wwPDB EM Validation Summary Report (i)

Nov 29, 2022 – 02:55 AM JST

PDB ID	:	7VOY
EMDB ID	:	EMD-32062
Title	:	Rba sphaeroides PufX-KO RC-LH1
Authors	:	Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on	:	2021-10-15
Resolution	:	4.20 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 4.20 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		0.0%
Sidechain outliers		1.2%

Worse　　　　　　　*Better*

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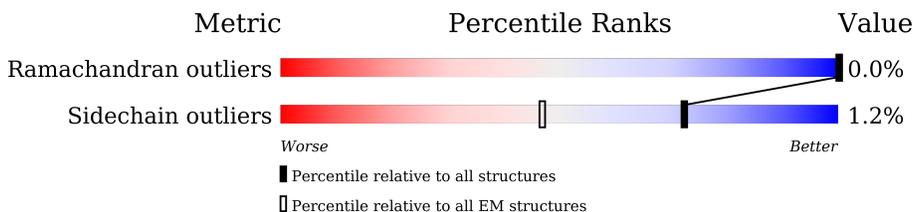
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1	58	9% / 88% · 9%
1	4	58	40% / 91% · 7%
1	6	58	28% / 93% 7%
1	7	58	24% / 79% 21%
1	9	58	36% / 93% 7%
1	A	58	41% / 93% 7%
1	C	58	19% / 93% 7%
1	D	58	47% / 93% 7%
1	F	58	38% / 93% 7%

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Mol	Chain	Length	Quality of chain
1	I	58	31% 91% 7%
1	K	58	16% 91% 7%
1	O	58	9% 93% 7%
1	Q	58	10% 93% 7%
1	S	58	16% 93% 7%
1	U	58	10% 93% 7%
1	W	58	21% 93% 7%
1	Y	58	16% 91% 7%
2	0	49	41% 86% 10%
2	2	49	16% 80% 18%
2	3	49	35% 88% 8%
2	5	49	41% 90% 8%
2	8	49	39% 86% 10%
2	B	49	49% 90% 8%
2	E	49	45% 86% 12%
2	G	49	41% 86% 12%
2	J	49	22% 86% 12%
2	N	49	16% 86% 12%
2	P	49	20% 84% 12%
2	R	49	18% 86% 12%
2	T	49	20% 86% 12%
2	V	49	18% 82% 6% 12%
2	X	49	18% 86% 12%
2	Z	49	16% 84% 14%
2	t	49	39% 90% 8%

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Mol	Chain	Length	Quality of chain
3	L	282	96% ■■■■■■■■■■■■■■■■■■■■■ 99%
4	M	308	94% ■■■■■■■■■■■■■■■■■■■■■ 99% .
5	H	260	93% ■■■■■■■■■■■■■■■■■■■■■ 95% 5%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 22119 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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	D	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	F	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	K	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	O	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	Q	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	S	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	U	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	W	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	Y	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	1	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
1	7	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
1	9	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	4	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	6	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
1	C	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

- Molecule 2 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	45	Total 365	C 243	N 57	O 64	S 1	0	0
2	E	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	G	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	J	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	N	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	P	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	R	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	T	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	V	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	X	43	Total 351	C 236	N 55	O 59	S 1	0	0
2	Z	42	Total 343	C 230	N 54	O 58	S 1	0	0
2	2	40	Total 327	C 219	N 52	O 55	S 1	0	0
2	8	44	Total 359	C 240	N 56	O 62	S 1	0	0
2	0	44	Total 359	C 240	N 56	O 62	S 1	0	0
2	t	45	Total 365	C 243	N 57	O 64	S 1	0	0
2	5	45	Total 365	C 243	N 57	O 64	S 1	0	0
2	3	45	Total 365	C 243	N 57	O 64	S 1	0	0

- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	281	Total 2232	C 1507	N 355	O 362	S 8	0	0

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		

- Molecule 5 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	247	Total	C	N	O	S	0	0
			1875	1202	318	345	10		

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).


BCL

Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	B	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	E	1	Total	C	Mg	N	O	0
			92	70	2	8	12	
6	E	1	Total	C	Mg	N	O	0
			92	70	2	8	12	
6	F	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	I	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
6	J	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	K	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	O	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	P	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	Q	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	T	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	0	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
6	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	t	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	5	1	Total	C	Mg	N	O	0
			92	70	2	8	12	
6	5	1	Total	C	Mg	N	O	0
			92	70	2	8	12	
6	C	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	L	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	M	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
6	M	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
6	M	1	Total	C	Mg	N	O	0
			138	105	3	12	18	

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).
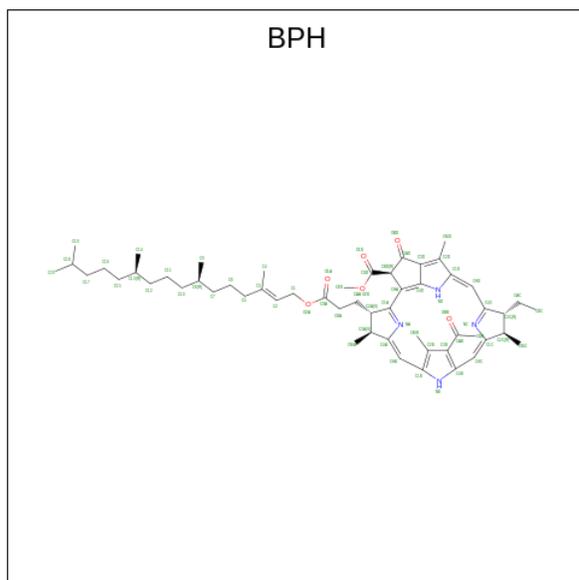
BPH

Mol	Chain	Residues	Atoms				AltConf
7	L	1	Total	C	N	O	0
			45	35	4	6	

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Mol	Chain	Residues	Atoms				AltConf
7	M	1	Total	C	N	O	0
			45	35	4	6	

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

U10
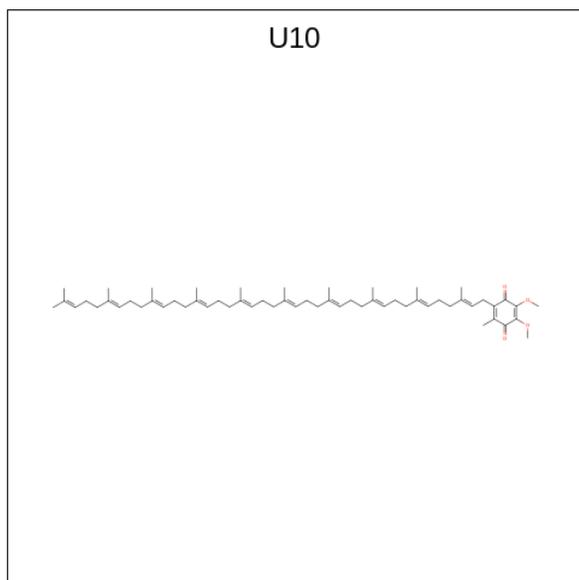
Mol	Chain	Residues	Atoms			AltConf
8	L	1	Total	C	O	0
			14	10	4	
8	M	1	Total	C	O	0
			14	10	4	

- Molecule 9 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	M	1	Total	Fe	0
			1	1	

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).

SPN
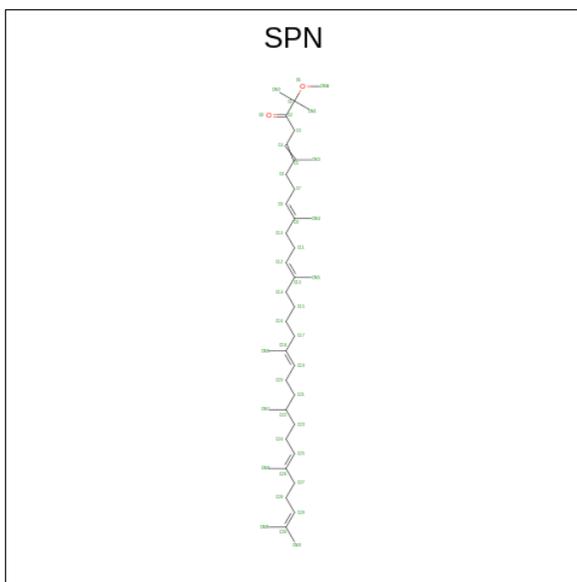
Mol	Chain	Residues	Atoms			AltConf
10	M	1	Total	C	O	0
			43	41	2	

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.
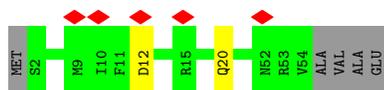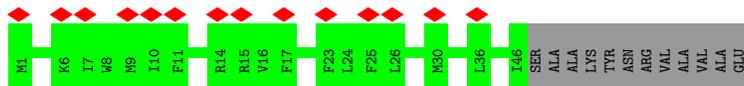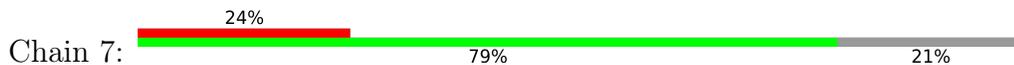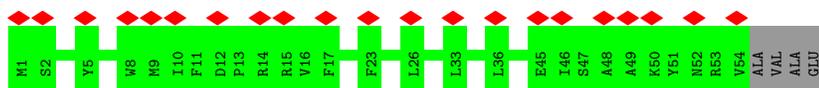
- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain A:

- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain D:

- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain F:

- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain I:

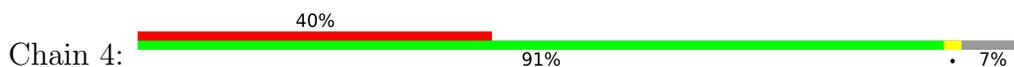- Molecule 1: Light-harvesting protein B-875 alpha chain

Chain K:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain O:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain Q:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain S:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain U:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain W:

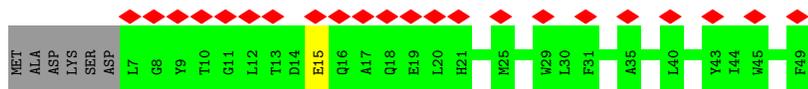• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain Y:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain 1:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain 7:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain 9:

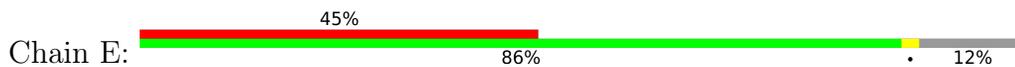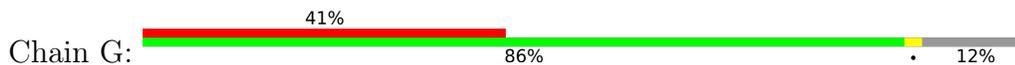• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain 4:

• Molecule 1: Light-harvesting protein B-875 alpha chain
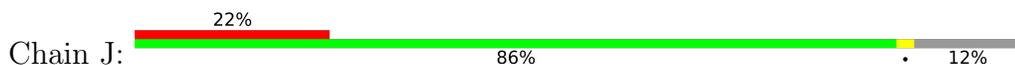
Chain 6:

• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain C:

• Molecule 2: Light-harvesting protein B-875 beta chain

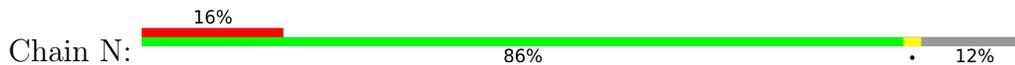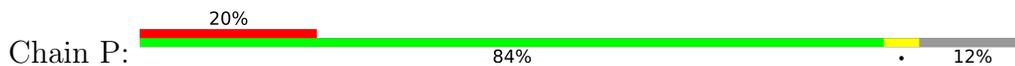Chain B:

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain E:

45%

86%   ·   12%

MET ALA ASP LYS SER ASP L7 G8 Y9 T10 G11 L12 T13 D14 E15 Q16 A17 Q18 E19 L20 H21 M25 W29 L30 F31 A35 L40 Y43 I44 W45 F49

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain G:

41%

86%   ·   12%

MET ALA ASP LYS SER ASP L7 G8 Y9 T10 G11 L12 T13 D14 E15 Q16 A17 Q18 E19 L20 H21 M25 S26 W29 L30 A33 V34 A35 I36 F49

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain J:

22%

86%   ·   12%

MET ALA ASP LYS SER ASP L7 G11 L12 T13 D14 E15 Q16 A17 Q18 G27 I44 W45 R46 F49

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain N:

16%

86%   ·   12%

MET ALA ASP LYS SER ASP L7 G8 G11 L12 T13 D14 E15 E19 M25 L40 F49

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain P:

20%

84%   ·   12%

MET ALA ASP LYS SER ASP L7 G8 Y9 T10 G11 L12 T13 D14 E15 Q16 A17 Q18 E19 M25 F49

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain R:

18%

86%   ·   12%

MET ALA ASP LYS SER ASP L7 G8 Y9 T10 G11 E15 H21 M25 Y43 I44 F49

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain T:

20%

86%   ·   12%

MET ALA ASP LYS SER ASP L7 G8 Y9 T10 G11 L12 T13 D14 E15 M25 S26 G27 L40 F49
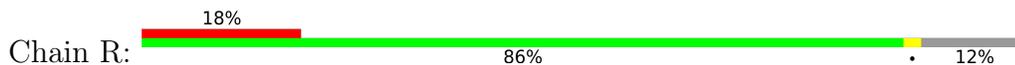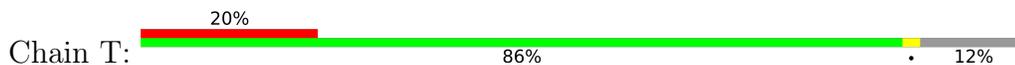
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain V:

• Molecule 2: Light-harvesting protein B-875 beta chain
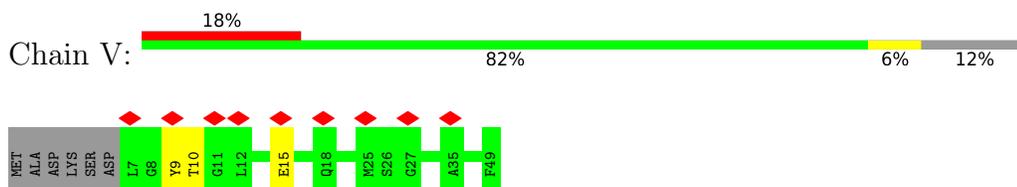
Chain X:

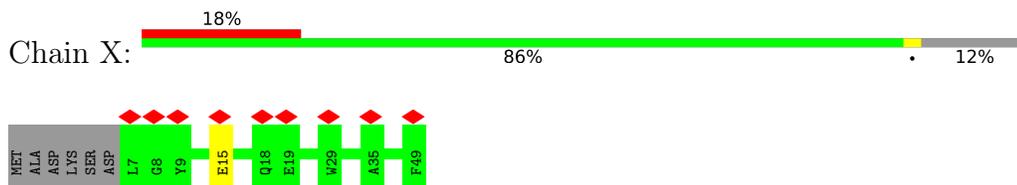• Molecule 2: Light-harvesting protein B-875 beta chain

Chain Z:

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain 2:

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain 8:

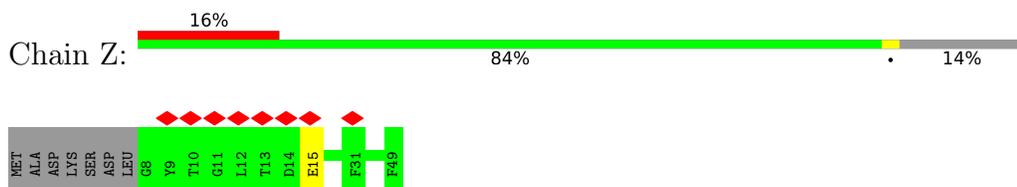• Molecule 2: Light-harvesting protein B-875 beta chain

Chain 0:

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain t:

• Molecule 2: Light-harvesting protein B-875 beta chain

Chain 5:

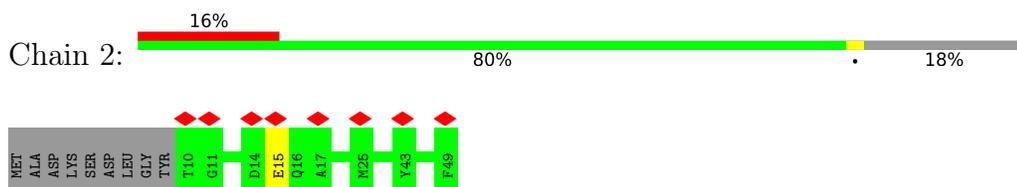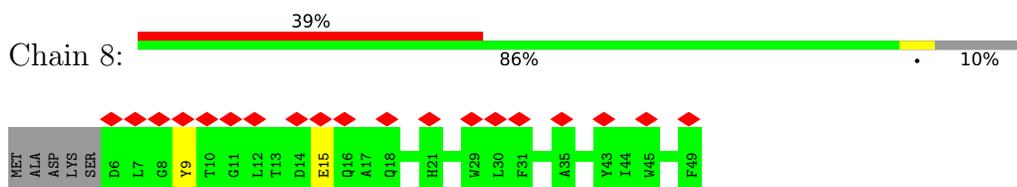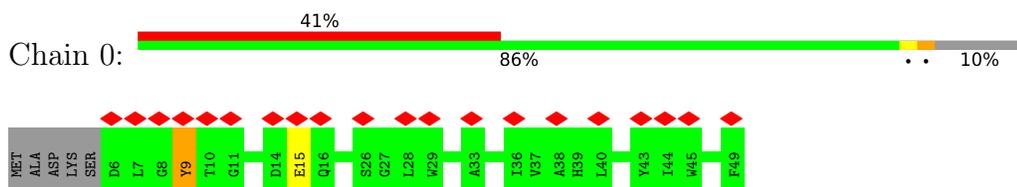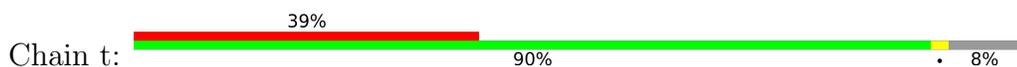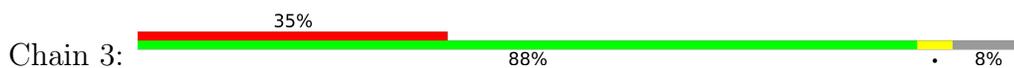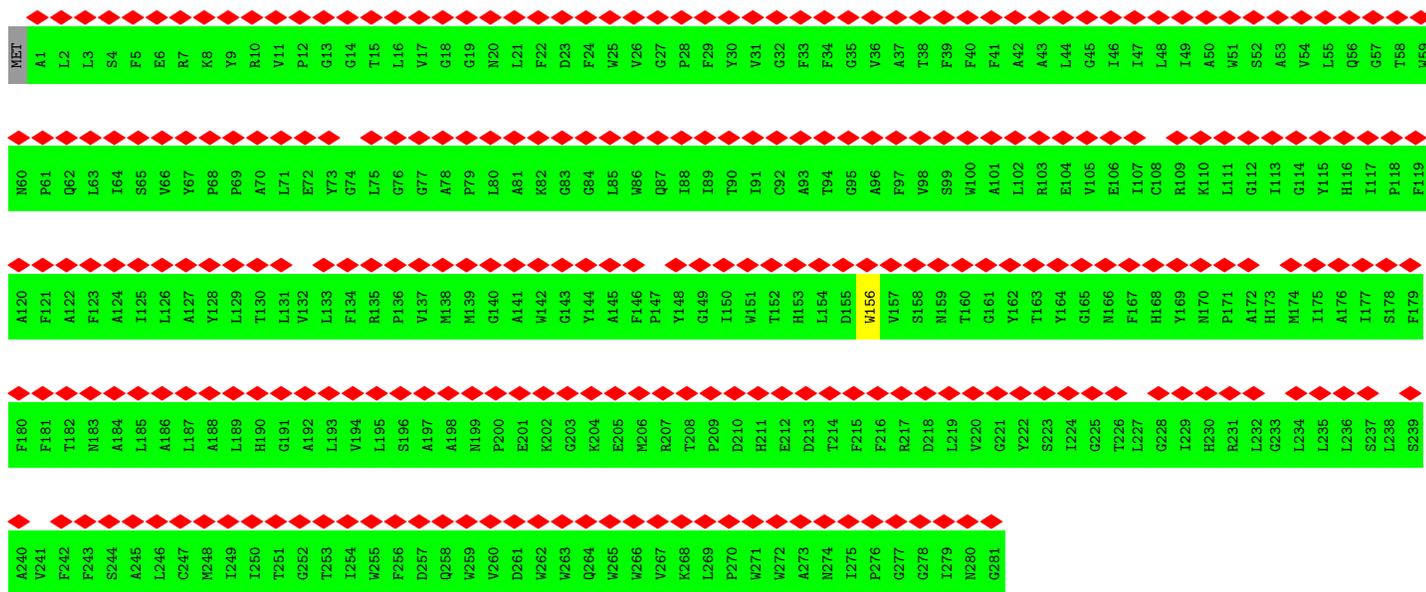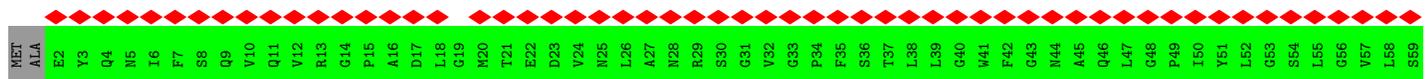• Molecule 2: Light-harvesting protein B-875 beta chain
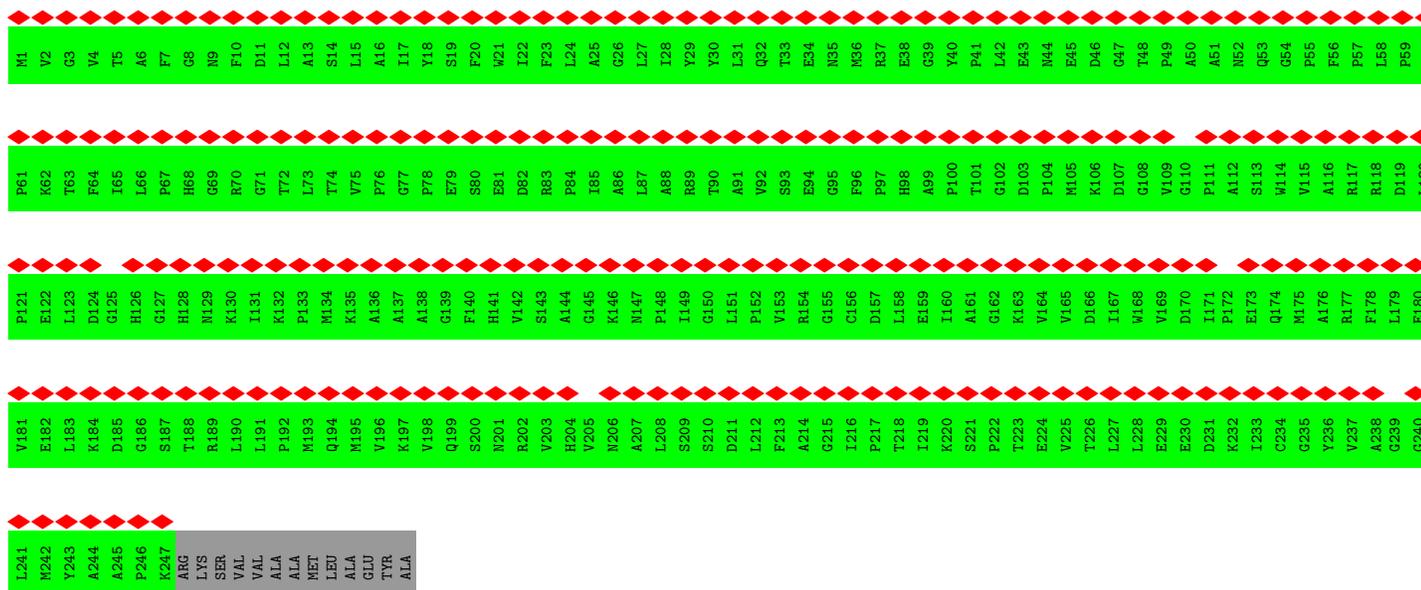
Chain 3:

• Molecule 3: Reaction center protein L chain

Chain L:

• Molecule 4: Reaction center protein M chain

Chain M:

L60 F61 S62 G63 L64 M65 W66 F67 F68 T69 I70 G71 I72 W73 F74 W75 Y76 Q77 A78 G79 W80 N81 P82 A83 V84 F85 L86 R87 D88 L89 F90 F91 F92 E95 P96 P97 A98 P99 E100 Y101 G102 L103 S104 F105 A106 A107 P108 L109 K110 E111 G112 G113 L114 W115 L116 I117 A118 S119 F120

F121 M122 F123 V124 A125 V126 W127 S128 W129 W130 G131 R132 T133 Y134 L135 R136 A137 Q138 A139 L140 G141 M142 G143 K144 H145 T146 A147 W148 A149 F150 L151 S152 A153 I154 W155 L156 W157 M158 V159 L160 G161 F162 I163 R164 P165 I166 L167 M168 G169 S170 W171 S172 E173 A174 V175 P176 Y177 G178 I179 F180

S181 H182 L183 D184 W185 T186 N187 N188 F189 S190 L191 V192 H193 G194 N195 L196 F197 Y198 N199 P200 F201 H202 G203 L204 S205 I206 A207 F208 L209 Y210 G211 S212 A213 L214 L215 F216 A217 M218 H219 G220 A221 T222 I223 L224 A225 V226 S227 R228 F229 G230 G231 E232 R233 E234 L235 E236 Q237 I238 A239 D240

R241 G242 T243 A244 A245 E246 R247 A248 A249 L250 F251 W252 R253 W254 T255 M256 G257 F258 N259 A260 T261 M262 E263 G264 I265 H266 R267 W268 A269 I270 W271 M272 A273 V274 L275 V276 T277 L278 T279 T280 G281 I282 G283 I284 L285 L286 S287 G288 T289 V290 V291 D292 N293 W294 Y295 V296 W297 G298 Q299 N300

H301 G302 M303 A304 P305 L306 ASN

• Molecule 5: Reaction center protein H chain

Chain H:

93%
95% 5%

M1 V2 G3 V4 T5 A6 F7 G8 N9 F10 D11 L12 A13 S14 L15 A16 I17 Y18 S19 F20 W21 I22 F23 L24 A25 G26 L27 I28 Y29 Y30 L31 Q32 T33 E34 N35 M36 R37 E38 G39 Y40 P41 L42 E43 N44 E45 D46 G47 T48 P49 A50 A51 N52 Q53 G54 P55 F56 P57 L58 P59 K60

P61 K62 T63 F64 I65 L66 P67 H68 G69 R70 G71 T72 L73 T74 V75 P76 G77 P78 E79 S80 E81 D82 R83 P84 I85 A86 L87 A88 R89 T90 A91 V92 S93 E94 G95 F96 P97 H98 A99 P100 T101 G102 D103 P104 M105 K106 D107 G108 V109 G110 P111 A112 S113 W114 V115 A116 R117 R118 D119 L120

P121 E122 L123 D124 G125 H126 G127 H128 N129 K130 I131 K132 P133 M134 K135 A136 A137 A138 G139 F140 H141 V142 S143 A144 G145 K146 N147 P148 I149 G150 L151 P152 V153 R154 G155 C156 D157 L158 E159 I160 A161 G162 K163 V164 V165 D166 I167 W168 V169 D170 I171 P172 E173 Q174 M175 A176 R177 F178 L179 E180

V181 E182 L183 K184 D185 G186 S187 T188 R189 L190 L191 P192 M193 Q194 M195 V196 K197 V198 Q199 S200 N201 R202 V203 H204 V205 N206 A207 L208 S209 S210 D211 L212 F213 A214 G215 I216 P217 T218 I219 K220 S221 P222 T223 E224 V225 T226 L227 L228 E229 E230 D231 K232 I233 C234 G235 Y236 V237 A238 G239 G240

L241 M242 Y243 A244 A245 P246 K247 ARG LYS SER VAL VAL ALA ALA MET LEU ALA GLU TYR ALA

4   Experimental information   ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	46.549	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0254	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5　Model quality　ⓘ

5.1　Standard geometry　ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, FE2, SPN, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	1	0.42	0/461	0.47	0/625
1	4	0.43	0/469	0.46	0/635
1	6	0.38	0/469	0.45	0/635
1	7	0.40	0/405	0.48	0/549
1	9	0.38	0/469	0.47	0/635
1	A	0.48	0/469	0.45	0/635
1	C	0.43	0/469	0.44	0/635
1	D	0.40	0/469	0.45	0/635
1	F	0.41	0/469	0.46	0/635
1	I	0.40	0/469	0.45	0/635
1	K	0.41	0/469	0.48	0/635
1	O	0.40	0/469	0.51	0/635
1	Q	0.46	0/469	0.49	0/635
1	S	0.44	0/469	0.48	0/635
1	U	0.48	0/469	0.49	0/635
1	W	0.42	0/469	0.47	0/635
1	Y	0.43	0/469	0.49	0/635
2	0	0.38	0/372	0.52	1/510 (0.2%)
2	2	0.36	0/339	0.36	0/465
2	3	0.37	0/378	0.48	0/518
2	5	0.41	0/378	0.45	0/518
2	8	0.36	0/372	0.45	1/510 (0.2%)
2	B	0.37	0/378	0.39	0/518
2	E	0.38	0/364	0.38	0/499
2	G	0.37	0/364	0.38	0/499
2	J	0.36	0/364	0.42	0/499
2	N	0.38	0/364	0.45	0/499
2	P	0.36	0/364	0.44	0/499
2	R	0.36	0/364	0.40	0/499
2	T	0.35	0/364	0.40	0/499
2	V	0.38	0/364	0.40	0/499
2	X	0.36	0/364	0.38	0/499

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Z	0.40	0/356	0.42	0/488
2	t	0.39	0/378	0.50	0/518
3	L	0.30	0/2320	0.47	0/3175
4	M	0.30	0/2524	0.46	0/3446
5	H	0.28	0/1925	0.49	0/2620
All	All	0.37	0/20897	0.46	2/28476 (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
2	0	0	1
2	3	0	1
2	P	0	1
2	V	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	9	TYR	C-N-CA	-6.27	106.03	121.70
2	8	9	TYR	C-N-CA	5.10	134.44	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0	9	TYR	Peptide
2	3	9	TYR	Peptide
2	P	9	TYR	Peptide
2	V	9	TYR	Peptide

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	1	51/58 (88%)	48 (94%)	3 (6%)	0	100	100
1	4	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	6	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	7	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
1	9	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	A	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
1	C	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	D	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	F	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	I	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	K	52/58 (90%)	52 (100%)	0	0	100	100
1	O	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	Q	52/58 (90%)	52 (100%)	0	0	100	100
1	S	52/58 (90%)	52 (100%)	0	0	100	100
1	U	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	W	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	Y	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
2	0	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
2	2	38/49 (78%)	37 (97%)	1 (3%)	0	100	100
2	3	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
2	5	43/49 (88%)	40 (93%)	3 (7%)	0	100	100
2	8	42/49 (86%)	39 (93%)	3 (7%)	0	100	100
2	B	43/49 (88%)	40 (93%)	3 (7%)	0	100	100
2	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	G	41/49 (84%)	39 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	N	41/49 (84%)	37 (90%)	4 (10%)	0	100	100
2	P	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	R	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	T	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	V	41/49 (84%)	39 (95%)	1 (2%)	1 (2%)	6	36
2	X	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
2	Z	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	t	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
3	L	279/282 (99%)	257 (92%)	22 (8%)	0	100	100
4	M	303/308 (98%)	285 (94%)	18 (6%)	0	100	100
5	H	245/260 (94%)	229 (94%)	16 (6%)	0	100	100
All	All	2405/2669 (90%)	2294 (95%)	110 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	10	THR

5.3.2　Protein sidechains　ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	48/51 (94%)	46 (96%)	2 (4%)	30	55
1	4	49/51 (96%)	48 (98%)	1 (2%)	55	73
1	6	49/51 (96%)	49 (100%)	0	100	100
1	7	43/51 (84%)	43 (100%)	0	100	100
1	9	49/51 (96%)	49 (100%)	0	100	100
1	A	49/51 (96%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	49/51 (96%)	49 (100%)	0	100	100
1	D	49/51 (96%)	49 (100%)	0	100	100
1	F	49/51 (96%)	49 (100%)	0	100	100
1	I	49/51 (96%)	48 (98%)	1 (2%)	55	73
1	K	49/51 (96%)	48 (98%)	1 (2%)	55	73
1	O	49/51 (96%)	49 (100%)	0	100	100
1	Q	49/51 (96%)	49 (100%)	0	100	100
1	S	49/51 (96%)	49 (100%)	0	100	100
1	U	49/51 (96%)	49 (100%)	0	100	100
1	W	49/51 (96%)	49 (100%)	0	100	100
1	Y	49/51 (96%)	48 (98%)	1 (2%)	55	73
2	0	36/40 (90%)	35 (97%)	1 (3%)	43	65
2	2	33/40 (82%)	32 (97%)	1 (3%)	41	63
2	3	37/40 (92%)	36 (97%)	1 (3%)	44	66
2	5	37/40 (92%)	36 (97%)	1 (3%)	44	66
2	8	36/40 (90%)	35 (97%)	1 (3%)	43	65
2	B	37/40 (92%)	36 (97%)	1 (3%)	44	66
2	E	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	G	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	J	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	N	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	P	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	R	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	T	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	V	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	X	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	Z	34/40 (85%)	33 (97%)	1 (3%)	42	64
2	t	37/40 (92%)	36 (97%)	1 (3%)	44	66
3	L	220/221 (100%)	219 (100%)	1 (0%)	88	93
4	M	239/241 (99%)	238 (100%)	1 (0%)	91	94
5	H	199/208 (96%)	199 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2086/2217 (94%)	2061 (99%)	25 (1%)	72 83

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	12	ASP
2	8	15	GLU
4	M	195	ASN
2	2	15	GLU
2	0	15	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	M	46	GLN
4	M	182	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 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	#$|Z| > 2$
7	BPH	L	302	-	31,50,70	1.04	2 (6%)	28,77,101	1.59	7 (25%)
6	BCL	X	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	7	101	-	38,54,74	1.45	5 (13%)	45,91,115	1.88	12 (26%)
7	BPH	M	405	-	31,50,70	1.12	3 (9%)	28,77,101	1.44	6 (21%)
6	BCL	4	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.87	12 (26%)
6	BCL	9	101	-	38,54,74	1.45	7 (18%)	45,91,115	1.85	11 (24%)
6	BCL	3	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	A	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.84	12 (26%)
6	BCL	Q	101	-	38,54,74	1.54	9 (23%)	45,91,115	1.78	11 (24%)
6	BCL	5	101	-	38,54,74	1.52	6 (15%)	45,91,115	1.84	14 (31%)
10	SPN	M	407	-	40,42,42	3.37	12 (30%)	50,52,52	2.37	18 (36%)
6	BCL	T	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	K	101	-	38,54,74	1.46	5 (13%)	45,91,115	1.80	10 (22%)
6	BCL	W	101	-	38,54,74	1.47	7 (18%)	45,91,115	1.66	9 (20%)
6	BCL	J	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	I	101	-	38,54,74	1.42	5 (13%)	45,91,115	1.84	13 (28%)
6	BCL	N	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
8	U10	M	406	-	14,14,63	2.63	6 (42%)	18,20,79	0.91	0
6	BCL	t	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	B	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	0	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	F	101	-	38,54,74	1.45	6 (15%)	45,91,115	1.75	10 (22%)
6	BCL	5	102	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	R	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	S	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.79	10 (22%)
6	BCL	1	101	-	38,54,74	1.52	7 (18%)	45,91,115	1.90	10 (22%)
6	BCL	2	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	E	102	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	V	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	M	401	-	38,54,74	1.46	3 (7%)	45,91,115	1.85	12 (26%)
6	BCL	P	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	U	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.89	12 (26%)
8	U10	L	303	-	14,14,63	2.64	6 (42%)	18,20,79	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	BCL	L	301	-	38,54,74	1.34	4 (10%)	45,91,115	1.91	10 (22%)
6	BCL	Y	101	-	38,54,74	1.59	6 (15%)	45,91,115	1.68	11 (24%)
6	BCL	O	101	-	38,54,74	1.40	5 (13%)	45,91,115	1.86	12 (26%)
6	BCL	E	101	-	38,54,74	1.35	5 (13%)	45,91,115	5.26	12 (26%)
6	BCL	C	101	-	38,54,74	1.53	8 (21%)	45,91,115	1.81	12 (26%)
6	BCL	M	403	-	38,54,74	1.47	4 (10%)	45,91,115	1.79	12 (26%)
6	BCL	M	404	-	38,54,74	1.38	3 (7%)	45,91,115	1.72	8 (17%)
6	BCL	Z	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	8	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	G	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)

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
7	BPH	L	302	-	-	3/13/81/105	0/5/6/6
6	BCL	X	101	-	-	5/13/113/137	-
6	BCL	7	101	-	-	6/13/113/137	-
7	BPH	M	405	-	-	5/13/81/105	0/5/6/6
6	BCL	4	101	-	-	4/13/113/137	-
6	BCL	9	101	-	-	8/13/113/137	-
6	BCL	3	101	-	-	5/13/113/137	-
6	BCL	A	101	-	-	1/13/113/137	-
6	BCL	Q	101	-	-	2/13/113/137	-
6	BCL	5	101	-	-	7/13/113/137	-
10	SPN	M	407	-	-	25/50/51/51	-
6	BCL	T	101	-	-	5/13/113/137	-
6	BCL	K	101	-	-	2/13/113/137	-
6	BCL	W	101	-	-	5/13/113/137	-
6	BCL	J	101	-	-	5/13/113/137	-
6	BCL	I	101	-	-	6/13/113/137	-
6	BCL	N	101	-	-	5/13/113/137	-
8	U10	M	406	-	-	3/4/28/87	0/1/1/1
6	BCL	t	101	-	-	5/13/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	B	101	-	-	5/13/113/137	-
6	BCL	0	101	-	-	5/13/113/137	-
6	BCL	F	101	-	-	4/13/113/137	-
6	BCL	5	102	-	-	5/13/113/137	-
6	BCL	R	101	-	-	5/13/113/137	-
6	BCL	S	101	-	-	2/13/113/137	-
6	BCL	1	101	-	-	4/13/113/137	-
6	BCL	2	101	-	-	5/13/113/137	-
6	BCL	E	102	-	-	5/13/113/137	-
6	BCL	V	101	-	-	5/13/113/137	-
6	BCL	M	401	-	-	4/13/113/137	-
6	BCL	P	101	-	-	5/13/113/137	-
6	BCL	U	101	-	-	2/13/113/137	-
8	U10	L	303	-	-	1/4/28/87	0/1/1/1
6	BCL	L	301	-	-	2/13/113/137	-
6	BCL	Y	101	-	-	5/13/113/137	-
6	BCL	O	101	-	-	4/13/113/137	-
6	BCL	E	101	-	-	2/13/113/137	-
6	BCL	C	101	-	-	5/13/113/137	-
6	BCL	M	403	-	-	2/13/113/137	-
6	BCL	M	404	-	-	6/13/113/137	-
6	BCL	Z	101	-	-	5/13/113/137	-
6	BCL	8	101	-	-	5/13/113/137	-
6	BCL	G	101	-	-	5/13/113/137	-

The worst 5 of 233 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	407	SPN	C8-C9	8.69	1.53	1.33
10	M	407	SPN	C29-C30	7.85	1.54	1.32
10	M	407	SPN	CM8-C26	-7.20	1.32	1.50
10	M	407	SPN	CM5-C13	-6.49	1.34	1.50
10	M	407	SPN	CM3-C5	-6.15	1.34	1.50

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	101	BCL	OBB-CAB-C3B	-26.10	73.67	119.99
6	E	101	BCL	OBB-CAB-CBB	-17.76	80.21	120.17
6	E	101	BCL	CBB-CAB-C3B	11.30	153.89	120.34
6	L	301	BCL	CAD-C3D-C4D	-8.36	103.81	108.47
10	M	407	SPN	C7-C8-C9	-6.72	111.48	127.66

There are no chirality outliers.

5 of 205 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	101	BCL	CHA-CBD-CGD-O1D
6	B	101	BCL	CHA-CBD-CGD-O2D
6	E	101	BCL	C4C-C3C-CAC-CBC
6	E	102	BCL	CHA-CBD-CGD-O1D
6	E	102	BCL	CHA-CBD-CGD-O2D

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 BPH L 302

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL X 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 7 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH M 405

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 4 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 9 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 3 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL A 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL Q 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 5 101

Bond lengths

Bond angles

Torsions

Rings

Ligand SPN M 407

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL T 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL K 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL W 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL J 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL I 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL N 101

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 M 406

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL t 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL B 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 0 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL F 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 5 102

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL R 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL S 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 1 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 2 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL E 102

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL V 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 401

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL P 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL U 101

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 L 303

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 301

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL Y 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL O 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL E 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL C 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 403

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 404

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL Z 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 8 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL G 101

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-32062. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

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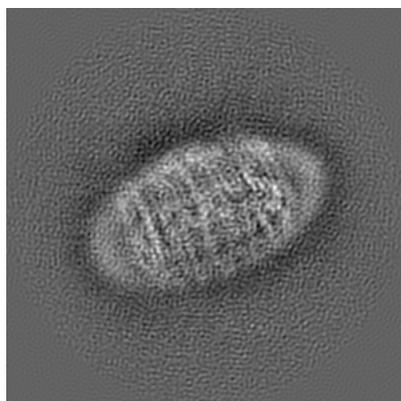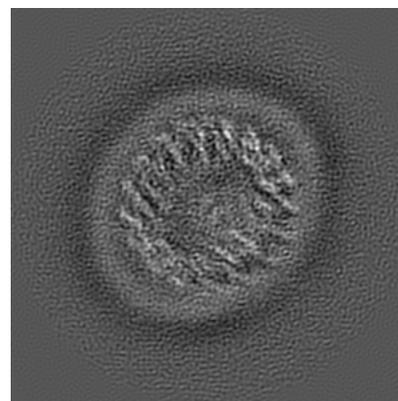
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
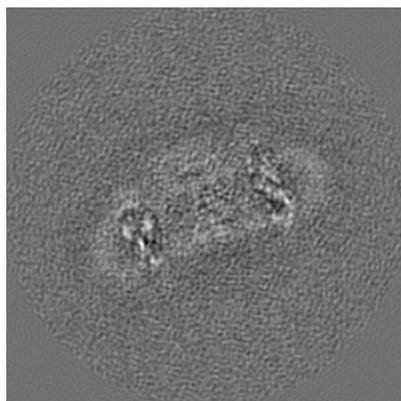
6.2.1 Primary map
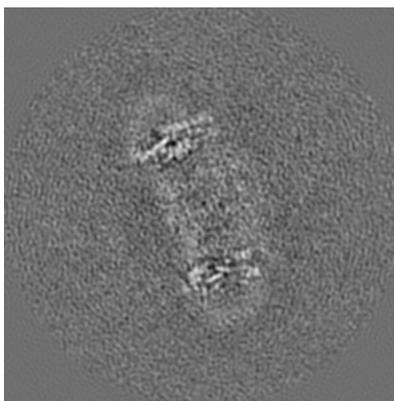
| X Index: 125 | Y Index: 125 | Z Index: 125 |
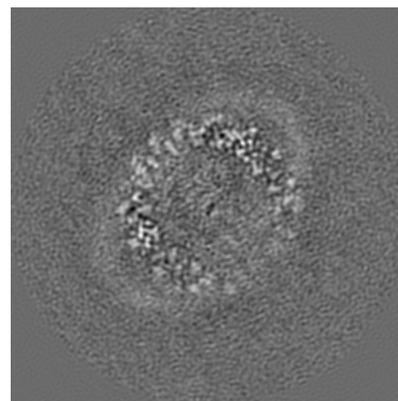
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices (i)

6.3.1   Primary map
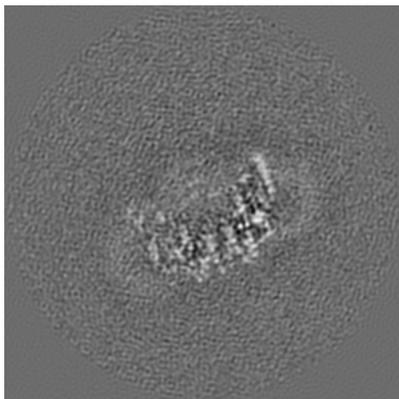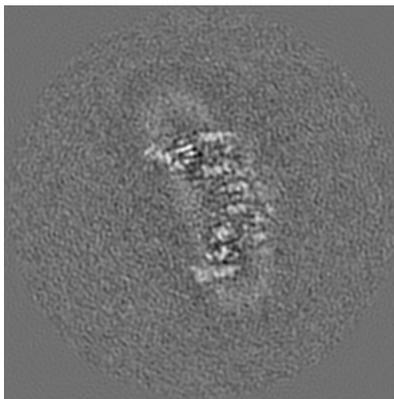
| X Index: 155 | Y Index: 155 | Z Index: 124 |
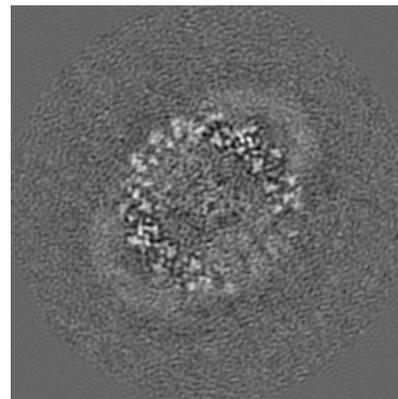
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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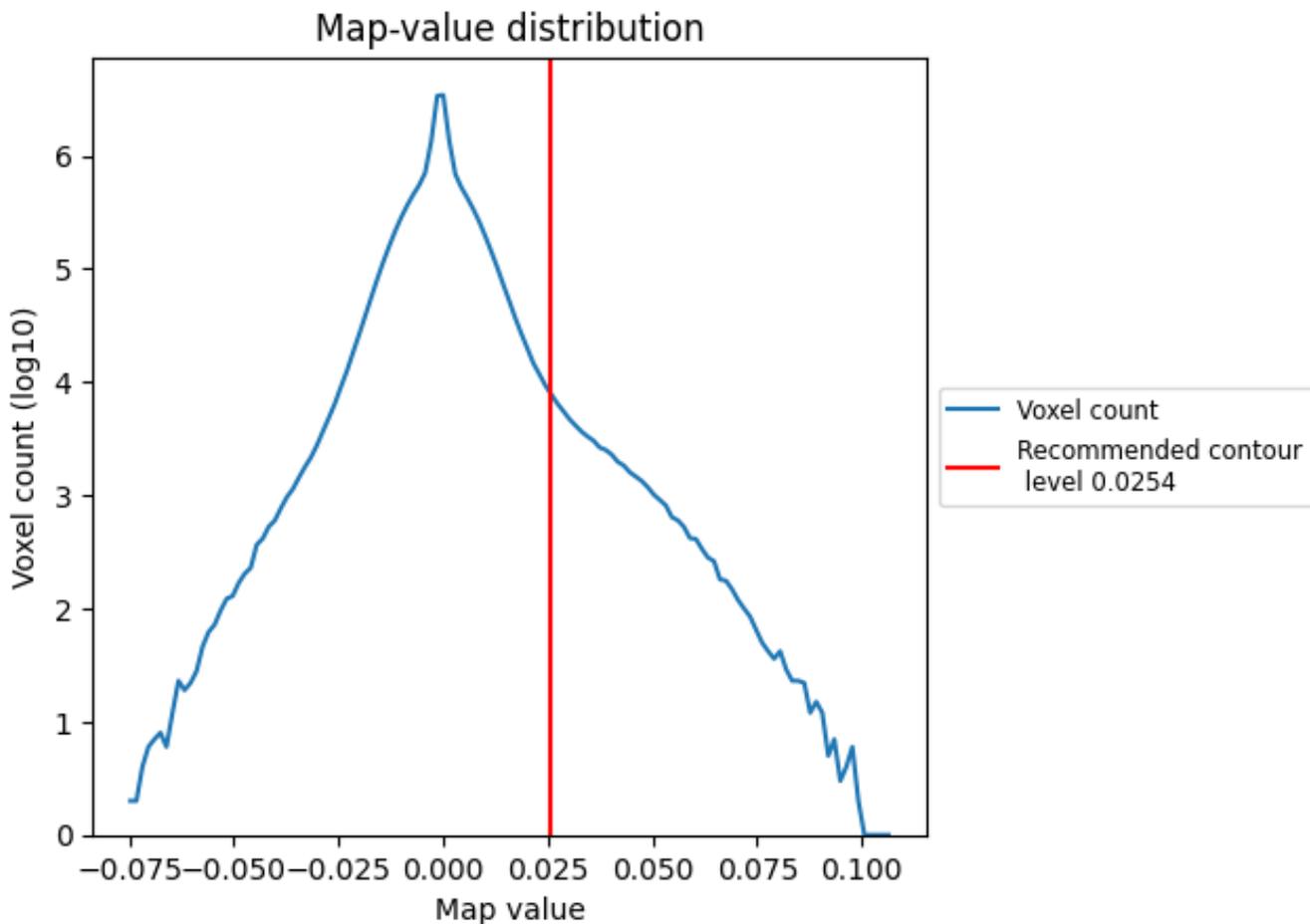
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
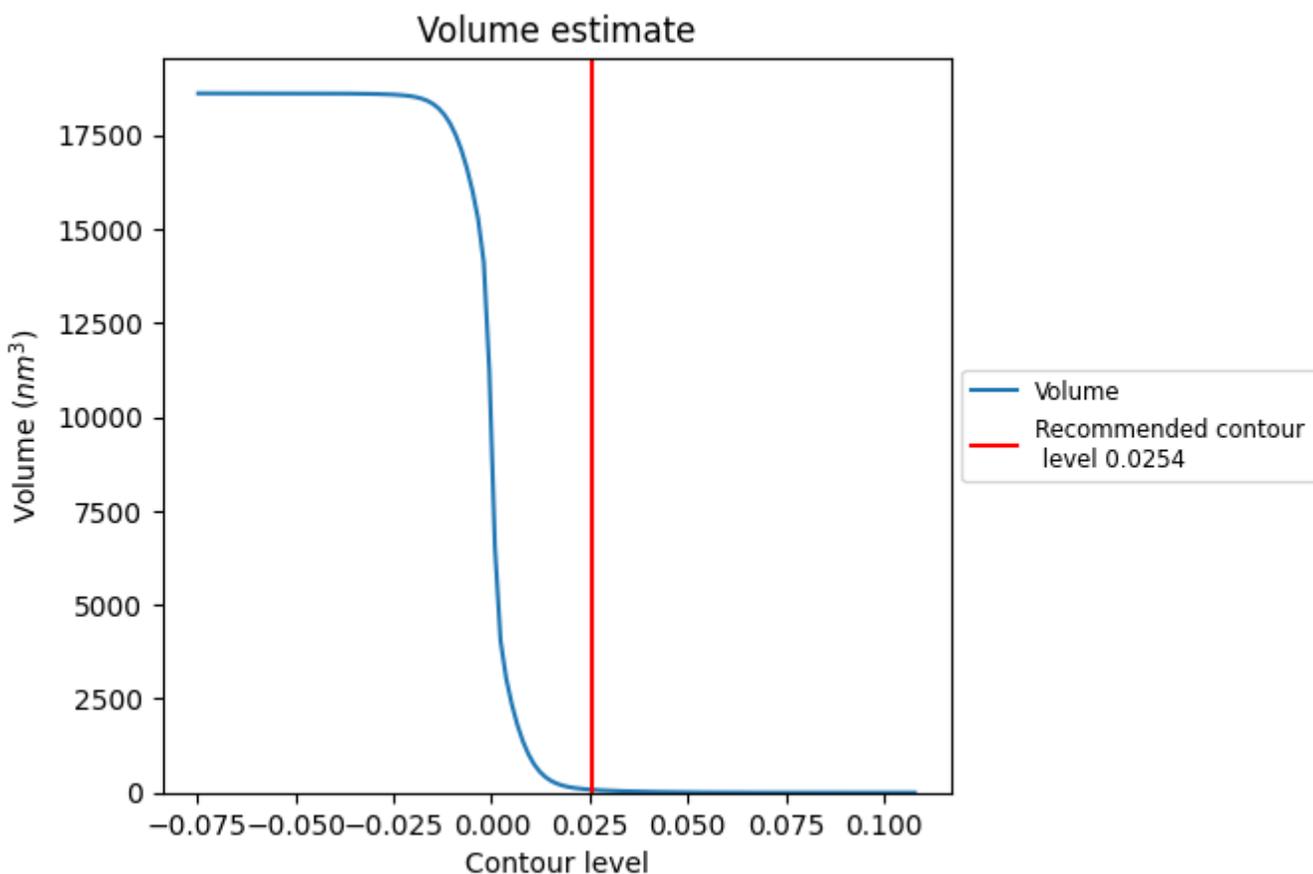
The volume at the recommended contour level is 79 nm^3; this corresponds to an approximate mass of 71 kDa.

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 ⓘ
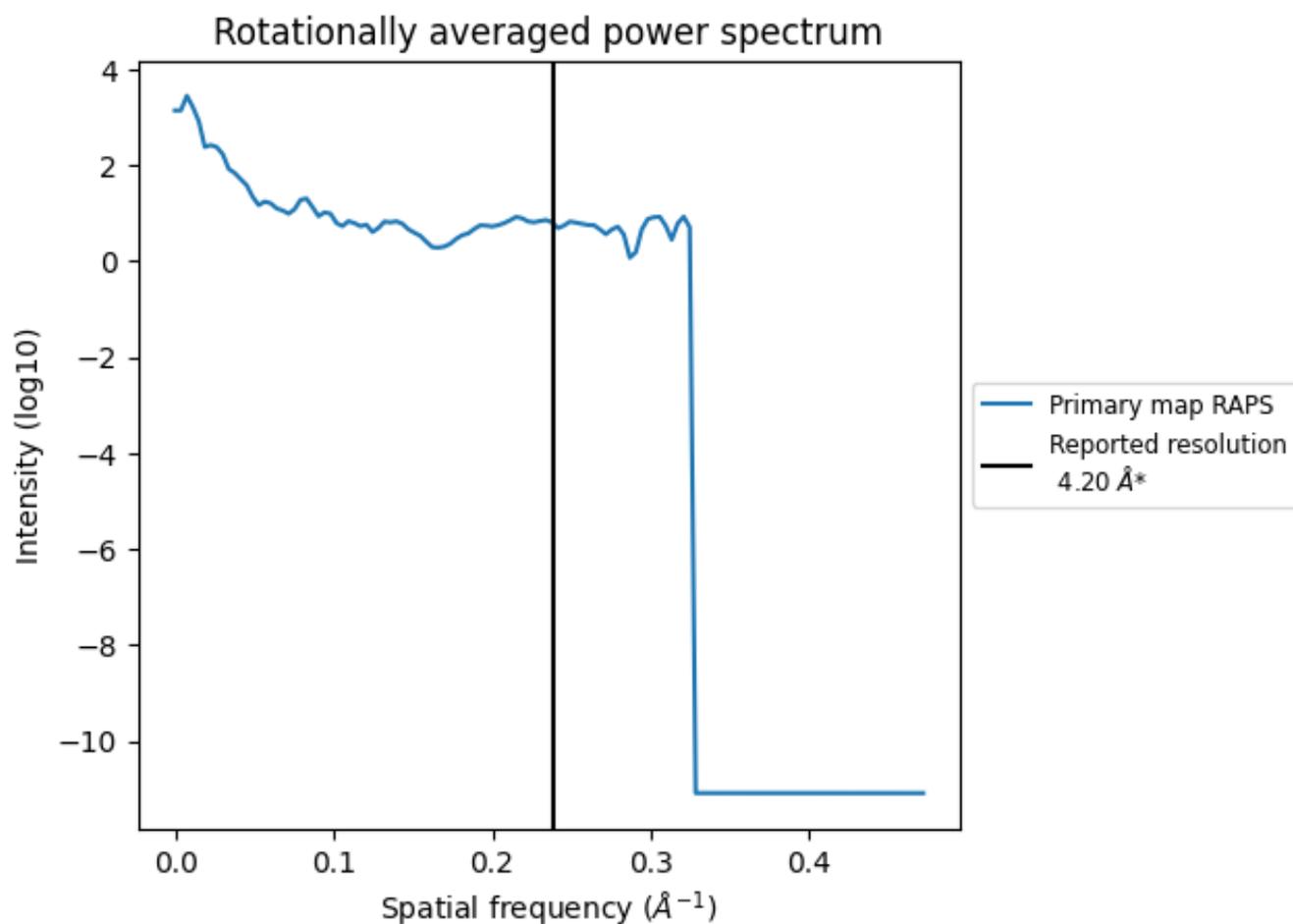
*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 ⓘ
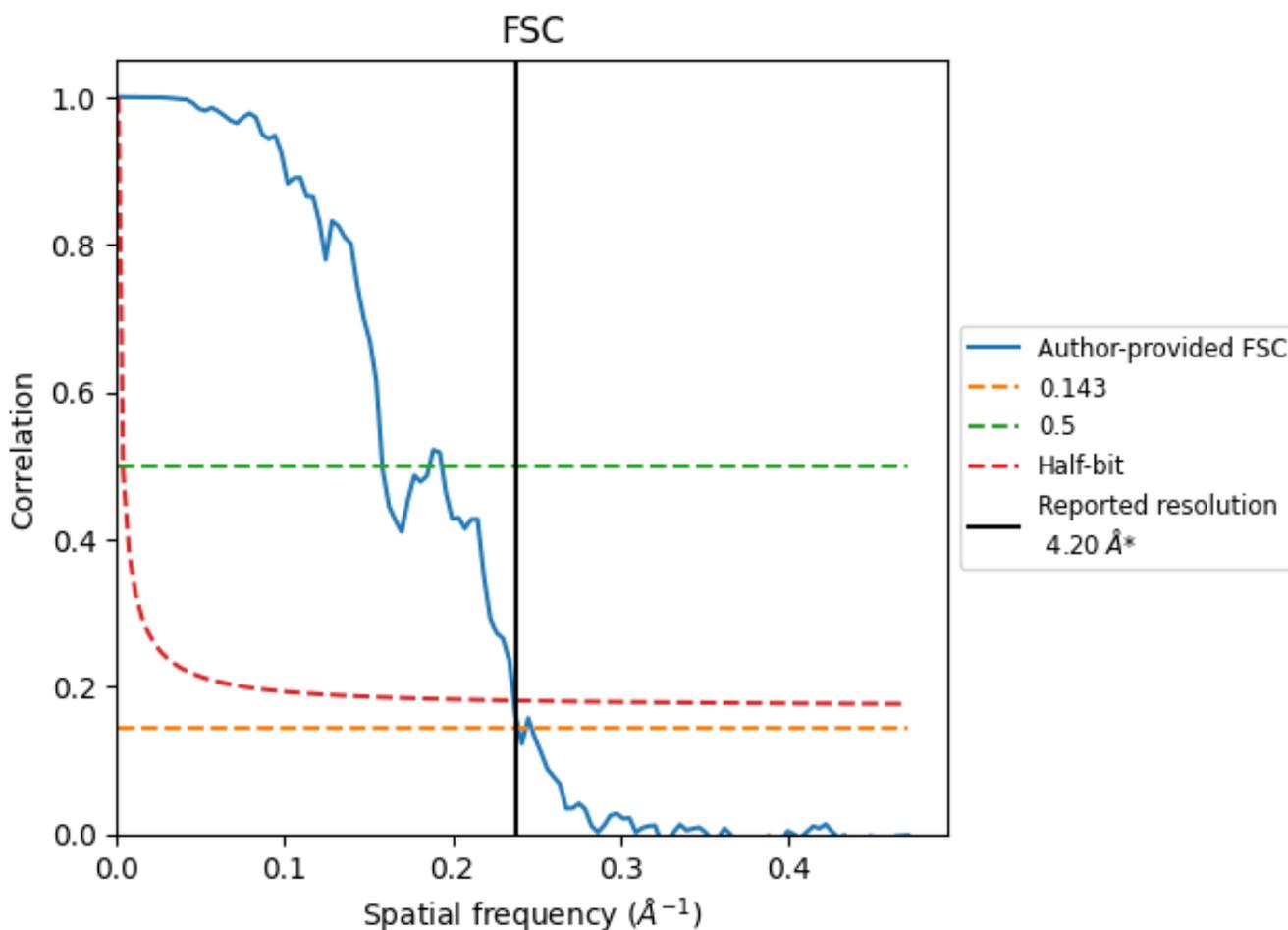
*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.32	4.22
Unmasked-calculated*	-	-	-

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

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32062 and PDB model 7VOY. Per-residue inclusion information can be found in section 3 on page 12.

9.1   Map-model overlay ⓘ
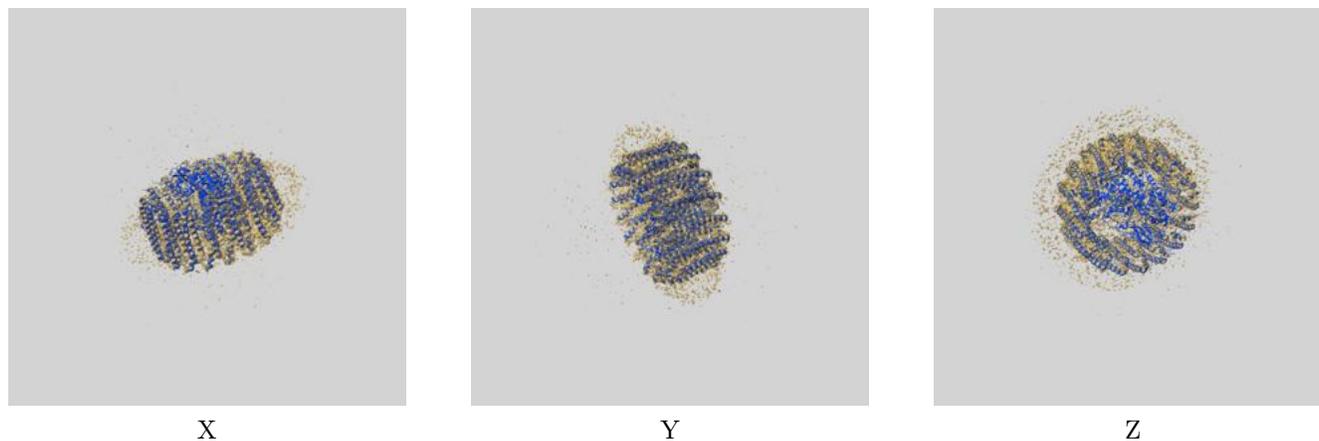
X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0254 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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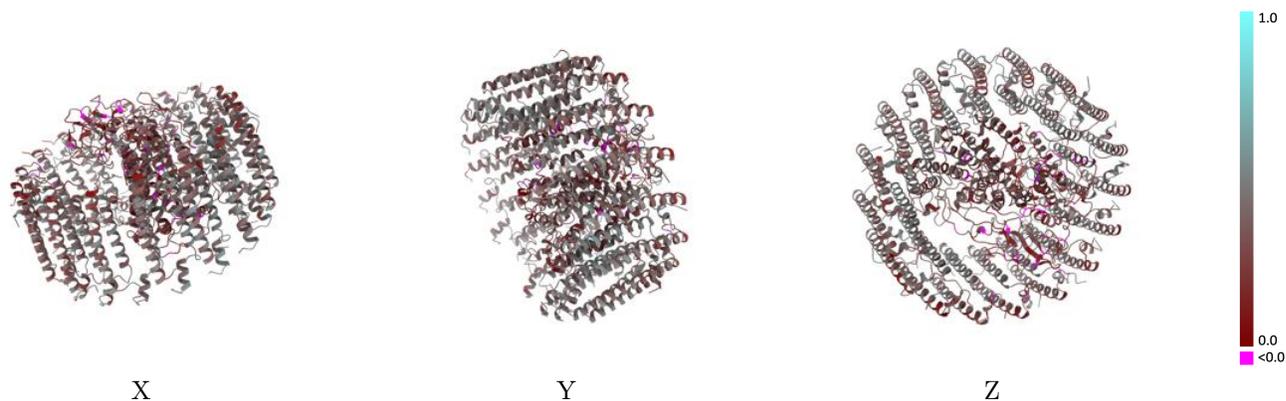
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
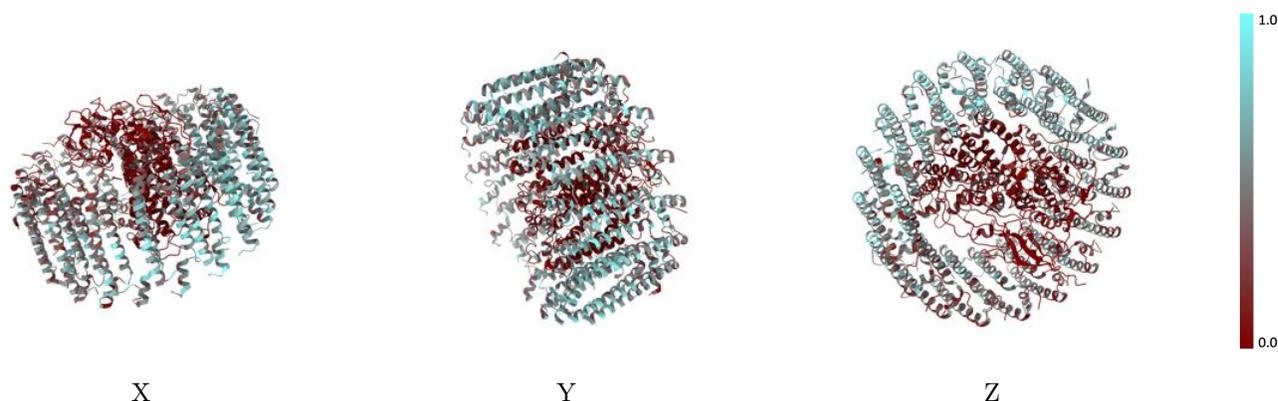
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0254).

9.4　Atom inclusion ⓘ
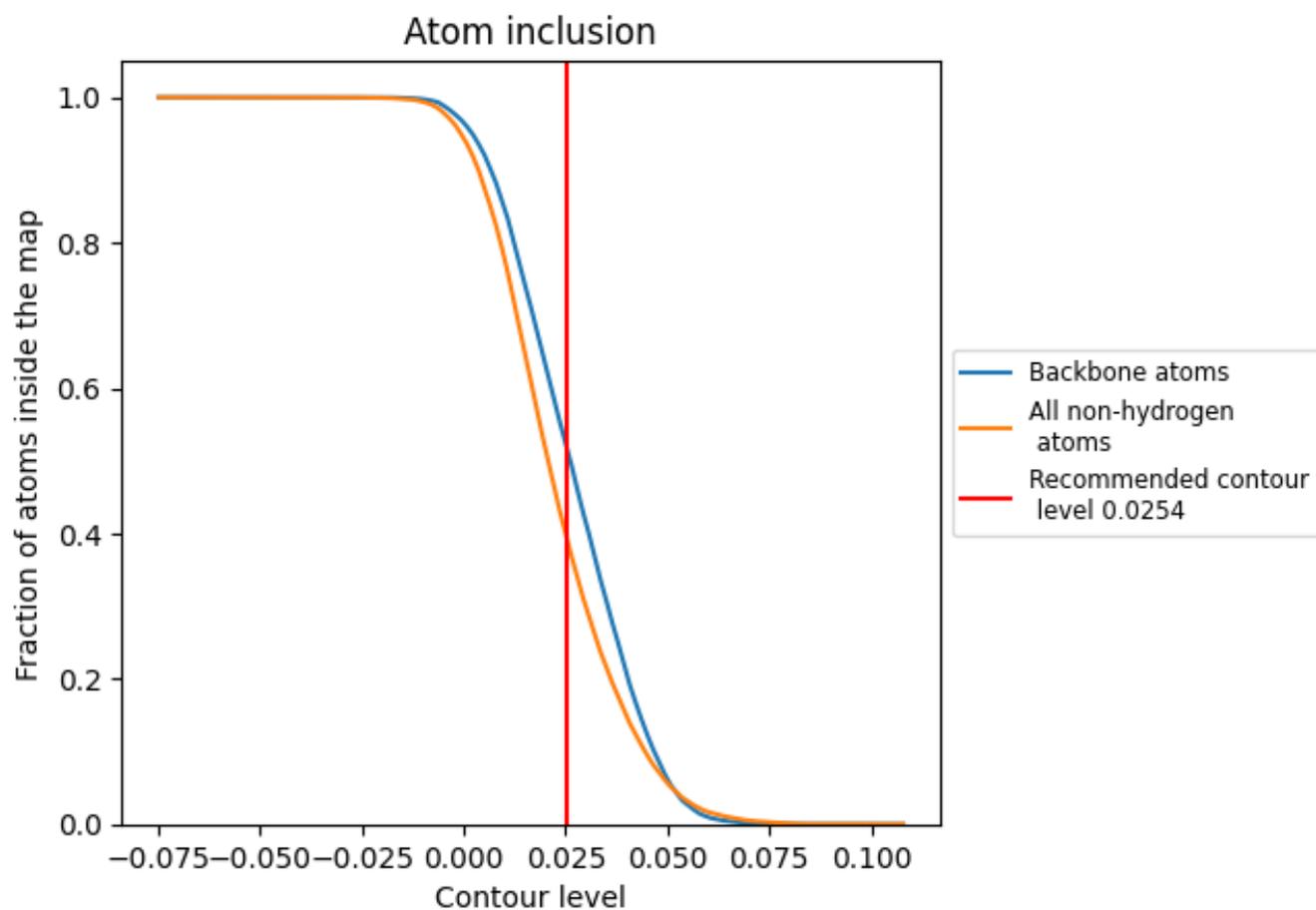
At the recommended contour level, 52% of all backbone atoms, 39% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0254) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3918	0.3720
0	0.4198	0.3390
1	0.5879	0.4410
2	0.5442	0.4090
3	0.4812	0.3960
4	0.5041	0.4300
5	0.4717	0.3810
6	0.5248	0.4430
7	0.5117	0.4320
8	0.4249	0.3480
9	0.4938	0.4270
A	0.4547	0.4190
B	0.3860	0.3570
C	0.5905	0.4580
D	0.4257	0.3990
E	0.4403	0.3540
F	0.4753	0.4180
G	0.4623	0.3790
H	0.0466	0.2360
I	0.5370	0.4380
J	0.5299	0.3840
K	0.5905	0.4430
L	0.0932	0.2730
M	0.1007	0.3040
N	0.5896	0.4260
O	0.6235	0.4690
P	0.5948	0.4060
Q	0.6255	0.4520
R	0.5688	0.3930
S	0.6132	0.4590
T	0.5636	0.4030
U	0.6481	0.4590
V	0.5662	0.4120
W	0.6152	0.4600
X	0.5584	0.3950

1.0

0.0
<0.0

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Chain	Atom inclusion	Q-score
Y	0.5947	0.4500
Z	0.5729	0.3960
t	0.4336	0.3520