WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

May 5, 2025 – 04:10 AM EDT

PDB ID	:	7TRA / pdb_00007tra
EMDB ID	:	EMD-26084
Title	:	Cascade complex from type I-A CRISPR-Cas system
Authors	:	Hu, C.; Ni, D.; Nam, K.H.; Majumdar, S.; McLean, J.; Stahlberg, H.; Terns, M.; Ke, A.
Deposited on	:	2022-01-28
Resolution	:	3.30 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

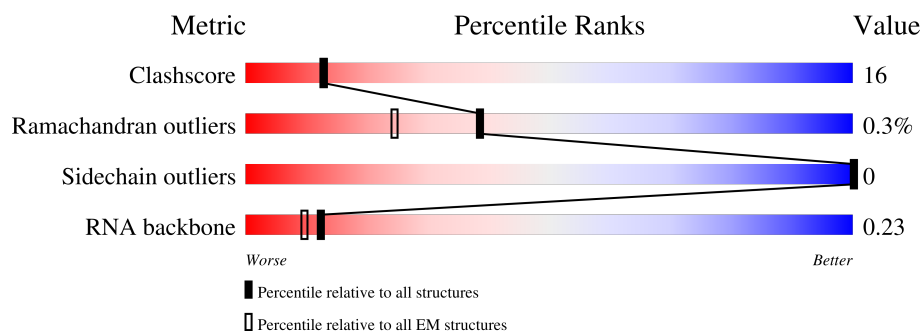|		
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
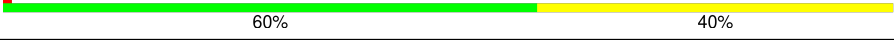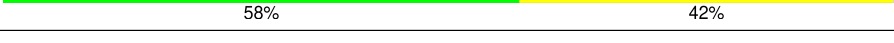
Metric	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		0.3%
Sidechain outliers		0
RNA backbone		0.23

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
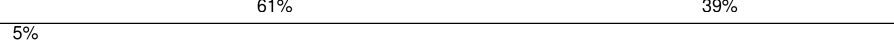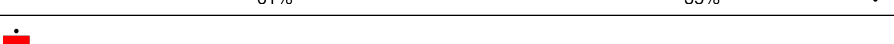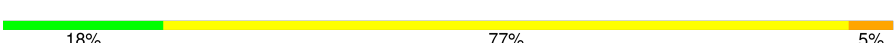
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	572	29% / 77% / 22%
2	B	341	7% / 64% / 34%
3	C	108	• / 65% / 34%
3	D	108	• / 64% / 36%
3	E	108	• / 68% / 31%
3	F	108	• / 68% / 31%
3	G	108	7% / 68% / 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	H	336	59% 40%
4	I	336	61% 39%
4	J	336	60% 40%
4	K	336	58% 42%
4	L	336	61% 39%
4	M	336	5% 61% 35%
4	N	336	55% 27% 18%
5	O	256	56% 38% 6%
6	Q	219	5% 61% 39%
7	R	44	18% 77% 5%
8	S	44	52% 48%
9	T	25	24% 64% 36%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 34872 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 CRISPR-associated helicase Cas3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	572	4315	2756	746	805	8	0	0

There are 97 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	LYS	ARG	conflict	UNP A0A5C0XNV5
A	?	-	VAL	deletion	UNP A0A5C0XNV5
A	364	ALA	GLU	conflict	UNP A0A5C0XNV5
A	365	ALA	ASN	conflict	UNP A0A5C0XNV5
A	366	ALA	CYS	conflict	UNP A0A5C0XNV5
A	367	ALA	ILE	conflict	UNP A0A5C0XNV5
A	368	ALA	GLU	conflict	UNP A0A5C0XNV5
A	369	ALA	HIS	conflict	UNP A0A5C0XNV5
A	370	ALA	GLU	conflict	UNP A0A5C0XNV5
A	371	ALA	LYS	conflict	UNP A0A5C0XNV5
A	372	ALA	ILE	conflict	UNP A0A5C0XNV5
A	373	ALA	VAL	conflict	UNP A0A5C0XNV5
A	374	ALA	ARG	conflict	UNP A0A5C0XNV5
A	375	ALA	GLY	conflict	UNP A0A5C0XNV5
A	376	ALA	LEU	conflict	UNP A0A5C0XNV5
A	377	ALA	SER	conflict	UNP A0A5C0XNV5
A	378	ALA	GLU	conflict	UNP A0A5C0XNV5
A	379	ALA	LEU	conflict	UNP A0A5C0XNV5
A	380	ALA	MET	conflict	UNP A0A5C0XNV5
A	381	ALA	GLU	conflict	UNP A0A5C0XNV5
A	382	ALA	LYS	conflict	UNP A0A5C0XNV5
A	383	ALA	ILE	conflict	UNP A0A5C0XNV5
A	384	ALA	GLY	conflict	UNP A0A5C0XNV5
A	385	ALA	GLU	conflict	UNP A0A5C0XNV5
A	386	ALA	ASP	conflict	UNP A0A5C0XNV5
A	387	ALA	THR	conflict	UNP A0A5C0XNV5
A	388	ALA	VAL	conflict	UNP A0A5C0XNV5
A	389	ALA	VAL	conflict	UNP A0A5C0XNV5

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	ALA	PHE	conflict	UNP A0A5C0XNV5
A	392	VAL	THR	conflict	UNP A0A5C0XNV5
A	451	PRO	-	insertion	UNP A0A5C0XNV5
A	?	-	ALA	deletion	UNP A0A5C0XNV5
A	517	LYS	-	expression tag	UNP A0A5C0XNV5
A	518	ALA	-	expression tag	UNP A0A5C0XNV5
A	519	ALA	-	expression tag	UNP A0A5C0XNV5
A	520	ALA	-	expression tag	UNP A0A5C0XNV5
A	521	ALA	-	expression tag	UNP A0A5C0XNV5
A	522	ALA	-	expression tag	UNP A0A5C0XNV5
A	523	ALA	-	expression tag	UNP A0A5C0XNV5
A	524	ALA	-	expression tag	UNP A0A5C0XNV5
A	525	ALA	-	expression tag	UNP A0A5C0XNV5
A	526	ALA	-	expression tag	UNP A0A5C0XNV5
A	527	ALA	-	expression tag	UNP A0A5C0XNV5
A	528	ALA	-	expression tag	UNP A0A5C0XNV5
A	529	ALA	-	expression tag	UNP A0A5C0XNV5
A	530	ALA	-	expression tag	UNP A0A5C0XNV5
A	531	ALA	-	expression tag	UNP A0A5C0XNV5
A	580	ALA	-	expression tag	UNP A0A5C0XNV5
A	581	ALA	-	expression tag	UNP A0A5C0XNV5
A	582	ALA	-	expression tag	UNP A0A5C0XNV5
A	583	ALA	-	expression tag	UNP A0A5C0XNV5
A	584	ALA	-	expression tag	UNP A0A5C0XNV5
A	585	ALA	-	expression tag	UNP A0A5C0XNV5
A	586	ALA	-	expression tag	UNP A0A5C0XNV5
A	587	ALA	-	expression tag	UNP A0A5C0XNV5
A	588	ALA	-	expression tag	UNP A0A5C0XNV5
A	589	ALA	-	expression tag	UNP A0A5C0XNV5
A	590	ALA	-	expression tag	UNP A0A5C0XNV5
A	591	ALA	-	expression tag	UNP A0A5C0XNV5
A	592	ALA	-	expression tag	UNP A0A5C0XNV5
A	593	ALA	-	expression tag	UNP A0A5C0XNV5
A	594	ALA	-	expression tag	UNP A0A5C0XNV5
A	595	ALA	-	expression tag	UNP A0A5C0XNV5
A	596	ALA	-	expression tag	UNP A0A5C0XNV5
A	597	ALA	-	expression tag	UNP A0A5C0XNV5
A	598	ALA	-	expression tag	UNP A0A5C0XNV5
A	599	ALA	-	expression tag	UNP A0A5C0XNV5
A	600	ALA	-	expression tag	UNP A0A5C0XNV5
A	601	ILE	-	expression tag	UNP A0A5C0XNV5
A	602	ASP	-	expression tag	UNP A0A5C0XNV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	-	expression tag	UNP A0A5C0XNV5
A	604	LYS	-	expression tag	UNP A0A5C0XNV5
A	605	TYR	-	expression tag	UNP A0A5C0XNV5
A	606	TYR	-	expression tag	UNP A0A5C0XNV5
A	607	ASN	-	expression tag	UNP A0A5C0XNV5
A	608	SER	-	expression tag	UNP A0A5C0XNV5
A	609	GLU	-	expression tag	UNP A0A5C0XNV5
A	610	LEU	-	expression tag	UNP A0A5C0XNV5
A	611	ALA	-	expression tag	UNP A0A5C0XNV5
A	612	ALA	-	expression tag	UNP A0A5C0XNV5
A	613	ALA	-	expression tag	UNP A0A5C0XNV5
A	614	ALA	-	expression tag	UNP A0A5C0XNV5
A	615	ALA	-	expression tag	UNP A0A5C0XNV5
A	616	ALA	-	expression tag	UNP A0A5C0XNV5
A	617	ALA	-	expression tag	UNP A0A5C0XNV5
A	618	ALA	-	expression tag	UNP A0A5C0XNV5
A	619	ALA	-	expression tag	UNP A0A5C0XNV5
A	620	ALA	-	expression tag	UNP A0A5C0XNV5
A	621	ALA	-	expression tag	UNP A0A5C0XNV5
A	622	ALA	-	expression tag	UNP A0A5C0XNV5
A	623	ALA	-	expression tag	UNP A0A5C0XNV5
A	624	ALA	-	expression tag	UNP A0A5C0XNV5
A	625	ALA	-	expression tag	UNP A0A5C0XNV5
A	626	ALA	-	expression tag	UNP A0A5C0XNV5
A	627	ALA	-	expression tag	UNP A0A5C0XNV5
A	628	ALA	-	expression tag	UNP A0A5C0XNV5
A	629	ALA	-	expression tag	UNP A0A5C0XNV5

- Molecule 2 is a protein called Cas8a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	333	2662	1730	439	484	9	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	VAL	GLU	conflict	UNP Q8U338
B	64	SER	GLU	conflict	UNP Q8U338
B	110	LEU	VAL	conflict	UNP Q8U338
B	?	-	SER	deletion	UNP Q8U338
B	?	-	LEU	deletion	UNP Q8U338

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP Q8U338

- Molecule 3 is a protein called Cas11a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	107	Total 856	C 550	N 144	O 160	S 2	0	0
3	D	108	Total 860	C 552	N 145	O 161	S 2	0	0
3	E	107	Total 856	C 550	N 144	O 160	S 2	0	0
3	F	107	Total 856	C 550	N 144	O 160	S 2	0	0
3	G	107	Total 856	C 550	N 144	O 160	S 2	0	0

- Molecule 4 is a protein called Cas7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	335	Total 2597	C 1655	N 450	O 487	S 5	0	0
4	I	336	Total 2603	C 1659	N 451	O 488	S 5	0	0
4	J	336	Total 2596	C 1656	N 448	O 487	S 5	0	0
4	K	336	Total 2597	C 1656	N 448	O 488	S 5	0	0
4	L	336	Total 2597	C 1656	N 448	O 488	S 5	0	0
4	M	321	Total 2494	C 1595	N 431	O 463	S 5	0	0
4	N	274	Total 2134	C 1370	N 364	O 396	S 4	0	0

- Molecule 5 is a protein called Cas5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	240	Total 1936	C 1266	N 315	O 349	S 6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	?	-	THR	deletion	UNP A0A5C0XNV9

- Molecule 6 is a protein called CRISPR-associated endonuclease Cas3-HD.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	219	Total 1733	C 1113	N 296	O 311	S 13	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	LEU	deletion	UNP Q8U336
Q	217	ALA	-	expression tag	UNP Q8U336
Q	218	ALA	-	expression tag	UNP Q8U336
Q	219	ALA	-	expression tag	UNP Q8U336
Q	220	ALA	-	expression tag	UNP Q8U336

- Molecule 7 is a RNA chain called crRNA (44-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	44	Total 890	C 417	N 161	O 269	P 43	0	0

- Molecule 8 is a DNA chain called Target strand DNA (44-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	44	Total 913	C 433	N 173	O 263	P 44	0	0

- Molecule 9 is a DNA chain called Non-Target strand DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	25	Total 519	C 247	N 113	O 134	P 25	0	0

- Molecule 10 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

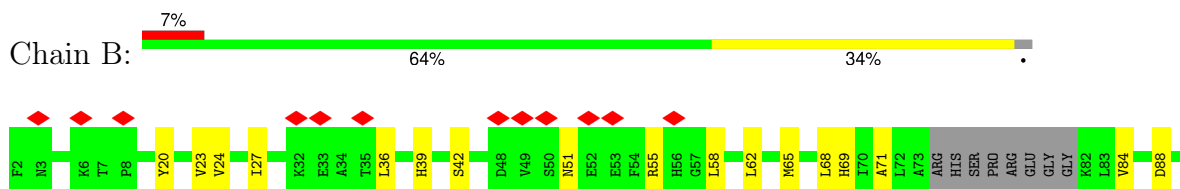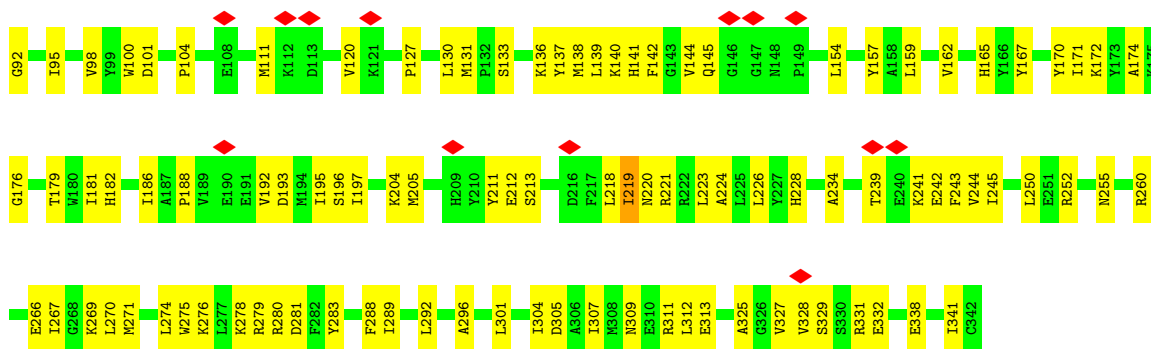| Mol	Chain	Residues	Atoms		AltConf
10	Q	2	Total 2	Ni 2	0

3 Residue-property plots ⓘ

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

• Molecule 1: CRISPR-associated helicase Cas3

Chain A:

• Molecule 2: Cas8a

Chain B:

G92 I95 V98 Y99 W100 D101 P104 E108 M111 K112 D113 V120 K121 P127 L130 M131 P132 S133 K136 Y137 M138 L139 K140 H141 F142 G143 V144 Q145 G146 G147 N148 P149 L154 Y157 A158 L159 V162 H165 Y166 Y167 Y170 I171 K172 Y173 A174 K175

G176 T179 W180 I181 H182 I186 A187 P188 V189 E190 E191 V192 D193 M194 I195 S196 I197 K204 M205 H209 Y210 Y211 E212 S213 D216 F217 L218 I219 N220 R221 R222 L223 A224 L225 Y226 Y227 H228 A234 T239 E240 E242 F243 V244 I245 L250 E251 R252 N255 R260

E266 I267 G268 K269 L270 M271 L274 W275 K276 L277 K278 R279 R280 D281 F282 Y283 F288 I289 L292 A296 L301 I304 D305 A306 I307 M308 N309 E310 R311 L312 E313 A325 G326 V327 V328 S329 S330 R331 E332 E338 I341 C342

- Molecule 3: Cas11a

Chain C: 65%   34%

GLY G3 W4 I5 R6 N7 I8 G9 Y14 L15 V16 D17 D18 A24 Y25 D26 V27 K33 A34 R35 T36 Q37 E38 E39 E42 G43 V44 L48 R49 K55 P66 R67 I68 D73 E78 E79 E82 Q83 D89 L90 R91 K92 V95 W100 S104 W105

N106 P109

- Molecule 3: Cas11a

Chain D: 64%   36%

G2 G3 R6 R10 Y11 L12 S13 Y14 D17 F20 E21 E22 Y23 A24 Y25 D26 V27 A32 R35 T36 Q37 E38 E42 Y45 R49 L50 A51 K57 K61 R67 I68 P69 S70 P71 E72 E75 A76 L77 E78 E79 K80 K88 D89 L90 R91

L99 W100 A101 F102 A103 S104 P109

- Molecule 3: Cas11a

Chain E: 68%   31%

GLY G3 R6 R10 Y11 Y14 D17 D18 T19 F20 E21 E22 Y23 D29 G30 I31 R35 T36 Q37 E38 E39 L40 L41 E42 A47 L48 R49 P52 K53 L54 K55 E59 I68 L84 S85 N86 L90 R91 A98 L99 W100 A103 S104 W105 N106 N107

C108 P109

- Molecule 3: Cas11a

Chain F: 68%   31%

GLY G3 W4 N7 I8 G9 R10 Y11 Y14 E22 Y23 A24 Y25 D26 I31 R35 T36 Q37 E38 E39 L40 L41 V44 A47 L48 R49 L50 A51 P52 K53 L54 P66 S70 P71 L77 K80 L84 K88 D89 L90 A94 L97 W100 A101

F102 A103 S104 N107 C108 P109

• Molecule 3: Cas11a

Chain G:

7%

68%

31%

GLY G3 R6 N7 I8 L12 S13 Y14 L15 V16 A32 K33 A34 R35 E38 L41 E42 G43 K46 P52 K53 L54 K55 K56 P66 R67 I68 P69 S70 P71 E72 D73 I74 L77 E78 E79 K80 V81 E82 Q83 L84 S85 N86 P87 K88 D89 K92 V95 S96

L97 A101 F102 P109

• Molecule 4: Cas7a

Chain H:

59%

40%

M1 Y2 V3 R4 I5 S6 G7 R8 I9 R10 L11 N12 A13 H14 S15 L16 N17 A18 Q19 G20 N25 Y26 I27 E28 I29 T32 R37 T38 E39 N40 G41 W42 V45 E46 I50 T51 G52 N53 M54 L55 W58 V61 G62 F63 Y66 T70 P71 Y72 E78 R79

Y83 N84 R87 Q90 T93 T94 A95 T96 G100 A101 T102 V103 Q104 L105 N106 D107 E108 I111 I112 V120 H121 G122 F123 L124 A125 P126 K127 R130 R131 V133 K137 A138 S139 F140 I141 L142 P143 T144 E145 D146 F147 I148 R155 L156 I157 T158 H162 N163

R164 V165 D166 V167 D168 E169 T180 A181 Q182 M183 L184 F185 S186 R187 T191 Y194 G195 F196 V199 L200 D201 L202 V205 P212 F215 E216 E217 N218 Q219 P220 R221 V225 I226 R231 R234 I235 K240 A241 P244 Y249 I250 G251 L254 A255 F258

P259 V260 F261 K262 V263 E264 E265 L266 V267 A268 I269 P276 A277 L278 V279 D285 Y286 I287 N290 I294 A297 G301 F302 N303 I304 E305 V306 F307 T308 V311 D312 L313 D316 I317 V322 M335 VAL

• Molecule 4: Cas7a

Chain I:

61%

39%

M1 Y2 V3 R4 R8 L11 N12 S15 L16 N17 A18 Q19 N25 E28 T32 K33 V34 T35 V36 R37 T38 E39 N40 V44 I50 T51 M54 L55 K56 H57 W58 V64 F67 N75 E78 R79 A80 L81 R82 Y83 N84 G85 T86 K97 A98

L105 N106 D107 I111 I112 L115 A118 D119 V120 H121 G122 F123 L124 A125 P126 K127 T128 G129 R130 R131 R132 V133 S134 K137 A138 S139 F140 I141 L142 F147 I148 K149 E150 V151 E152 G153 E154 R155 T158 R164 V165 D166 V167 D168 E169 A172 Q182 M183 L184 F185 S186

R187 E188 Y194 G195 F196 S197 I198 V199 L200 D201 L202 G203 L204 V205 G206 I207 K214 F215 E216 E230 R231 R234 I235 E236 P244 M245 L246 Y249 I250 G251 A252 N253 L254 A255 R256 S257 F258 V263 E264 E265 L266 V267 A268 I269 A270 I275 P276 A277 H280 G281 F282

Y283 E284 D285 Y286 I287 N290 I294 G301 I304 E305 V306 F307 T308 Y309 N310 V311 D312 L313 G314 E315 V322 E327 L328 N331 L332 V333 K334 M335 V336

● Molecule 4: Cas7a

Chain J:

● Molecule 4: Cas7a

Chain K:

● Molecule 4: Cas7a

Chain L:

I287 E288 R298 A299 L300 G301 V306 Y309 D312 L313 G314 E315 D316 I317 E318 V322 S323 S324 V325 E326 E327 L328 N331 L332 V333 K334 M335 V336

● Molecule 4: Cas7a

Chain M:

5%

61% 35%

M1 Y2 V3 R4 R8 I9 R10 H14 S15 L16 N17 A18 Q19 G20 G21 T24 N25 Y26 I27 T30 K31 V34 W42 E46 V47 P48 A49 I50 T51 M54 L55 K56 H57 W58 F63 Y66 F67 K68 R79 R82 T86 R87 F88 G91 T94

A95 T102 V103 N106 T110 I111 I112 K113 E114 L115 A118 D119 F123 L124 K127 R130 R131 R132 L135 V136 K137 A138 S139 F140 I141 L142 P143 T144 V151 E152 G153 E154 R155 L156 I157 I160 R164 VAL ASP VAL ASP GLU LYS GLY ALA ILE GLY SER SER

LYS GLU GLY T180 M183 L184 F185 S186 R187 E188 Y189 A190 L193 Y194 G195 F196 S197 I198 V199 L200 D201 L202 G203 L204 V205 G206 I207 K214 P222 N223 R231 R234 I235 L239 K240 A241 L242 I243 P244 M245 L246 S247 G248 Y249 I250 G251 P259 V260 F261 K262 V263

L266 I269 I275 P276 F282 Y283 E284 D285 E288 R291 L300 V306 Y309 L313 D316 A319 T320 K321 E326 E327 L328 V329 A330 N331 K334 M335 V336

● Molecule 4: Cas7a

Chain N:

55% 27% 18%

M1 Y2 V3 G7 R8 I9 R10 L11 N17 ALA GLN GLY GLY GLY THR ASN TYR ILE GLU ILE T30 K31 V34 T35 V36 R37 T38 E39 N40 G41 W42 E46 V47 P48 A49 I50 T51 M54 L55 K56 H59 F60 V61 V64 T86 R87 F88 G89 Q90 G91 E92

T93 T94 A95 V103 E108 I112 K113 D117 A118 D119 K127 T128 G129 R130 S134 L135 V136 K137 I141 L142 P143 D146 F147 I148 V151 E152 GLY GLU ARG LEU ILE THR ALA ILE LYS HIS ASN ARG VAL ASP VAL ASP GLU LYS GLY ALA ILE GLY SER SER LYS

GLU GLY THR ALA GLN MET LEU PHE SER ARG GLU GLU TYR ALA THR G192 L193 Y194 G195 F196 V199 L200 D201 L202 L211 P212 E216 R221 P222 N223 I224 V225 I226 R231 R234 I235 L239 S247 GLY TYR ILE GLY ALA ASN LEU ALA ARG SER PHE P259 V260 F261 K262

V263 E264 E265 L266 I269 P274 A277 L278 V279 H280 Y283 E284 D285 E288 R291 S292 N296 L300 G301 F302 N303 I304 F307 T308 Y309 N310 V311 G314 E315 D316 T320 K321 V322 N331 L332 V333 K334 M335 V336

● Molecule 5: Cas5a

Chain O:

56% 38% 6%

M1 D2 I3 L4 L5 F10 P11 F12 F13 S14 V15 A16 K17 R18 S19 Y20 Q21 V22 R23 T24 S25 F26 L27 L28 P29 P30 P31 S32 A33 L34 K35 P47 E48 S52 E57 A58 K61 E67 L70 I73 K74 A75 A79 P80 L81 S82 P83 L84 I85 R86 N87

A88 F89 L90 L91 K92 R93 L94 R95 E98 S99 G100 K105 S106 D107 A108 M109 R110 R111 E112 Y113 E118 L119 L120 Y123 Q130 K133 M141 D144 V145 T149 E150 S151 L152 A153 T154 P163 E164 D165 P169 L170 A171 F172 Y176 L182 LEU SER SER

LYS ILE GLN ALA LYS GLY LYS ILE R194 M195 M200 R201 V202 S203 S207 LYS THR LYS GLY PRO Q213 E214 E215 I216 F217 Y218 L219 P220 I221 R225 Y226 K227 R228 I229 V230 Y231 Y232 A233 R234 P237 V240 E241 K242 T245 V250 L251 G252 P256

• Molecule 6: CRISPR-associated endonuclease Cas3-HD

Chain Q:

5%

61% 39%

S2 C3 K4 A5 F6 Q7 G8 Q9 T10 L11 R12 E13 H14 I15 E16 A17 M18 W22 E23 I24 V25 Y29 I34 R35 V36 M37 K43 F44 A49 D50 K51 K54 I57 I58 L59 H60 D61 V62 S66 Q70 R83 H84 E85 L86 A89 Y90 Y91 A92 Y93

N94 I95 L96 K97 D98 M99 F100 K101 I105 A106 F107 L111 V112 V113 M114 E118 P119 I120 L121 Q124 I125 R126 S127 L128 E132 L133 T134 P135 E136 V137 V138 K141 F145 V148 M149 E150 G151 T152 E153 S154 F155 I156 K157 S158 K163 L164 G165 V166 I167 P168 K169

V170 Q175 V178 L179 R180 E181 V182 I183 R184 R190 H191 R192 L198 R199 M200 V201 V202 L205 P208 G215 A220

• Molecule 7: crRNA (44-MER)

Chain R:

18% 77% 5%

A1 U2 U3 G4 A5 A6 A7 G8 A9 G10 U11 G12 C13 U14 U15 C16 C17 C18 C19 A20 A21 A22 C23 C24 C25 U26 U27 A28 A29 C30 U31 G32 G33 U34 U35 G36 U37 A38 A39 G42 U43 U44

• Molecule 8: Target strand DNA (44-MER)

Chain S:

52% 48%

T21 A24 C25 T26 T29 A30 C31 A32 C35 A36 G37 T38 T39 A40 A41 G42 G43 G44 T45 T46 G54 C55 A56 C57 G61 T64

• Molecule 9: Non-Target strand DNA (25-MER)

Chain T:

24%

64% 36%

A16 G17 A18 C21 A22 T25 A28 A33 A34 A37 A38 A42 A43 A44 A45

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44773	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.033	Depositor
Minimum map value	-0.425	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.145	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	A	0.12	0/4387	0.34	0/5960
2	B	0.11	0/2723	0.32	0/3684
3	C	0.11	0/876	0.34	0/1188
3	D	0.12	0/880	0.31	0/1193
3	E	0.11	0/876	0.34	0/1188
3	F	0.13	0/876	0.38	0/1188
3	G	0.15	0/876	0.42	0/1188
4	H	0.10	0/2645	0.31	0/3583
4	I	0.11	0/2651	0.32	0/3592
4	J	0.11	0/2644	0.31	0/3584
4	K	0.12	0/2645	0.32	0/3585
4	L	0.11	0/2645	0.31	0/3585
4	M	0.11	0/2541	0.30	0/3445
4	N	0.09	0/2173	0.27	0/2946
5	O	0.11	0/1977	0.34	0/2673
6	Q	0.15	0/1764	0.41	0/2376
7	R	0.15	0/998	0.34	0/1536
8	S	0.16	0/1026	0.32	0/1584
9	T	0.10	0/584	0.20	0/888
All	All	0.12	0/35787	0.33	0/48966

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
6	Q	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Q	134	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4315	0	4428	91	0
2	B	2662	0	2668	98	0
3	C	856	0	860	29	0
3	D	860	0	863	32	0
3	E	856	0	860	26	0
3	F	856	0	860	24	0
3	G	856	0	860	31	0
4	H	2597	0	2628	119	0
4	I	2603	0	2635	106	0
4	J	2596	0	2621	117	0
4	K	2597	0	2624	126	0
4	L	2597	0	2624	114	0
4	M	2494	0	2524	114	0
4	N	2134	0	2168	68	0
5	O	1936	0	2018	82	0
6	Q	1733	0	1801	63	0
7	R	890	0	470	64	0
8	S	913	0	496	29	0
9	T	519	0	282	8	0
10	Q	2	0	0	0	0
All	All	34872	0	34290	1117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1117 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:36:VAL:O	4:K:42:TRP:HA	1.68	0.93
4:H:164:ARG:O	4:H:182:GLN:HA	1.68	0.92
3:D:77:LEU:HA	3:D:80:LYS:HE2	1.54	0.88
2:B:219:ILE:HG13	2:B:220:ASN:H	1.38	0.88
4:H:165:VAL:HA	4:H:182:GLN:HG2	1.61	0.82

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/572 (99%)	488 (86%)	73 (13%)	7 (1%)	11	38
2	B	329/341 (96%)	301 (92%)	26 (8%)	2 (1%)	22	53
3	C	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
3	D	106/108 (98%)	99 (93%)	7 (7%)	0	100	100
3	E	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
3	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
3	G	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
4	H	333/336 (99%)	315 (95%)	18 (5%)	0	100	100
4	I	334/336 (99%)	314 (94%)	19 (6%)	1 (0%)	37	66
4	J	334/336 (99%)	319 (96%)	15 (4%)	0	100	100
4	K	334/336 (99%)	306 (92%)	27 (8%)	1 (0%)	37	66
4	L	334/336 (99%)	310 (93%)	24 (7%)	0	100	100
4	M	317/336 (94%)	292 (92%)	25 (8%)	0	100	100
4	N	266/336 (79%)	254 (96%)	12 (4%)	0	100	100
5	O	234/256 (91%)	214 (92%)	20 (8%)	0	100	100
6	Q	217/219 (99%)	202 (93%)	15 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	4126/4280 (96%)	3800 (92%)	315 (8%)	11 (0%)	38	66

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	219	ILE
1	A	492	ILE
4	K	313	LEU
1	A	284	ASN
1	A	458	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	A	424/427 (99%)	424 (100%)	0	100	100
2	B	282/292 (97%)	282 (100%)	0	100	100
3	C	91/91 (100%)	91 (100%)	0	100	100
3	D	91/91 (100%)	91 (100%)	0	100	100
3	E	91/91 (100%)	91 (100%)	0	100	100
3	F	91/91 (100%)	91 (100%)	0	100	100
3	G	91/91 (100%)	91 (100%)	0	100	100
4	H	275/277 (99%)	275 (100%)	0	100	100
4	I	276/277 (100%)	276 (100%)	0	100	100
4	J	274/277 (99%)	274 (100%)	0	100	100
4	K	275/277 (99%)	275 (100%)	0	100	100
4	L	275/277 (99%)	275 (100%)	0	100	100
4	M	264/277 (95%)	264 (100%)	0	100	100
4	N	230/277 (83%)	230 (100%)	0	100	100
5	O	211/224 (94%)	211 (100%)	0	100	100
6	Q	191/191 (100%)	191 (100%)	0	100	100

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3432/3528 (97%)	3432 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
4	M	290	ASN
4	N	331	ASN
4	M	296	ASN
4	N	104	GLN
4	H	99	ASN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	7/44 (15%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	2	U
7	R	4	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	T	4
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	531:ALA	C	580:ALA	N	39.61
1	T	34:DA	O3'	37:DA	P	10.51
1	T	25:DT	O3'	28:DA	P	8.77
1	T	40:DA	O3'	42:DA	P	7.92
1	T	44:DA	O3'	45:DA	P	3.28

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-26084. 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 |
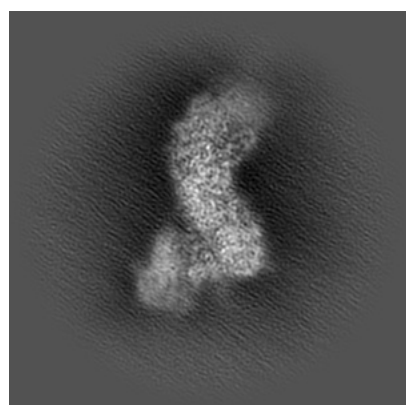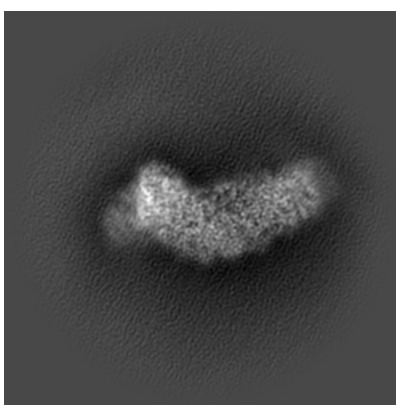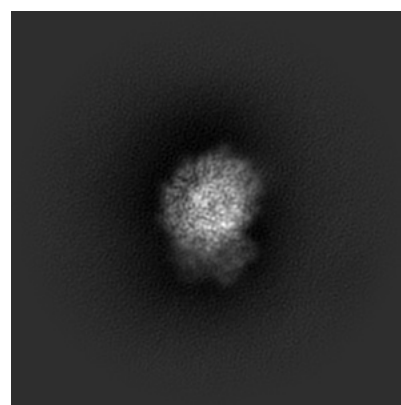
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
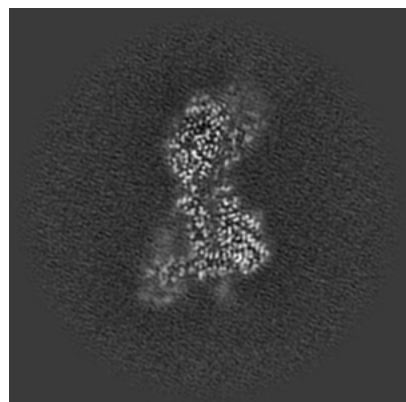
6.2.1 Primary map
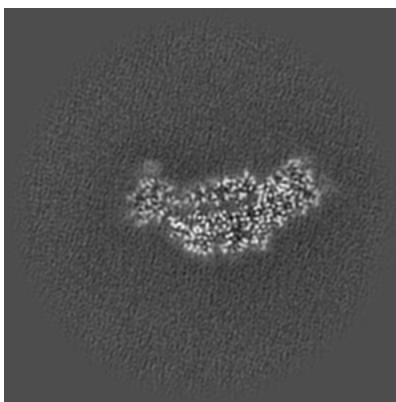
| X Index: 150 | Y Index: 150 | Z Index: 150 |
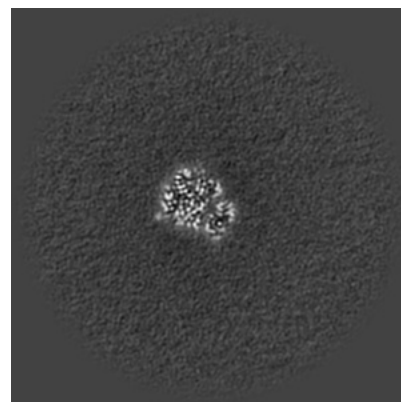
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
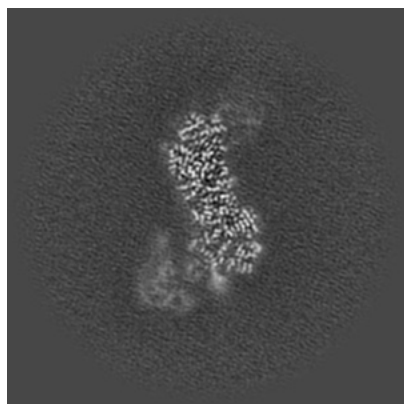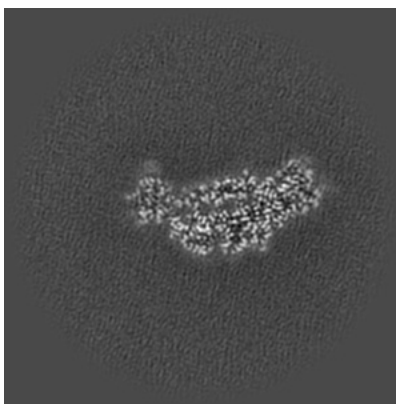
| X Index: 142 | Y Index: 149 | Z Index: 121 |
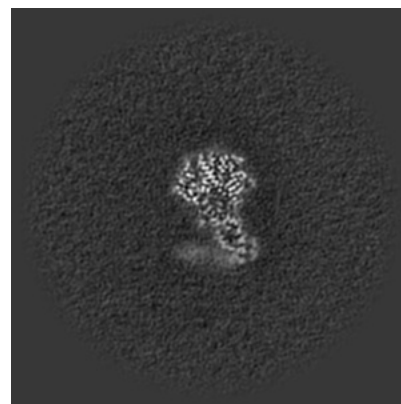
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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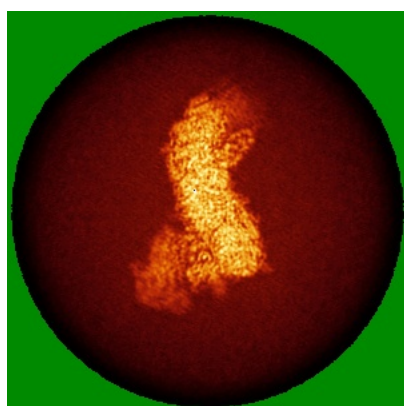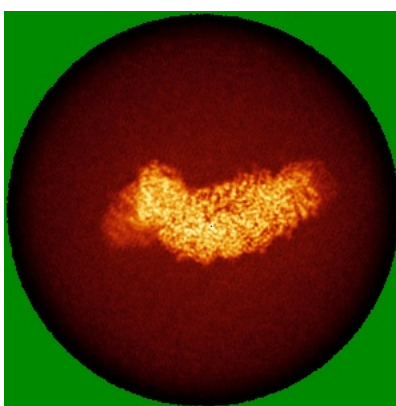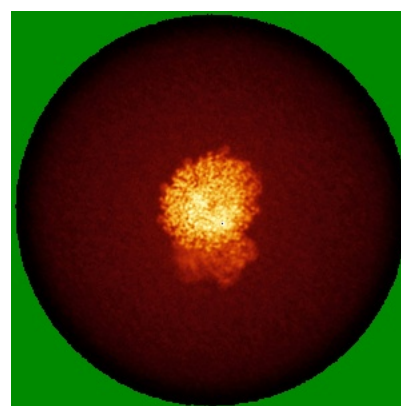
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5Orthogonal surface views(i)

6.5.1Primary map

X   Y   Z
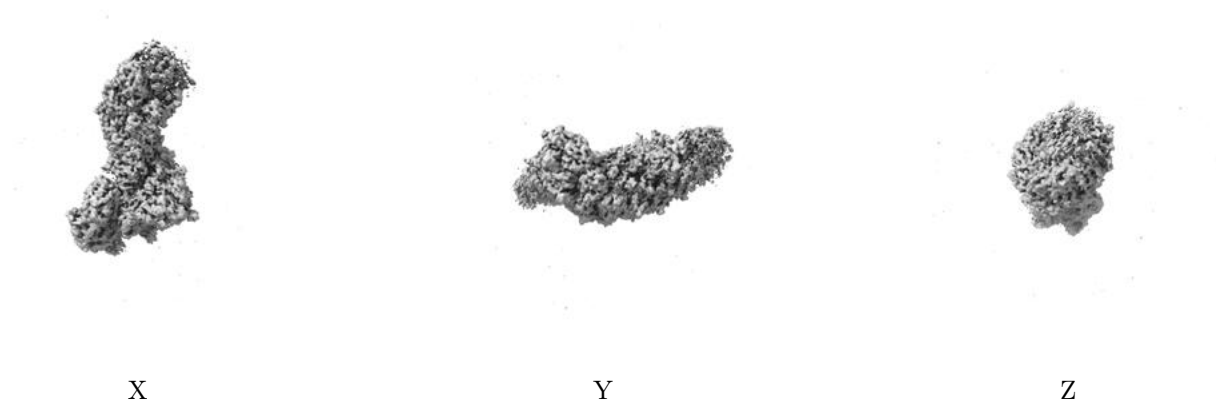
The images above show the 3D surface view of the map at the recommended contour level 0.145.
These images, in conjunction with the slice images, may facilitate assessment of whether an ap-
propriate contour level has been provided.

6.6Mask visualisation(i)

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

7　Map analysis ⓘ

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

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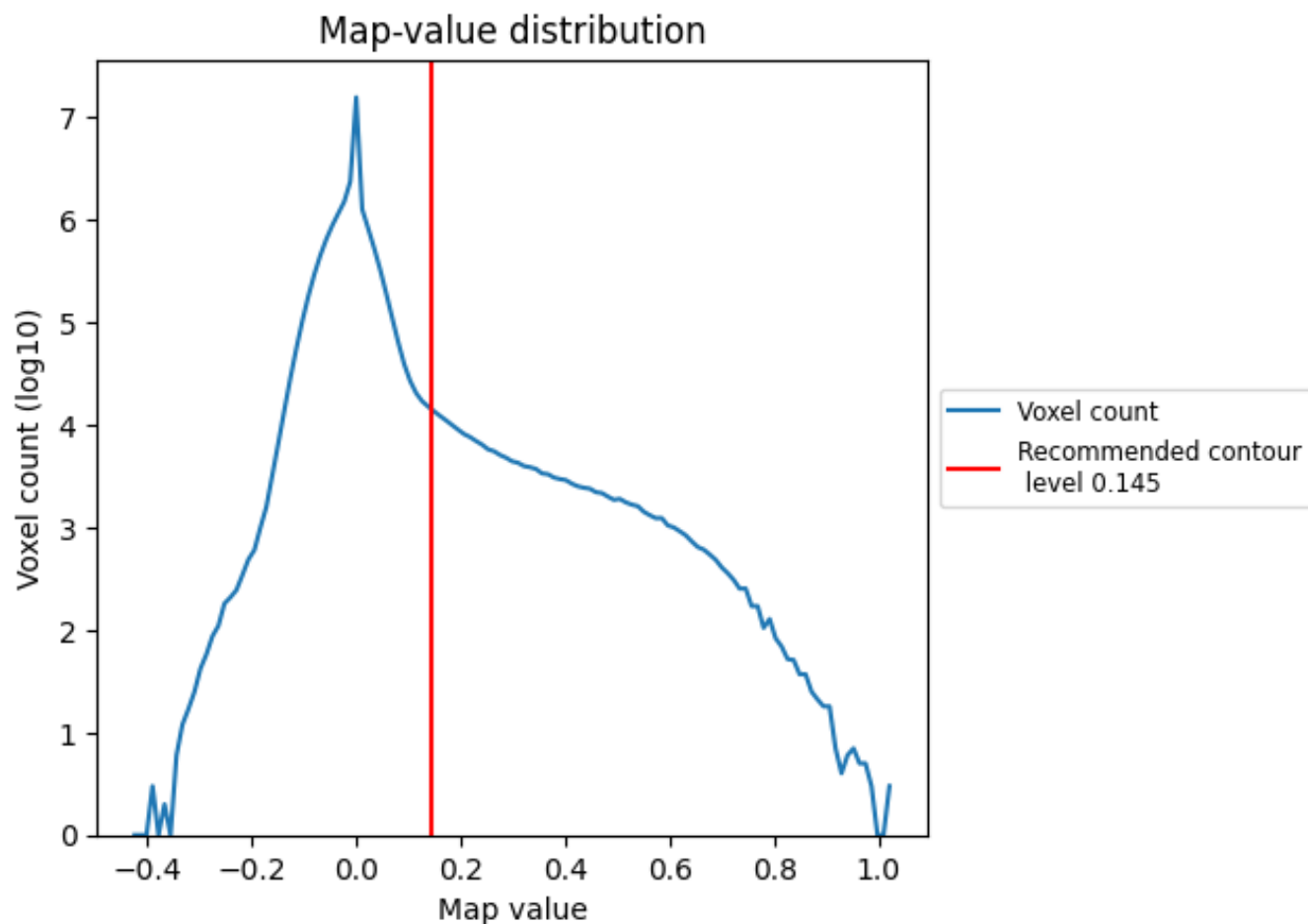
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
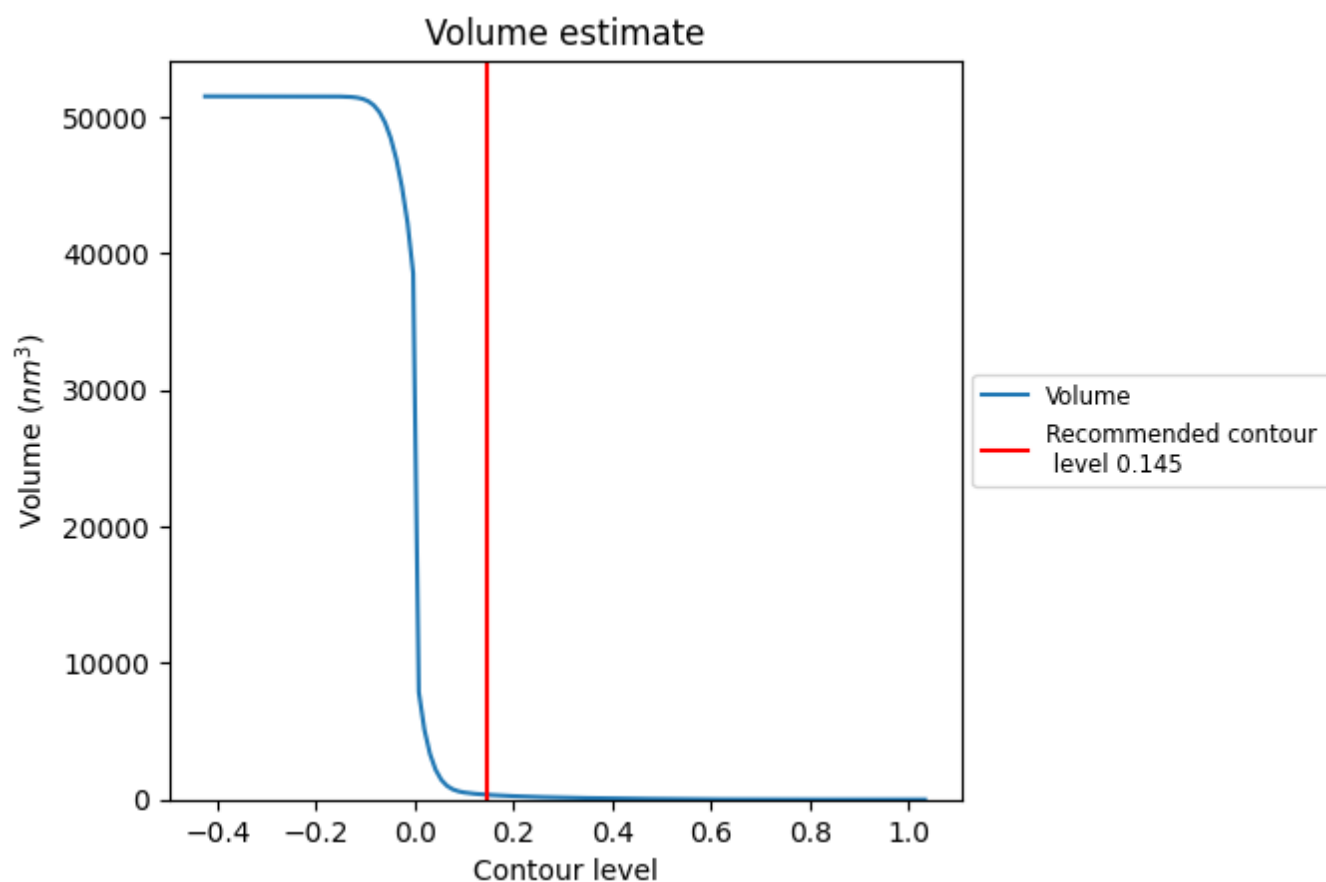
The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 322 kDa.

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 ⓘ
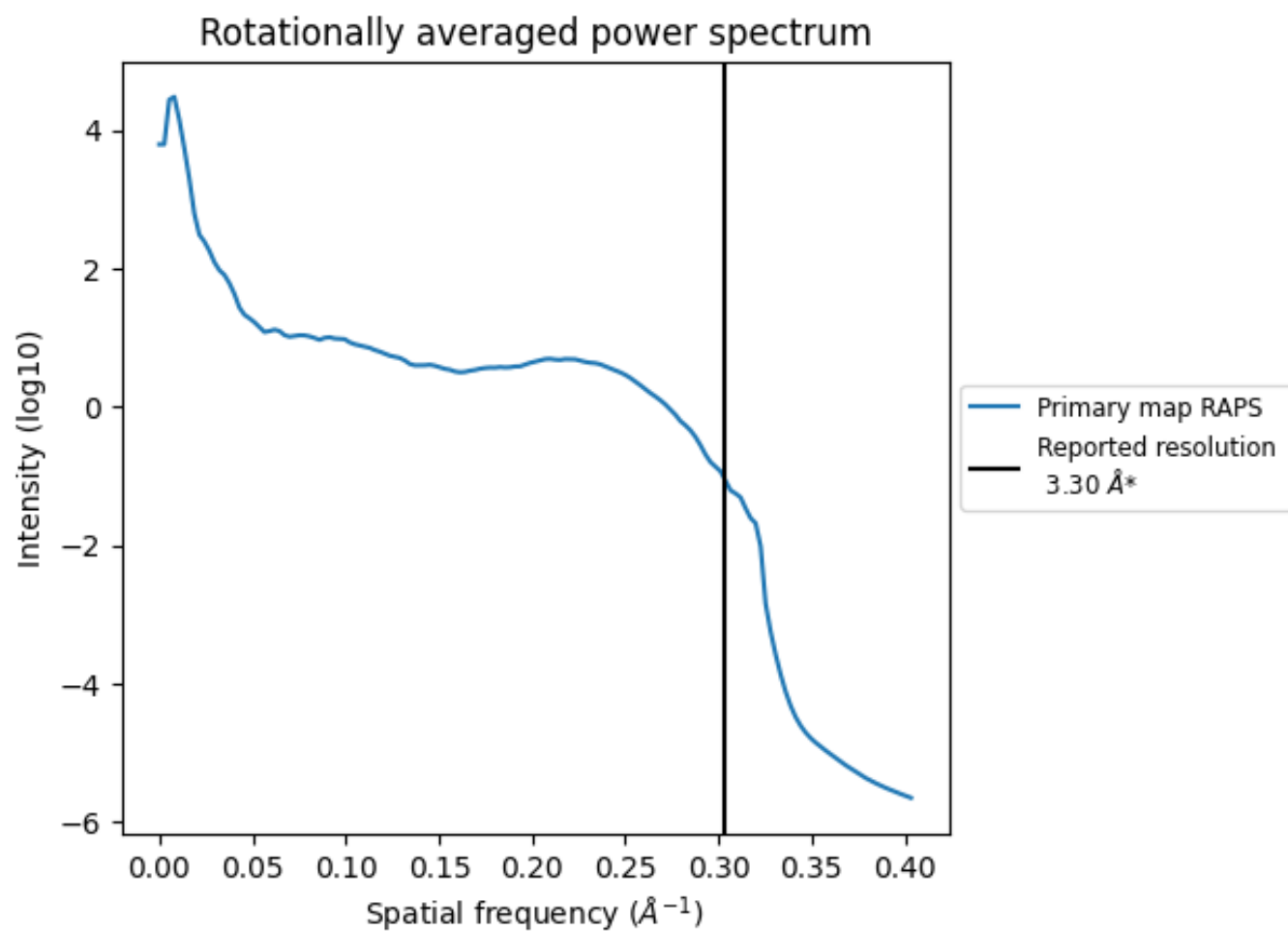
*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26084 and PDB model 7TRA. Per-residue inclusion information can be found in section 3 on page 9.

9.1   Map-model overlay (i)

| X | Y | Z |
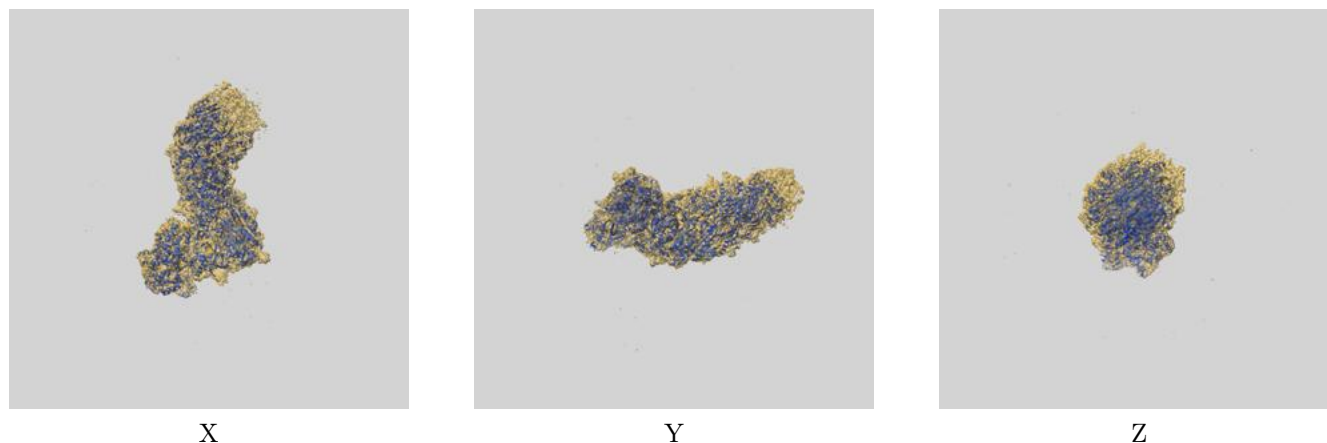
The images above show the 3D surface view of the map at the recommended contour level 0.145 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ
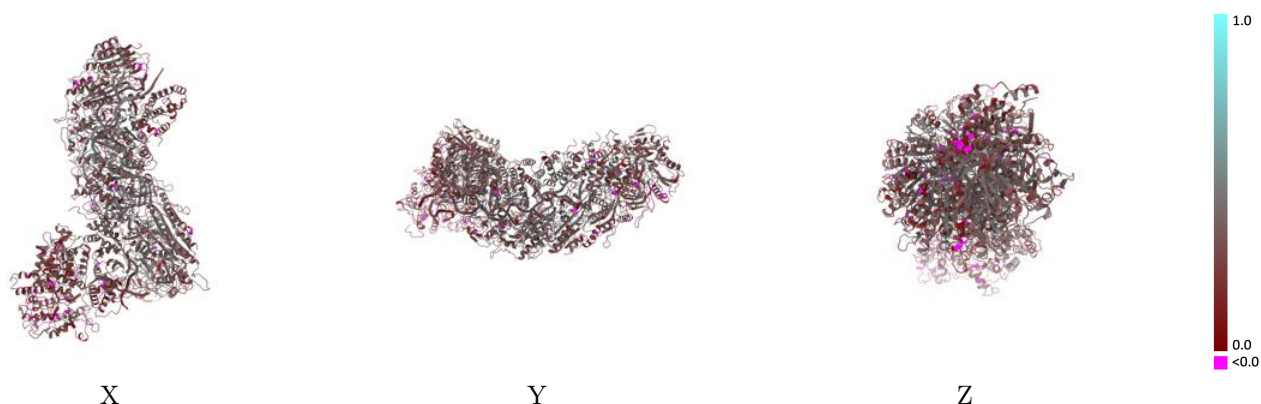
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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   ⓘ
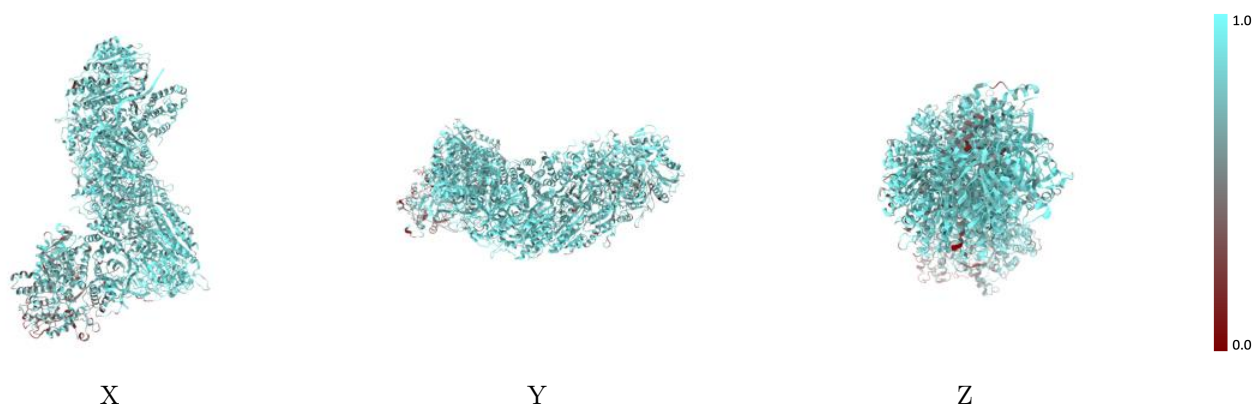
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.145).

9.4 Atom inclusion ⓘ
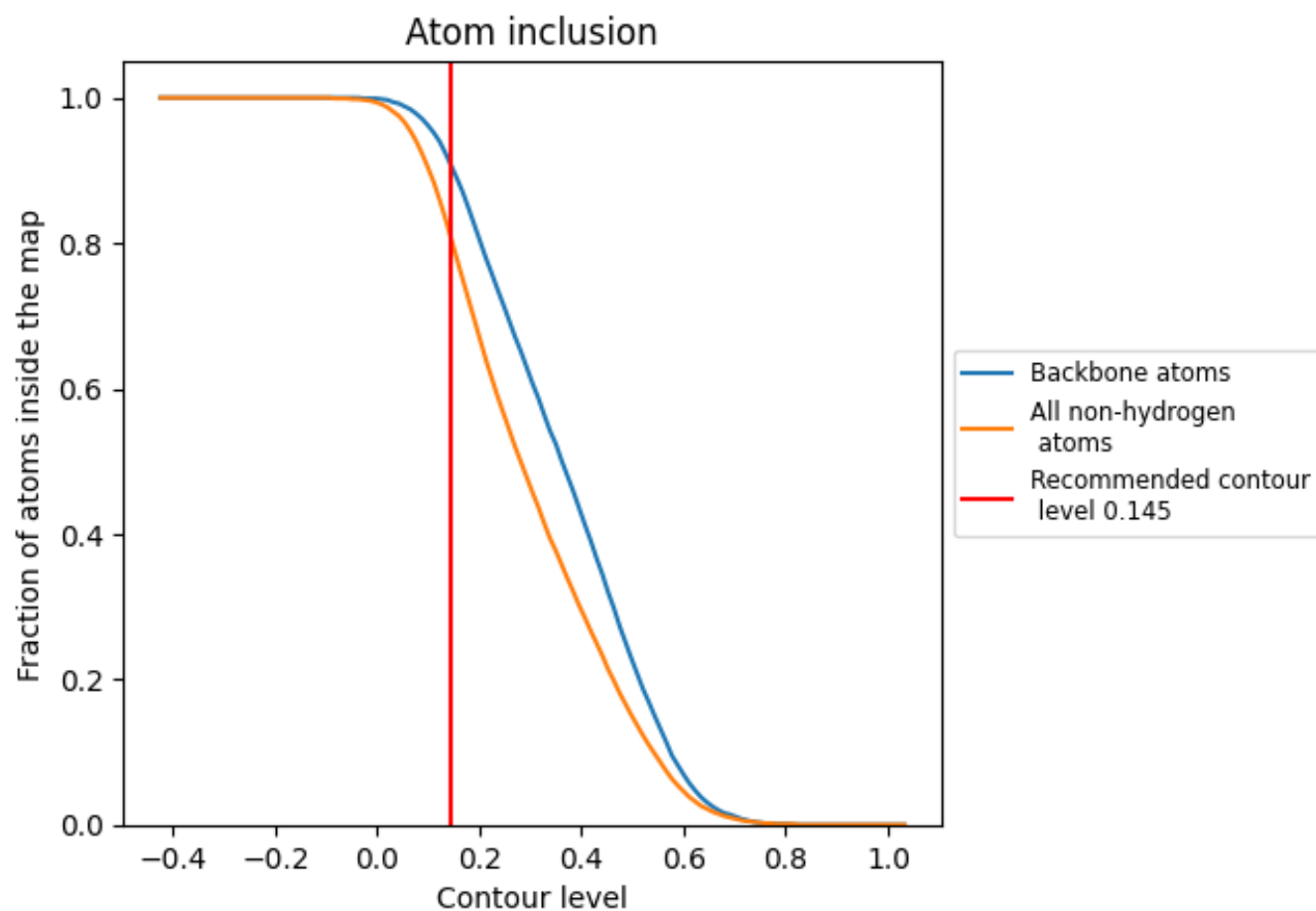
At the recommended contour level, 91% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8050	0.3240
A	0.5930	0.1970
B	0.7850	0.3150
C	0.8740	0.3600
D	0.8740	0.3510
E	0.8600	0.3680
F	0.8150	0.3270
G	0.7300	0.2690
H	0.8470	0.3420
I	0.8720	0.3560
J	0.8880	0.3870
K	0.8510	0.3510
L	0.8260	0.3480
M	0.8040	0.3310
N	0.8050	0.3240
O	0.8440	0.3480
Q	0.7680	0.2980
R	0.9610	0.4340
S	0.9470	0.3850
T	0.6220	0.1960

1.0

0.0
<0.0