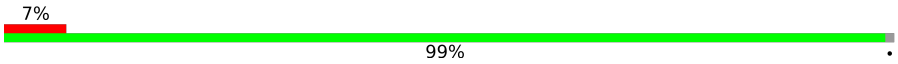
Chain K:

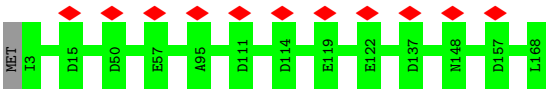




• Molecule 3: Tube PA0623

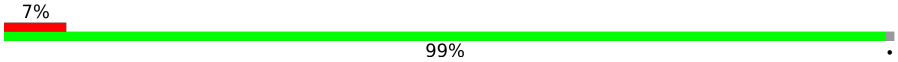
Chain L:

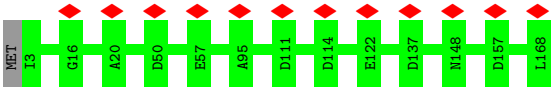




• Molecule 3: Tube PA0623

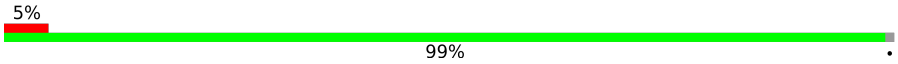
Chain I:

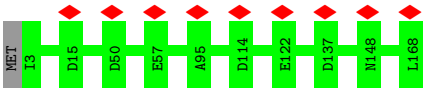




• Molecule 3: Tube PA0623

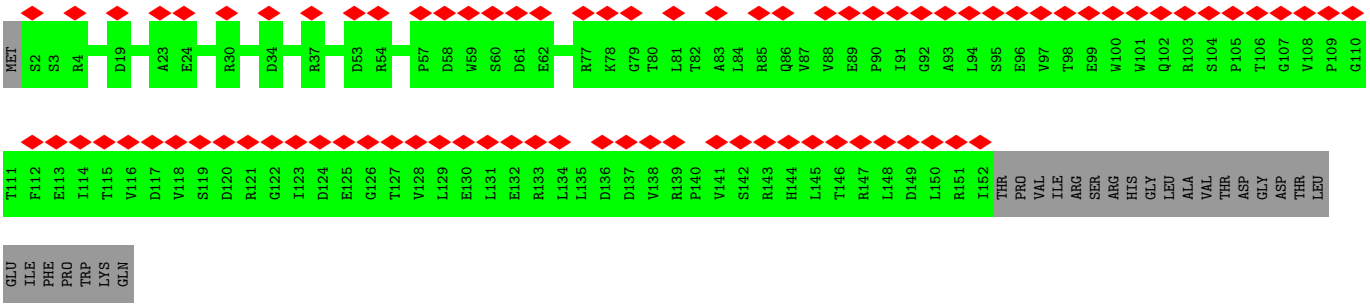
Chain J:





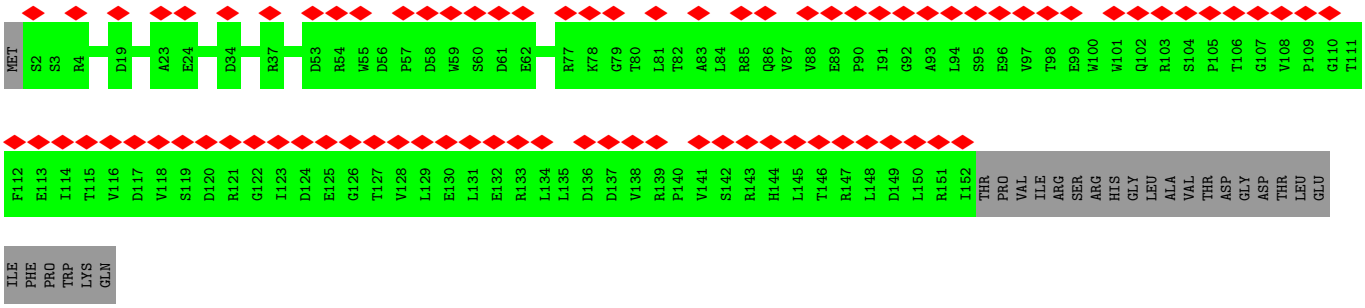
• Molecule 4: Tri2 PA0619

Chain 0:



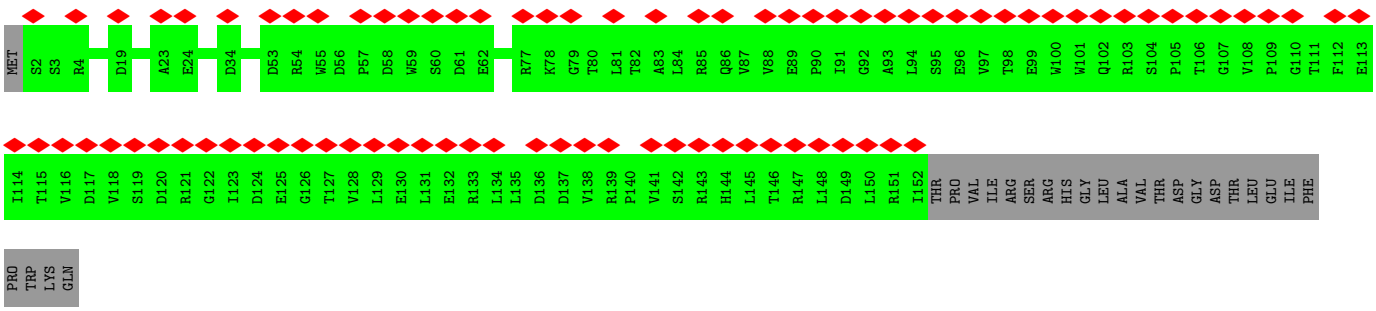
• Molecule 4: Tri2 PA0619

Chain 1:



• Molecule 4: Tri2 PA0619

Chain 4:



• Molecule 4: Tri2 PA0619

Chain 5:

- Molecule 4: Tri2 PA0619

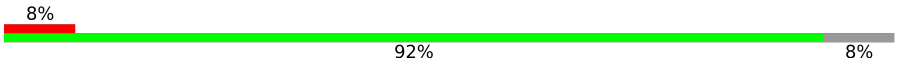
Chain 2:

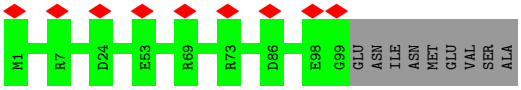
- Molecule 4: Tri2 PA0619

Chain 3:

- Molecule 5: Sheath Initiator PA0617

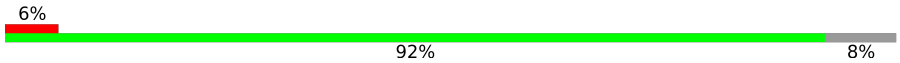
Chain a:

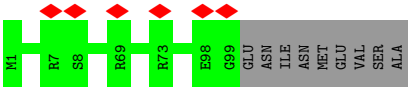




- Molecule 5: Sheath Initiator PA0617

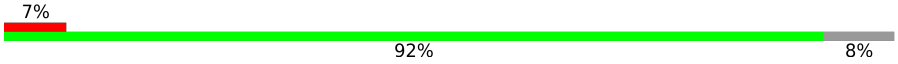
Chain b:

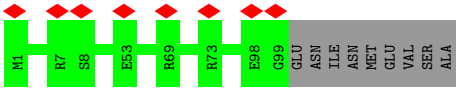




• Molecule 5: Sheath Initiator PA0617

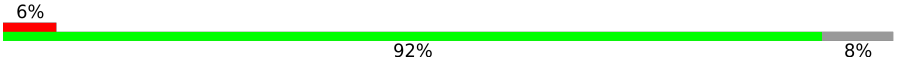
Chain e:

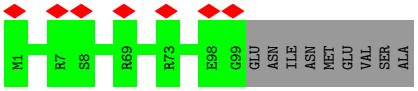




• Molecule 5: Sheath Initiator PA0617

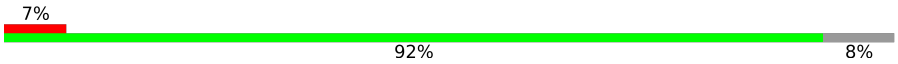
Chain f:

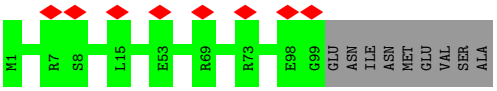




• Molecule 5: Sheath Initiator PA0617

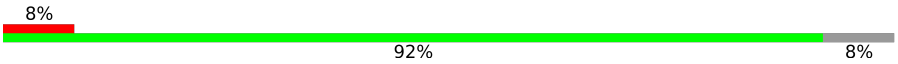
Chain c:

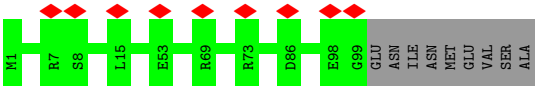




• Molecule 5: Sheath Initiator PA0617

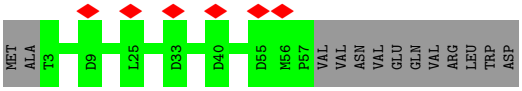
Chain d:





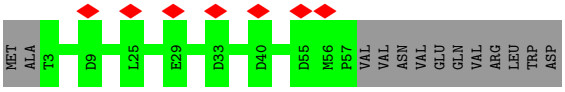
• Molecule 6: Glue PA0627

Chain 6:



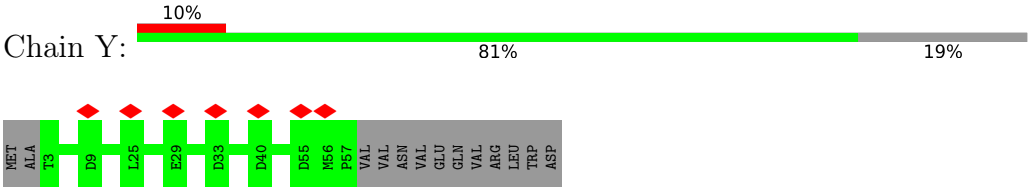
• Molecule 6: Glue PA0627

Chain 7:



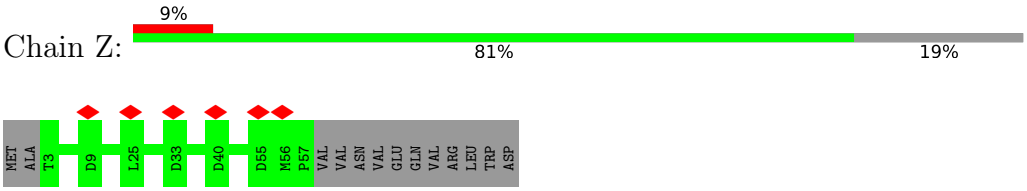
• Molecule 6: Glue PA0627

Chain Y:



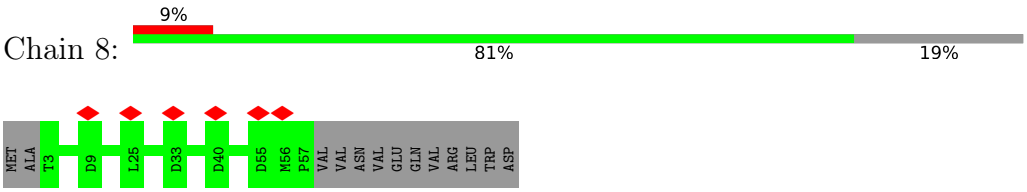
• Molecule 6: Glue PA0627

Chain Z:



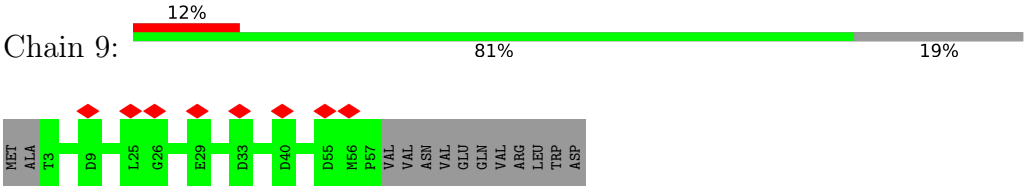
• Molecule 6: Glue PA0627

Chain 8:



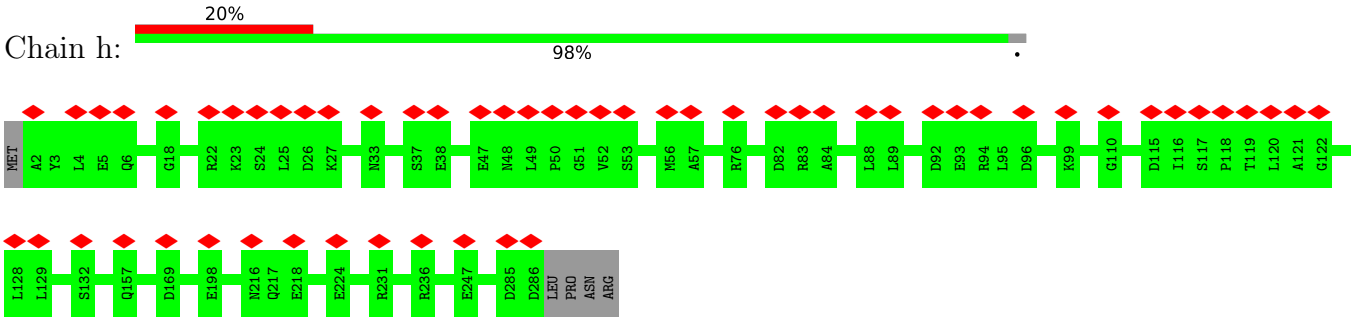
• Molecule 6: Glue PA0627

Chain 9:



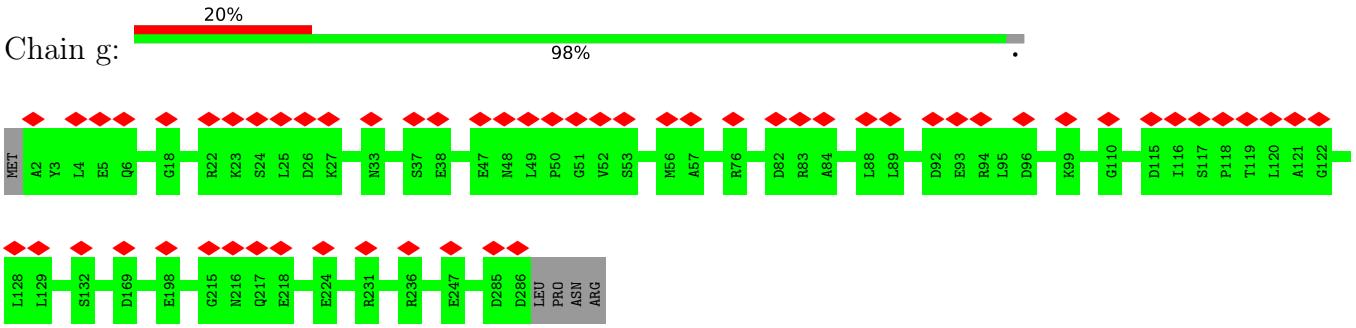
• Molecule 7: Ripcord PA0626

Chain h:



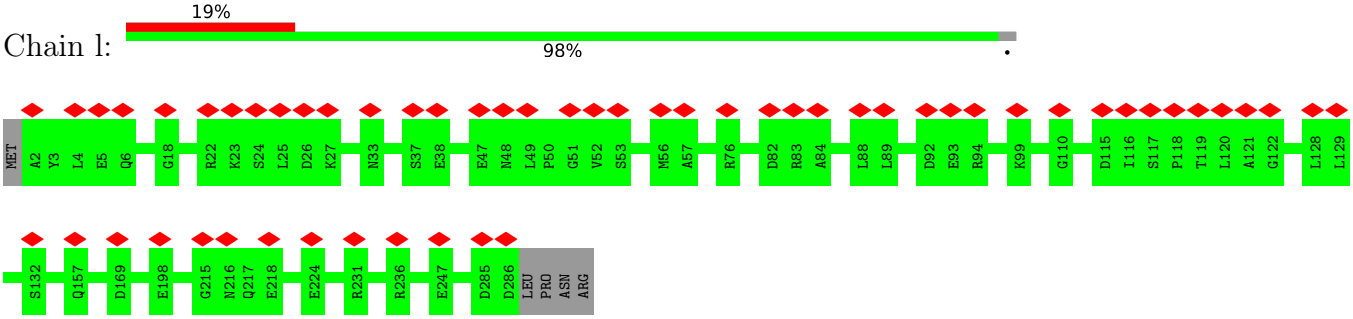
• Molecule 7: Ripcord PA0626

Chain g:



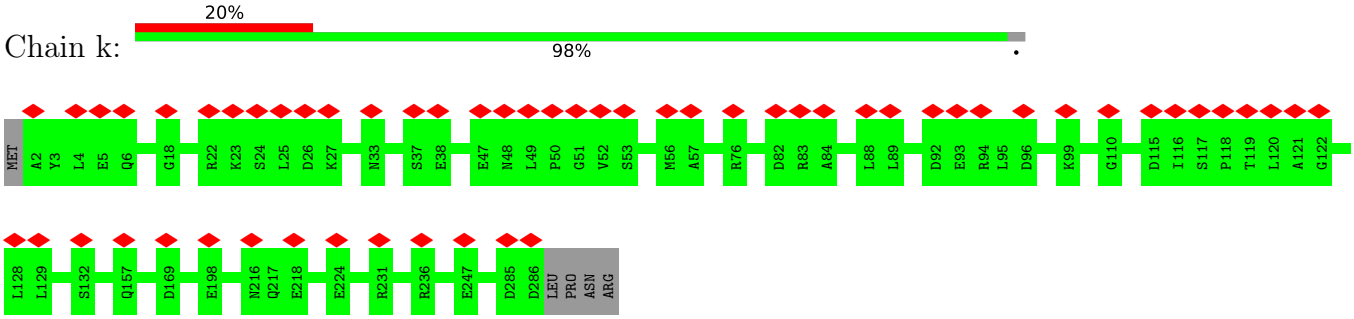
- Molecule 7: Ripcord PA0626

Chain l:



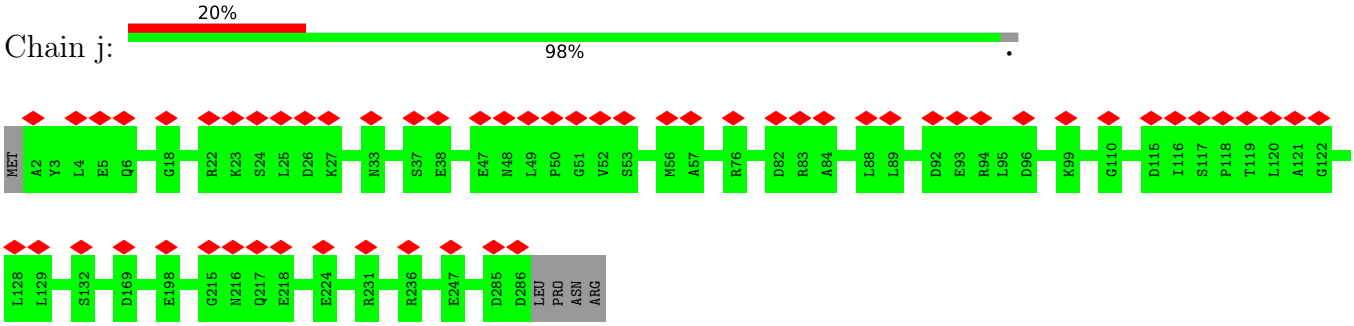
- Molecule 7: Ripcord PA0626

Chain k:



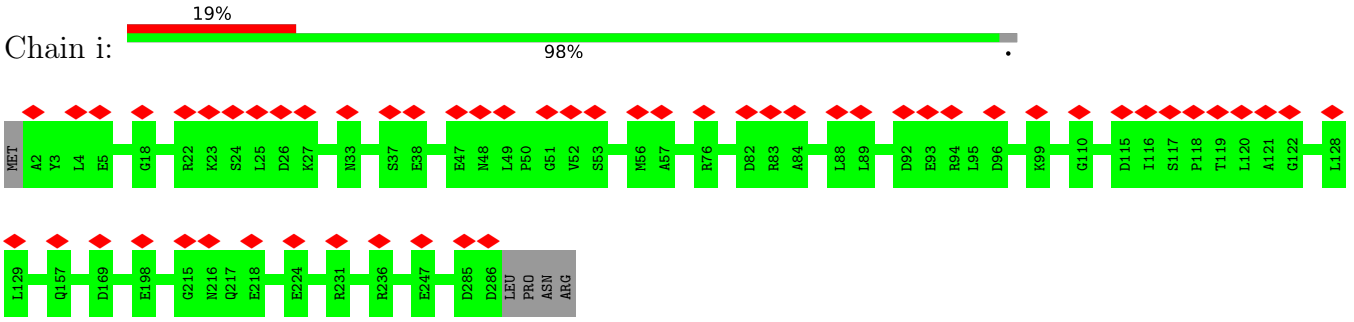
- Molecule 7: Ripcord PA0626

Chain j:



- Molecule 7: Ripcord PA0626

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	22001	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.086	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	333.12, 333.12, 333.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	m	0.28	0/2253	0.58	0/3069
1	n	0.28	0/2253	0.58	0/3069
1	o	0.28	0/2253	0.58	0/3069
1	p	0.28	0/2253	0.58	0/3069
1	q	0.28	0/2253	0.58	0/3069
1	r	0.28	0/2253	0.58	0/3069
1	s	0.30	0/2258	0.56	0/3076
1	t	0.30	0/2258	0.56	0/3076
1	u	0.29	0/2258	0.56	0/3076
1	v	0.29	0/2258	0.56	0/3076
1	w	0.29	0/2258	0.56	0/3076
1	x	0.30	0/2258	0.56	0/3076
2	A	0.30	0/2934	0.55	0/3999
2	B	0.30	0/2934	0.55	0/3999
2	C	0.29	0/2934	0.55	0/3999
2	D	0.29	0/2934	0.55	0/3999
2	E	0.29	0/2934	0.55	0/3999
2	F	0.29	0/2934	0.56	0/3999
2	M	0.30	0/2934	0.55	0/3999
2	N	0.30	0/2934	0.55	0/3999
2	O	0.30	0/2934	0.55	0/3999
2	P	0.30	0/2934	0.55	0/3999
2	Q	0.30	0/2934	0.55	0/3999
2	R	0.30	0/2934	0.55	0/3999
3	G	0.34	0/1277	0.59	0/1724
3	H	0.34	0/1277	0.60	0/1724
3	I	0.34	0/1277	0.60	0/1724
3	J	0.34	0/1277	0.60	0/1724
3	K	0.34	0/1277	0.60	0/1724
3	L	0.34	0/1277	0.60	0/1724
3	S	0.33	0/1272	0.58	0/1718
3	T	0.33	0/1272	0.58	0/1718
3	U	0.33	0/1272	0.58	0/1718
3	V	0.33	0/1272	0.58	0/1718

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	W	0.33	0/1272	0.58	0/1718
3	X	0.33	0/1272	0.58	0/1718
4	0	0.28	0/1229	0.59	0/1680
4	1	0.28	0/1229	0.59	0/1680
4	2	0.28	0/1229	0.59	0/1680
4	3	0.28	0/1229	0.59	0/1680
4	4	0.28	0/1229	0.59	0/1680
4	5	0.28	0/1229	0.59	0/1680
5	a	0.30	0/770	0.56	0/1036
5	b	0.30	0/770	0.56	0/1036
5	c	0.30	0/770	0.56	0/1036
5	d	0.30	0/770	0.56	0/1036
5	e	0.30	0/770	0.56	0/1036
5	f	0.30	0/770	0.56	0/1036
6	6	0.29	0/422	0.56	0/575
6	7	0.29	0/422	0.56	0/575
6	8	0.29	0/422	0.56	0/575
6	9	0.29	0/422	0.56	0/575
6	Y	0.29	0/422	0.56	0/575
6	Z	0.29	0/422	0.56	0/575
7	g	0.31	0/2194	0.58	0/2970
7	h	0.31	0/2194	0.58	0/2970
7	i	0.31	0/2194	0.58	0/2970
7	j	0.31	0/2194	0.58	0/2970
7	k	0.31	0/2194	0.58	0/2970
7	l	0.31	0/2194	0.58	0/2970
All	All	0.30	0/105258	0.57	0/143076

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	m	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	n	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	o	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	p	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	q	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	r	289/295 (98%)	265 (92%)	24 (8%)	0	100	100
1	s	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	t	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	u	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	v	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	w	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
1	x	290/295 (98%)	269 (93%)	21 (7%)	0	100	100
2	A	380/386 (98%)	345 (91%)	35 (9%)	0	100	100
2	B	380/386 (98%)	345 (91%)	35 (9%)	0	100	100
2	C	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	D	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	E	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	F	380/386 (98%)	346 (91%)	34 (9%)	0	100	100
2	M	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	N	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	O	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	P	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	Q	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
2	R	380/386 (98%)	341 (90%)	39 (10%)	0	100	100
3	G	164/167 (98%)	144 (88%)	20 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	I	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	J	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	K	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	L	164/167 (98%)	144 (88%)	20 (12%)	0	100	100
3	S	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	T	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	U	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	V	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	W	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
3	X	163/167 (98%)	149 (91%)	14 (9%)	0	100	100
4	0	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	1	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	2	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	3	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	4	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
4	5	149/177 (84%)	136 (91%)	13 (9%)	0	100	100
5	a	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	b	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	c	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	d	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	e	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
5	f	97/108 (90%)	90 (93%)	7 (7%)	0	100	100
6	6	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	7	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	8	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	9	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	Y	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
6	Z	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
7	g	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	h	283/290 (98%)	259 (92%)	24 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	i	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	j	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	k	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
7	l	283/290 (98%)	259 (92%)	24 (8%)	0	100	100
All	All	13488/14034 (96%)	12292 (91%)	1196 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	m	226/230 (98%)	226 (100%)	0	100	100
1	n	226/230 (98%)	226 (100%)	0	100	100
1	o	226/230 (98%)	226 (100%)	0	100	100
1	p	226/230 (98%)	226 (100%)	0	100	100
1	q	226/230 (98%)	226 (100%)	0	100	100
1	r	226/230 (98%)	226 (100%)	0	100	100
1	s	226/230 (98%)	225 (100%)	1 (0%)	91	96
1	t	226/230 (98%)	225 (100%)	1 (0%)	91	96
1	u	226/230 (98%)	225 (100%)	1 (0%)	91	96
1	v	226/230 (98%)	225 (100%)	1 (0%)	91	96
1	w	226/230 (98%)	225 (100%)	1 (0%)	91	96
1	x	226/230 (98%)	225 (100%)	1 (0%)	91	96
2	A	295/298 (99%)	295 (100%)	0	100	100
2	B	295/298 (99%)	295 (100%)	0	100	100
2	C	295/298 (99%)	295 (100%)	0	100	100
2	D	295/298 (99%)	295 (100%)	0	100	100
2	E	295/298 (99%)	295 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	295/298 (99%)	295 (100%)	0	100	100
2	M	295/298 (99%)	295 (100%)	0	100	100
2	N	295/298 (99%)	295 (100%)	0	100	100
2	O	295/298 (99%)	295 (100%)	0	100	100
2	P	295/298 (99%)	295 (100%)	0	100	100
2	Q	295/298 (99%)	295 (100%)	0	100	100
2	R	295/298 (99%)	295 (100%)	0	100	100
3	G	129/130 (99%)	129 (100%)	0	100	100
3	H	129/130 (99%)	129 (100%)	0	100	100
3	I	129/130 (99%)	129 (100%)	0	100	100
3	J	129/130 (99%)	129 (100%)	0	100	100
3	K	129/130 (99%)	129 (100%)	0	100	100
3	L	129/130 (99%)	129 (100%)	0	100	100
3	S	129/130 (99%)	128 (99%)	1 (1%)	81	91
3	T	129/130 (99%)	128 (99%)	1 (1%)	81	91
3	U	129/130 (99%)	128 (99%)	1 (1%)	81	91
3	V	129/130 (99%)	128 (99%)	1 (1%)	81	91
3	W	129/130 (99%)	128 (99%)	1 (1%)	81	91
3	X	129/130 (99%)	128 (99%)	1 (1%)	81	91
4	0	134/157 (85%)	134 (100%)	0	100	100
4	1	134/157 (85%)	134 (100%)	0	100	100
4	2	134/157 (85%)	134 (100%)	0	100	100
4	3	134/157 (85%)	134 (100%)	0	100	100
4	4	134/157 (85%)	134 (100%)	0	100	100
4	5	134/157 (85%)	134 (100%)	0	100	100
5	a	82/90 (91%)	82 (100%)	0	100	100
5	b	82/90 (91%)	82 (100%)	0	100	100
5	c	82/90 (91%)	82 (100%)	0	100	100
5	d	82/90 (91%)	82 (100%)	0	100	100
5	e	82/90 (91%)	82 (100%)	0	100	100
5	f	82/90 (91%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	45/57 (79%)	45 (100%)	0	100	100
6	7	45/57 (79%)	45 (100%)	0	100	100
6	8	45/57 (79%)	45 (100%)	0	100	100
6	9	45/57 (79%)	45 (100%)	0	100	100
6	Y	45/57 (79%)	45 (100%)	0	100	100
6	Z	45/57 (79%)	45 (100%)	0	100	100
7	g	221/226 (98%)	221 (100%)	0	100	100
7	h	221/226 (98%)	221 (100%)	0	100	100
7	i	221/226 (98%)	221 (100%)	0	100	100
7	j	221/226 (98%)	221 (100%)	0	100	100
7	k	221/226 (98%)	221 (100%)	0	100	100
7	l	221/226 (98%)	221 (100%)	0	100	100
All	All	10692/11076 (96%)	10680 (100%)	12 (0%)	93	98

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

Mol	Chain	Res	Type
3	S	154	ASN
3	T	154	ASN
3	W	154	ASN
3	X	154	ASN
3	U	154	ASN
3	V	154	ASN
1	s	201	ARG
1	t	201	ARG
1	w	201	ARG
1	x	201	ARG
1	u	201	ARG
1	v	201	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	m	66	ASN
1	m	119	ASN
2	M	5	HIS
2	M	252	ASN

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Mol	Chain	Res	Type
3	S	154	ASN
3	S	158	GLN
4	0	144	HIS
7	h	150	GLN
1	n	66	ASN
1	n	119	ASN
1	q	66	ASN
1	q	119	ASN
1	r	66	ASN
1	r	119	ASN
1	o	119	ASN
1	p	24	GLN
1	p	119	ASN
4	1	144	HIS
4	4	144	HIS
4	5	144	HIS
4	2	144	HIS
4	3	144	HIS
3	T	37	GLN
3	T	154	ASN
3	T	158	GLN
3	W	37	GLN
3	W	154	ASN
3	W	158	GLN
3	X	37	GLN
3	X	154	ASN
3	X	158	GLN
3	U	154	ASN
3	U	158	GLN
3	V	154	ASN
3	V	158	GLN
2	N	5	HIS
2	N	252	ASN
2	Q	5	HIS
2	Q	252	ASN
2	R	5	HIS
2	R	252	ASN
2	R	369	ASN
2	O	5	HIS
2	O	252	ASN
2	P	5	HIS
2	P	252	ASN

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Mol	Chain	Res	Type
7	g	150	GLN
7	l	150	GLN
7	k	150	GLN
7	j	150	GLN
7	i	150	GLN
1	s	84	GLN
1	s	140	HIS
2	A	133	HIS
2	A	252	ASN
2	A	269	ASN
2	A	369	ASN
2	B	133	HIS
2	B	369	ASN
2	E	133	HIS
2	E	252	ASN
2	E	269	ASN
2	E	369	ASN
2	F	133	HIS
2	F	269	ASN
2	F	369	ASN
2	C	133	HIS
2	C	369	ASN
2	D	133	HIS
2	D	369	ASN
3	K	71	ASN
1	t	84	GLN
1	t	140	HIS
1	w	84	GLN
1	w	140	HIS
1	x	84	GLN
1	x	140	HIS
1	u	84	GLN
1	u	140	HIS
1	v	84	GLN
1	v	140	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

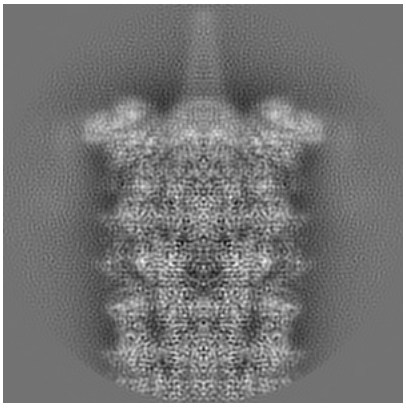
6 Map visualisation (i)

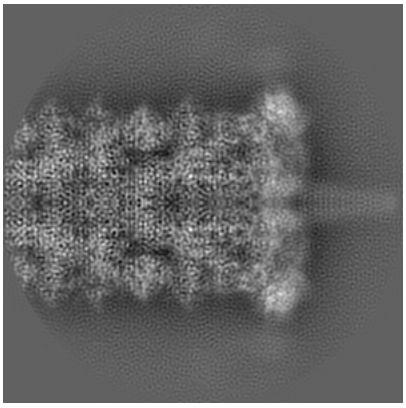
This section contains visualisations of the EMDB entry EMD-20643. These allow visual inspection of the internal detail of the map and identification of artifacts.

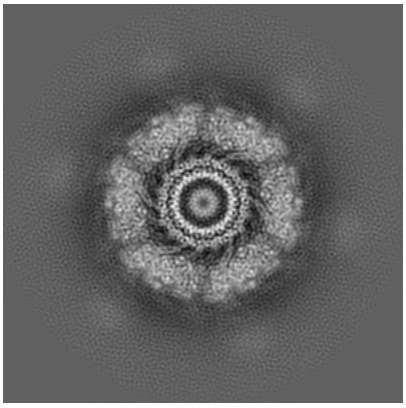
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

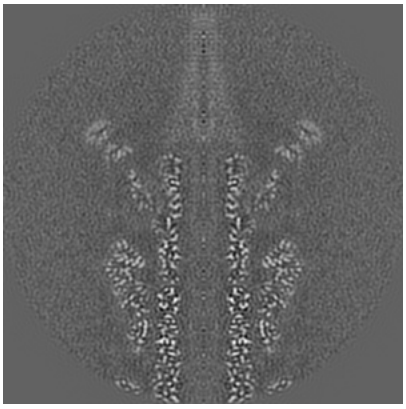

Y

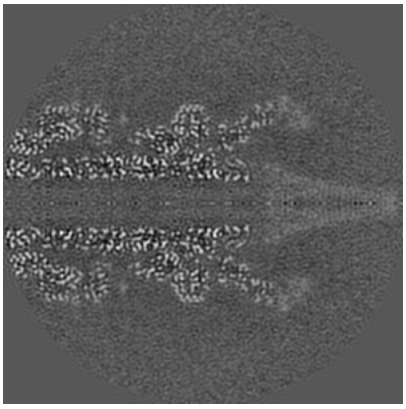

Z

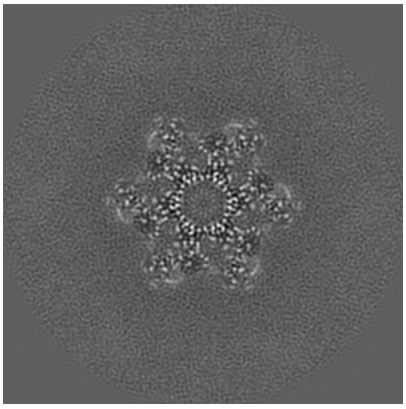
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 160

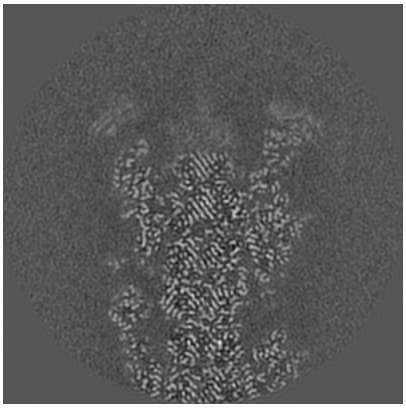

Y Index: 160

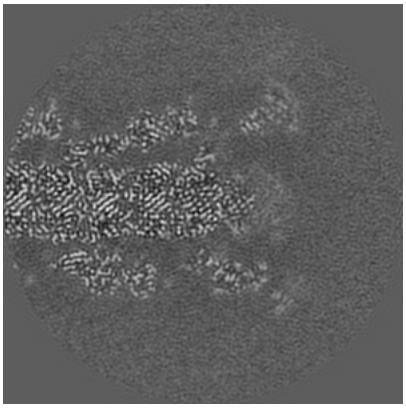

Z Index: 160

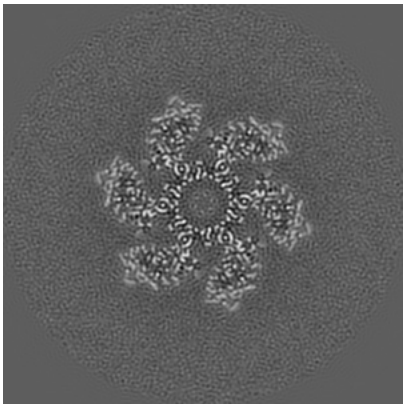
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 139

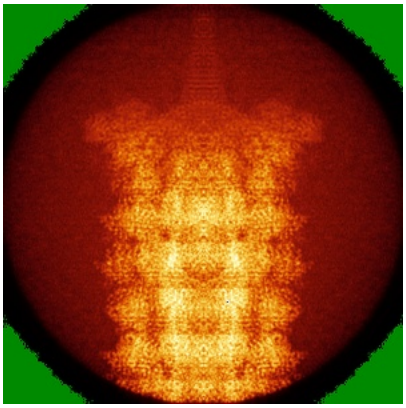

Y Index: 137

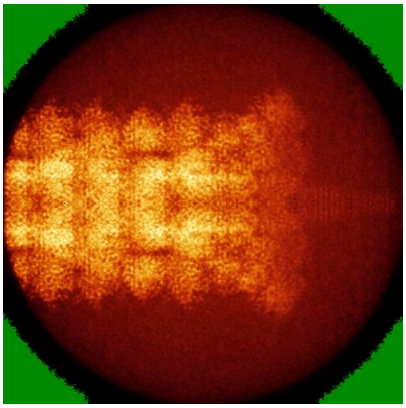

Z Index: 149

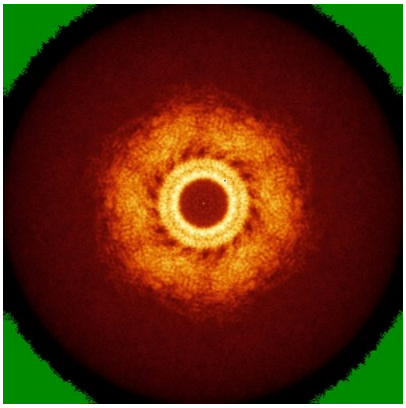
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

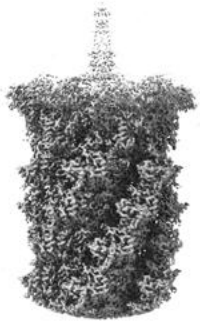

Y


Z

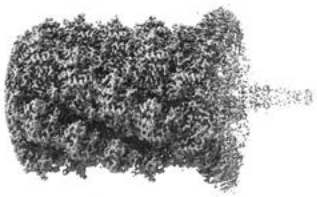
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

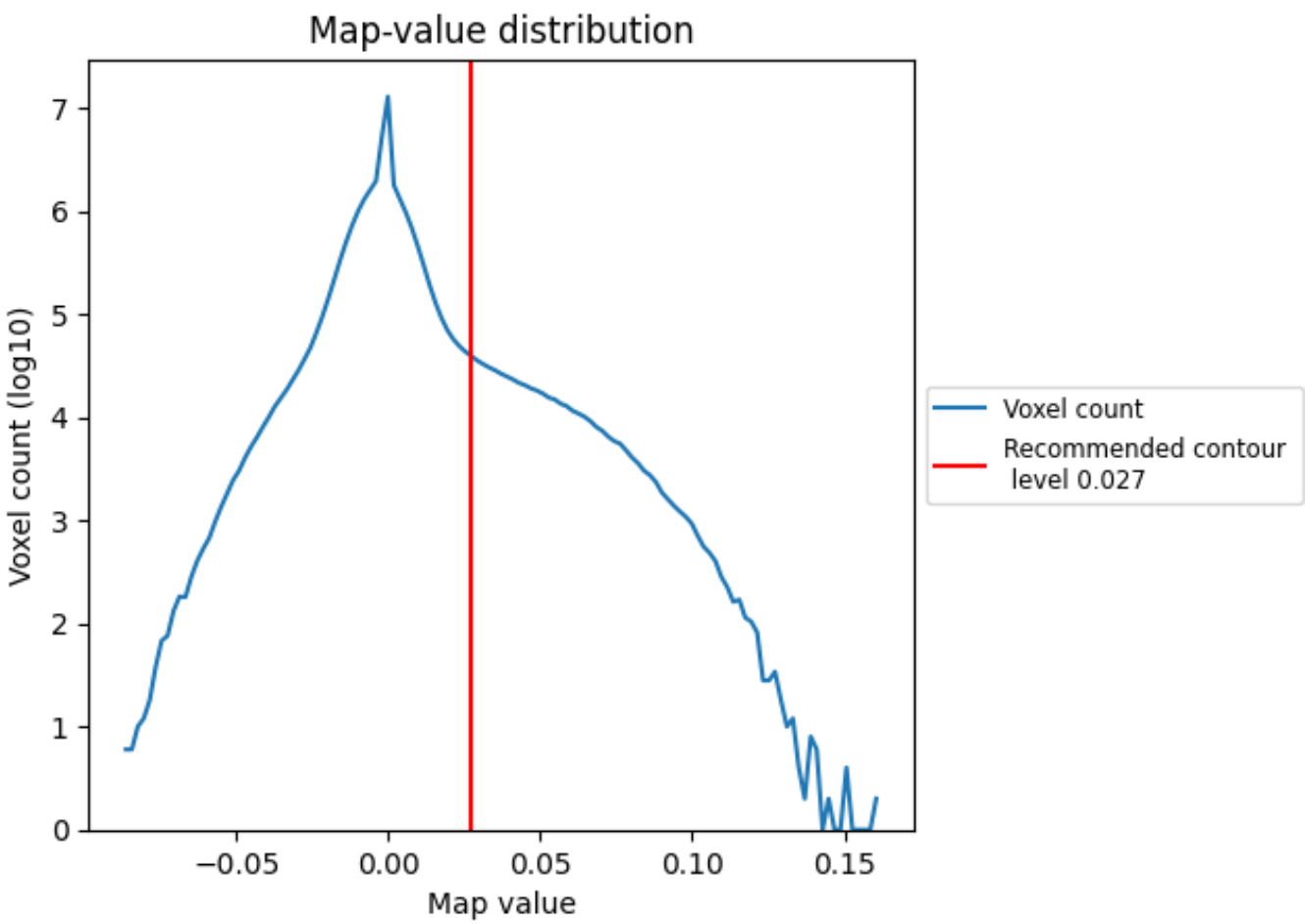
6.6 Mask visualisation (i)

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

7 Map analysis (i)

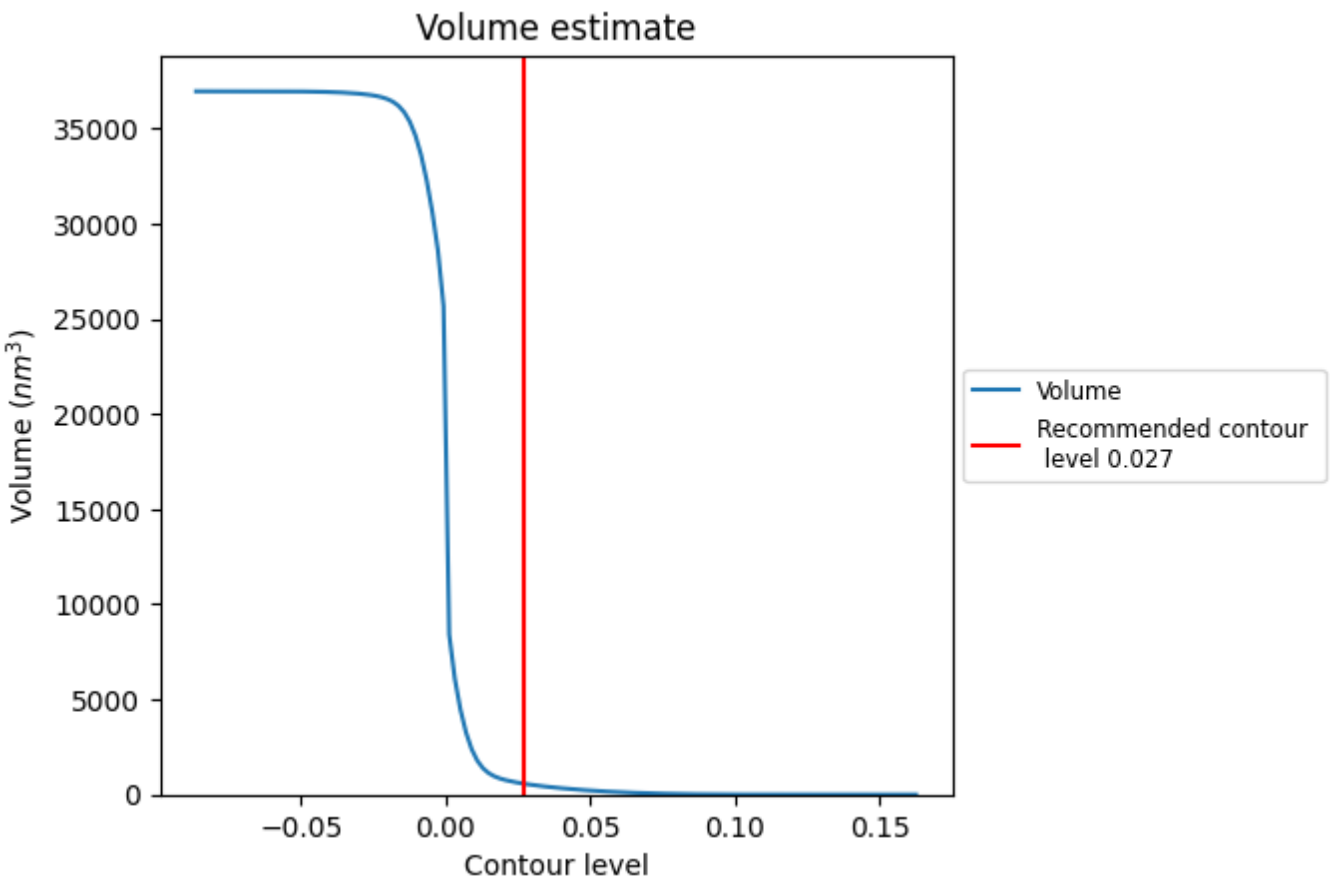
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

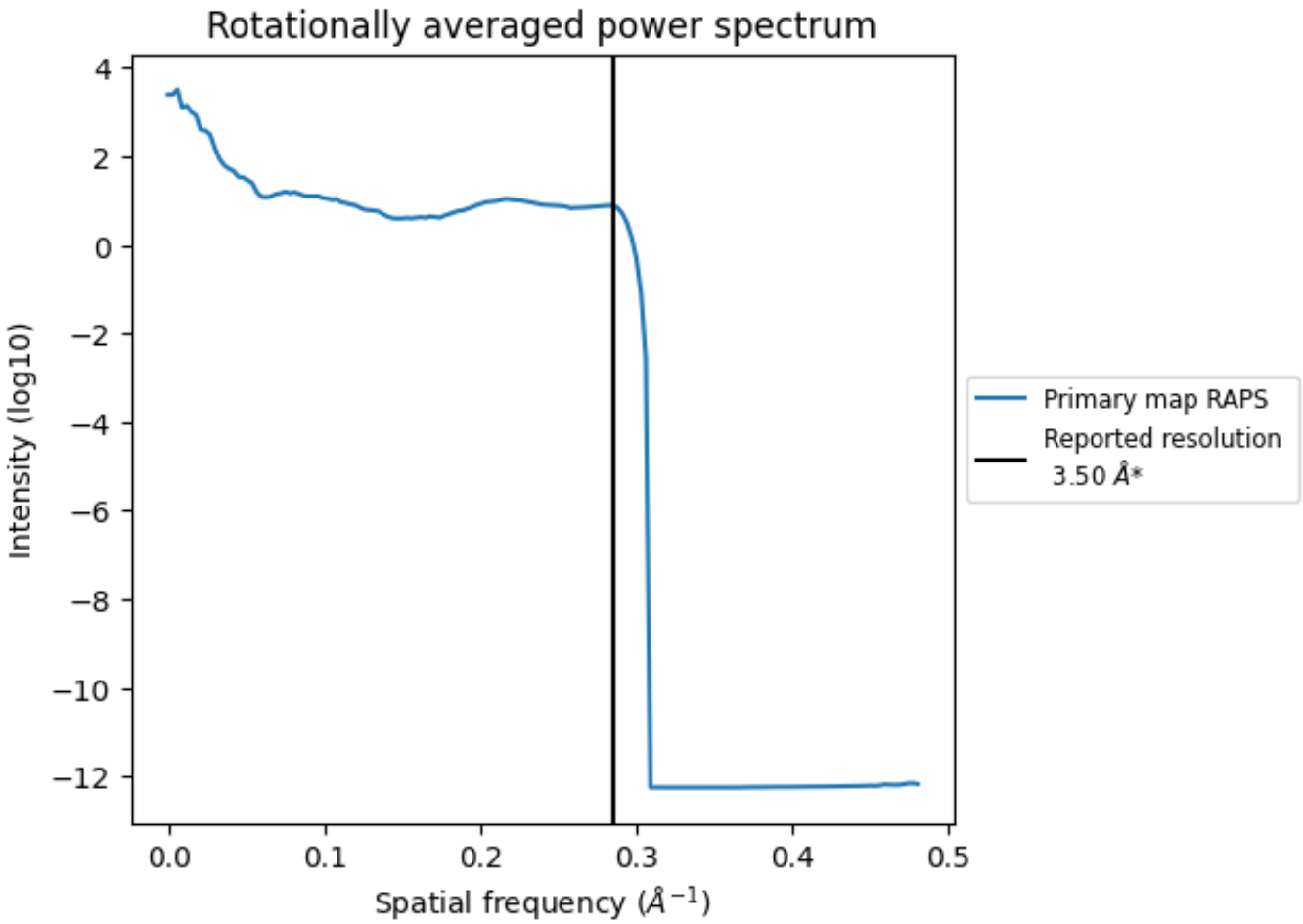
7.2 Volume estimate (i)



The volume at the recommended contour level is 571 nm^3; this corresponds to an approximate mass of 516 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)

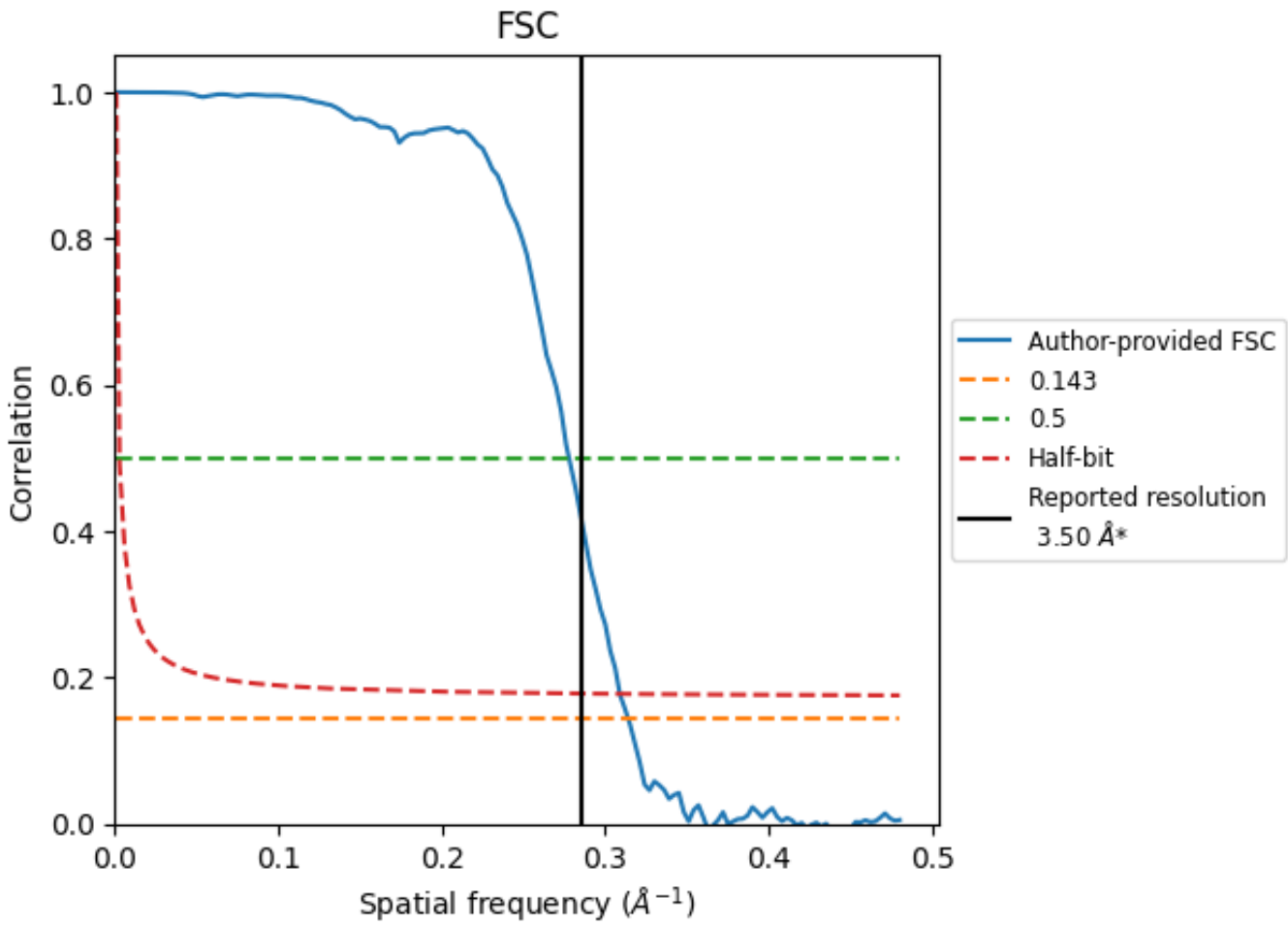


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

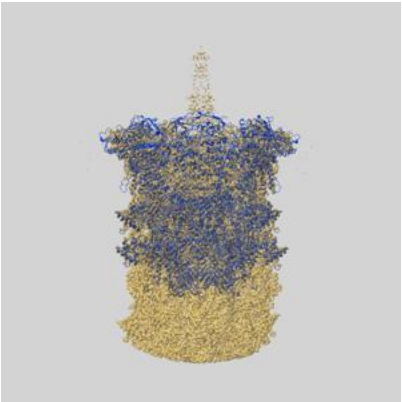
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.18	3.60	3.24
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

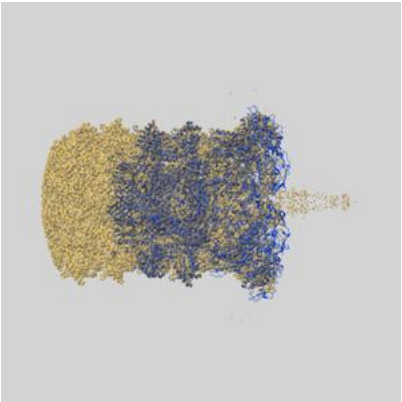
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20643 and PDB model 6U5B. Per-residue inclusion information can be found in section 3 on page 10.

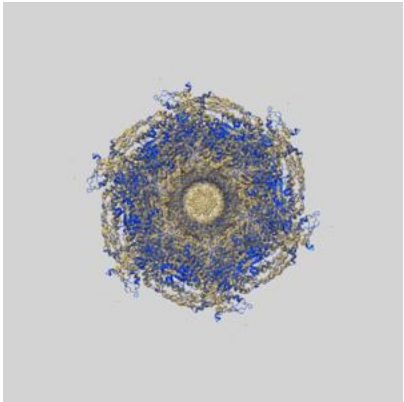
9.1 Map-model overlay (i)



X



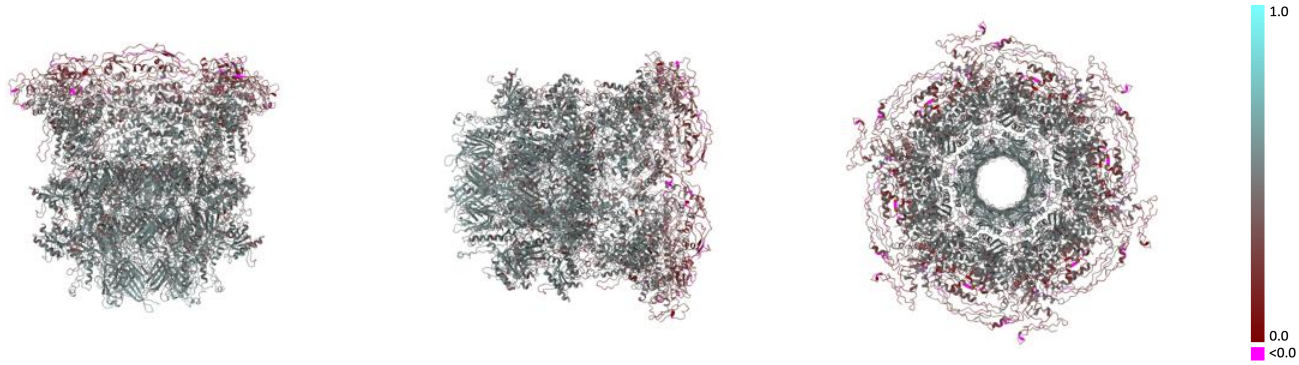
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

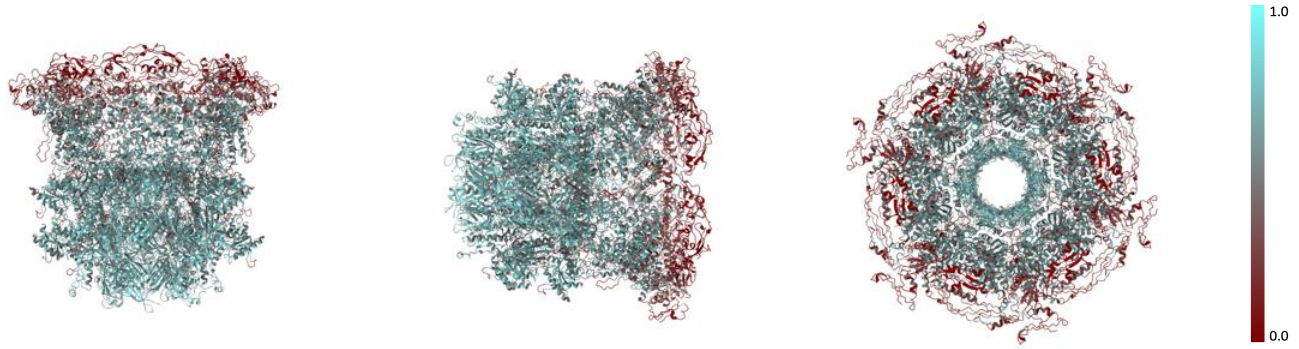
9.2 Q-score mapped to coordinate model (i)



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.

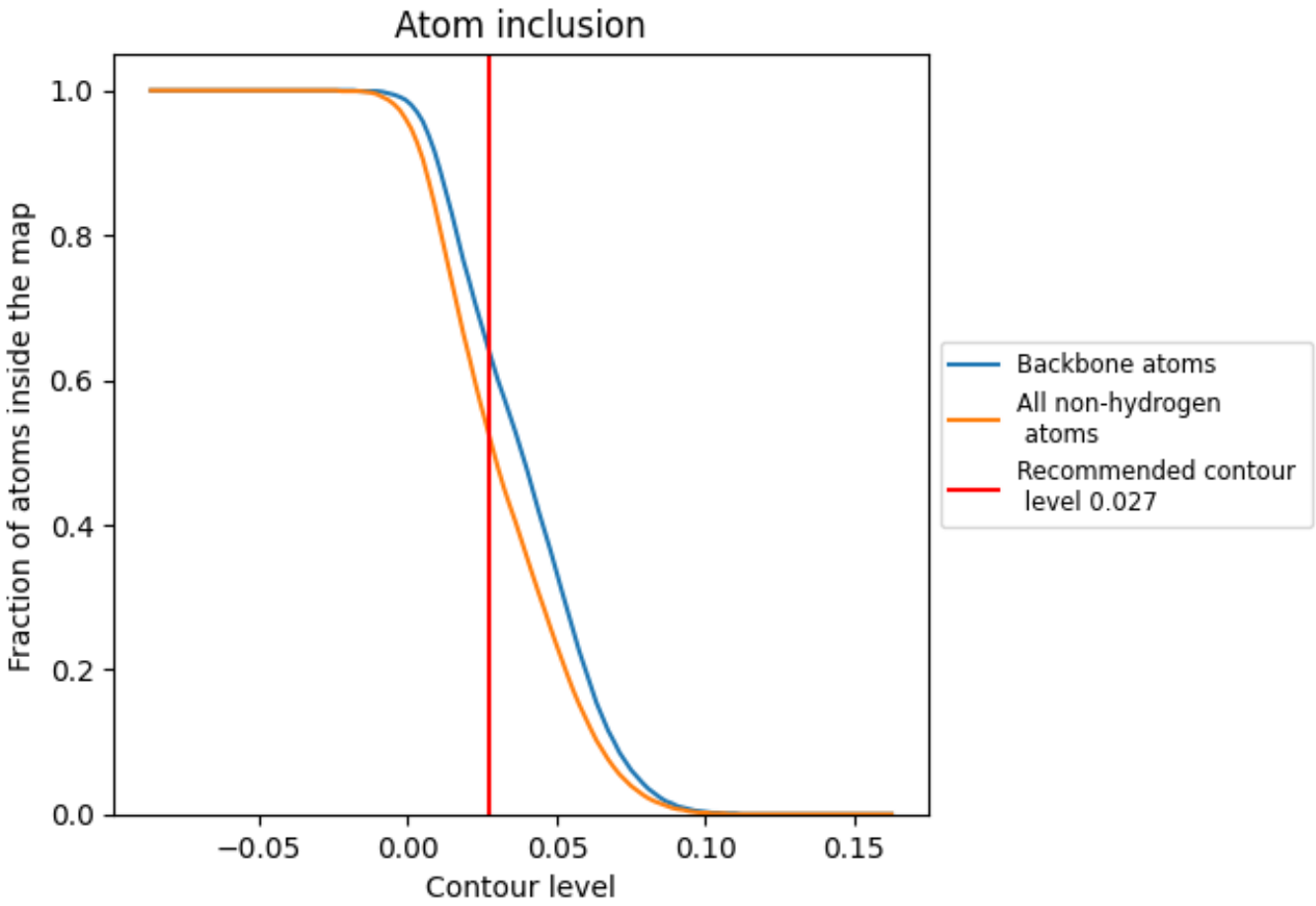
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.027).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 53% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5280	0.4480
0	0.3490	0.3770
1	0.3550	0.3740
2	0.3540	0.3730
3	0.3490	0.3740
4	0.3530	0.3730
5	0.3550	0.3750
6	0.6140	0.4970
7	0.6190	0.4930
8	0.6220	0.4900
9	0.6070	0.4990
A	0.6170	0.4870
B	0.6240	0.4870
C	0.6250	0.4880
D	0.6140	0.4870
E	0.6220	0.4830
F	0.6190	0.4870
G	0.6820	0.5240
H	0.6830	0.5230
I	0.6820	0.5230
J	0.6880	0.5220
K	0.6810	0.5220
L	0.6840	0.5250
M	0.5950	0.4780
N	0.5920	0.4780
O	0.5900	0.4760
P	0.5950	0.4760
Q	0.5900	0.4760
R	0.5940	0.4750
S	0.6770	0.5100
T	0.6760	0.5070
U	0.6780	0.5080
V	0.6780	0.5090
W	0.6770	0.5080
X	0.6810	0.5090

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Chain	Atom inclusion	Q-score
Y	0.6070	0.4960
Z	0.6140	0.4940
a	0.6370	0.4880
b	0.6370	0.4870
c	0.6420	0.4890
d	0.6410	0.4920
e	0.6390	0.4900
f	0.6390	0.4910
g	0.5910	0.4820
h	0.5890	0.4820
i	0.5960	0.4810
j	0.5910	0.4820
k	0.5930	0.4820
l	0.5930	0.4800
m	0.2620	0.3290
n	0.2630	0.3310
o	0.2680	0.3340
p	0.2640	0.3320
q	0.2600	0.3320
r	0.2680	0.3300
s	0.3910	0.3830
t	0.3880	0.3830
u	0.3910	0.3840
v	0.3900	0.3850
w	0.3860	0.3820
x	0.3910	0.3810