WORLDWIDE

wwPDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Mar 9, 2024 – 10:29 AM EST

PDB ID	:	6NUW
EMDB ID	:	EMD-0523
Title	:	Yeast Ctf19 complex
Authors	:	Hinshaw, S.M.; Harrison, S.C.
Deposited on	:	2019-02-03
Resolution	:	4.25 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 ⓘ 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 ⓘ) were used in the production of this report:
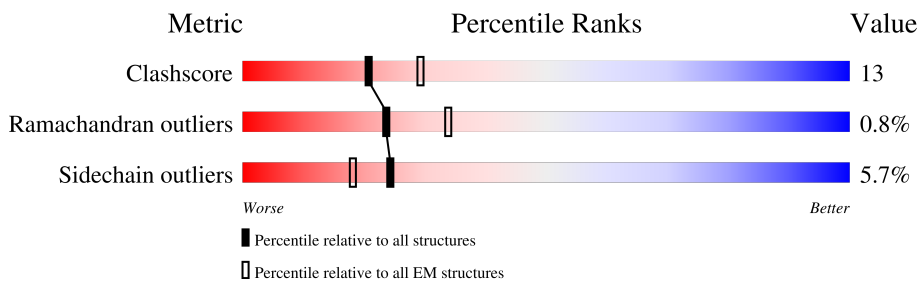
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1　Overall quality at a glance ⓘ

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

The reported resolution of this entry is 4.25 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.
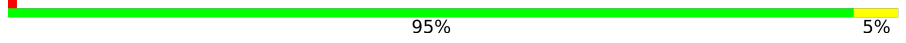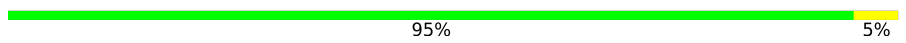
Metric	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		0.8%
Sidechain outliers		5.7%

Worse　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	B	248	6% — 62% / 35% / · ·
2	C	371	· 34% / 16% / · / 48%
3	D	369	· 29% / 19% / 5% · / 47%
4	E	461	6% — 54% / 23% / · / 20%
5	F	406	14% — 39% / 7% / 53%
6	G	241	17% — 65% / 7% · / 27%
7	I	330	11% — 41% / 10% / 49%
8	H	773	· 33% / 6% / 61%

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Mol	Chain	Length	Quality of chain
8	Y	773	19% · 81%
9	J	153	24% 75% 20% · ·
10	X	126	95% 5%
11	M	75	95% 5%
12	U	23	87% 100%

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 16292 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 Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	244	Total 1962	C 1256	N 324	O 370	S 12	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P38265
B	-1	ASN	-	expression tag	UNP P38265
B	0	ALA	-	expression tag	UNP P38265

- Molecule 2 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	194	Total 1601	C 1039	N 261	O 297	S 4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP Q06675
C	-1	ASN	-	expression tag	UNP Q06675
C	0	ALA	-	expression tag	UNP Q06675

- Molecule 3 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	196	Total 1578	C 1011	N 277	O 280	S 10	0	0

- Molecule 4 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	369	Total 2851	C 1848	N 492	O 500	S 11	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	expression tag	UNP P38907
E	-1	ASN	-	expression tag	UNP P38907
E	0	ALA	-	expression tag	UNP P38907

- Molecule 5 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	190	Total 1360	C 835	N 247	O 273	S 5	0	0

- Molecule 6 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	176	Total 1114	C 678	N 212	O 222	S 2	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	SER	-	expression tag	UNP Q12493
G	-1	ASN	-	expression tag	UNP Q12493
G	0	ALA	-	expression tag	UNP Q12493

- Molecule 7 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	168	Total 1295	C 807	N 231	O 253	S 4	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	325	HIS	-	expression tag	UNP P38313
I	326	HIS	-	expression tag	UNP P38313
I	327	HIS	-	expression tag	UNP P38313
I	328	HIS	-	expression tag	UNP P38313

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Chain	Residue	Modelled	Actual	Comment	Reference
I	329	HIS	-	expression tag	UNP P38313
I	330	HIS	-	expression tag	UNP P38313

- Molecule 8 is a protein called Inner kinetochore subunit CTF3,Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	302	Total	C	N	O	S	0	0
			1668	1026	319	322	1		
8	Y	150	Total	C	N	O		0	0
			746	446	150	150			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	SER	-	expression tag	UNP Q12748
H	-1	ASN	-	expression tag	UNP Q12748
H	0	ALA	-	expression tag	UNP Q12748
Y	-2	SER	-	expression tag	UNP Q12748
Y	-1	ASN	-	expression tag	UNP Q12748
Y	0	ALA	-	expression tag	UNP Q12748

- Molecule 9 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	147	Total	C	N	O	0	0
			997	618	184	195		

- Molecule 10 is a protein called Inner kinetochore subunit Mcm22.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	126	Total	C	N	O	0	0
			630	378	126	126		

- Molecule 11 is a protein called Inner kinetochore subunit Mcm16.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	75	Total	C	N	O	0	0
			375	225	75	75		

- Molecule 12 is a protein called Unknown (unassigned).

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	U	23	115	69	23	23	0	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: Inner kinetochore subunit IML3

Chain B:

- Molecule 2: Inner kinetochore subunit MCM21

Chain C:

- Molecule 3: Inner kinetochore subunit CTF19

Chain D:

MET ASP PHE THR SER ASP THR THR ASN SER HIS ASP THR SER ASN SER HIS LEU SER LEU GLU ASP ALA VAL GLY THR HIS HIS ALA GLY GLU GLU ALA ASP VAL ASN ILE ASP GLY ASP GLU LYS GLN GLN LEU SER LEU LEU ASP ASP GLN VAL ARG ALA LEU LYS LEU GLN GLU GLU

LYS ASP ALA LEU LEU THR ARG ARG ASN THR LEU LEU GLN GLU ILE GLN THR TYR GLN ASN ILE LEU MET LYS GLU ASN ASN SER LYS THR LYS ASN GLY ASP ILE LEU LEU GLN ASP ILE THR GLN ASP PHE LEU ASN LEU ILE SER ILE SER SER ASN PRO ASN SER ALA ILE SER

ASP ARG LYS ARG V125 E126 R127 I128 N129 G130 L131 T132 N133 L134 Q135 K136 E137 L138 D143 L147 L148 N149 M150 N151 L152 R153 L154 S155 Y156 P163 H164 L165 Q166 V167 S168 V169 Q170 S171 R172 D173 ARG VAL HIS N177 E181 V182 L183 V184 V185 N186 Y187 K188 N192 T193 M194

N195 P196 F197 E198 I199 Q200 F201 LYS MET PHE TYR LYS PHE GLU ASP S210 T211 L212 L213 K214 W215 E216 I217 L218 R219 R225 L226 K229 Q230 L231 L232 A233 T234 R235 N236 F237 Q238 K239 C240 L241 L242 S243 L244 Y245 E246 F247 I250 K251 S252 L261 L264 R267 K268

C271 Y272 LEU MET ASN ASN SER ASP S279 L280 R284 VAL ILE ARG GLY ARG LEU THR THR ILE LYS LEU Q297 I301 I302 T303 M304 E307 R308 G309 K310 N313 C314 P317 MET SER LYS ILE SER ILE ALA LEU TRP LYS GLY GLY GLU ARG PHE N333 D338 E339

I345 L354 K355 C358 L362 F363 P364 ASP MET TYR ALA ARG

• Molecule 4: Inner kinetochore subunit CHL4

Chain E:

6%

54%   23%   •   20%

SER ASN ALA MET SER ASN GLU LEU ARG GLU LEU GLU ASP ASN TYR VAL PRO THR SER D16 T17 L18 V19 V20 F21 K22 Q23 L24 M25 P28 V29 T30 V31 L32 Y33 L37 S38 W39 K42 PHE GLY GLY SER PHE ASP GLY D50 I51 Y52 L53 L54 T55 E56 L60 L61 I62 E63

K64 R67 R68 V72 N73 R74 I75 L76 Y77 W80 PRO ASP GLY L84 I92 D93 C94 H95 L96 M97 I98 S99 K100 P101 W106 L107 V120 F128 L132 K138 I139 Y140 H141 M146 F147 K148 H149 P150 S161 L152 P153 V154 L155 R158 I159 Q160 L161 F162

L167 PHE LEU SER THR PRO ASN ILE GLY GLY SER ILE ASN LYS GLU SER LEU TYR ASN LYS SER LEU ASP PHE GLN G191 K192 P193 P199 Y200 A203 F204 P205 L206 N207 S208 P209 I210 I211 F212 H213 S214 V215 D218 A221 S233 E234 R235 E236 T237 I238 Q244 K245 V248

K249 S250 N253 I254 L258 G259 P260 S261 R262 F263 A264 E265 S266 M267 G268 E271 C272 Y273 A274 N277 P282 L283 H284 G291 K295 R300 E301 F302 D303 F313 Y314 G315 K316 E317 E318 P319 E320 N329 F333 S336 ALA ASN GLY VAL MET ASP GLN LYS

TYR ASN ASP LEU LYS GLU PHE ASN GLU HIS VAL HIS ASN ILE ARG GLY LYS ASN GLU ASP SER GLY GLU PRO VAL TYR ILE S374 L379 V380 T388 L389 K390 N391 R396 I397 I400 L402 K403 F404 M407 D408 I409 G412 L413 H414 D418 I422 N423

T424 D425 L431 T441 I442 F447 A453 K454 GLY GLY LEU LEU

• Molecule 5: Inner kinetochore subunit OKP1

Chain F:

14%

39%   7%   53%

MET ALA ALA ASP ARG ASP ASN PHE LEU GLN ASN ILE ASN ASP SER ILE ASN ASN GLY GLN ALA MET ASP LEU SER PRO ASN ARG SER SER SER GLU ASP SER ASP SER ILE LEU MET ASN VAL ASN ASP ILE LYS THR LEU ARG LEU ASP VAL ALA PRO GLU ALA LYS SER THR GLN

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

GLY GLU GLY ASN VAL ARG PRO TRP GLU PHE ARG LYS VAL ILE GLN ALA GLU TYR ARG GLU ARG LEU PRO ARG ASN TYR GLU LEU LYS HIS TRP LYS LYS PRO SER LYS ILE MET ILE GLY SER **I162 L163 R164 L165 L166 E167 T168** **F178 E179 K180 Y181 E182 K183 E184 M185 N186 Q187 M188**

T189 H190 G191 D192 **V196** **I199** **F223 P224** SER ARG ILE SER GLU ARG ASP GLU LEU **D233 I234 E235** **N246** **Q250 E251 L252** **N255** **L262** **L269** **R273** **C276** **L279 K280 T281 N282 N283** **R286** **L287 T288 E289 K290 L291 I292 Q293 K294 D295** LEU HIS PRO VAL LEU

ASN LYS ALA MET GLU TYR THR TYR GLY LEU GLU SER THR ASN GLY PHE MET HIS PRO ASP GLY PRO **V323** **N327** **H330 E331 L332 N333 L334 M335** **L336 N337 D338 P339 I340 K341 S342 T343 A344 D345 V346 R347 L348 D349 K350** **V353** **L356 L357** **K365** **K368** **E369 L370 K371 E372**

I378 S379 D380 S381 H382 **E385 I386** LYS GLU VAL PHE VAL PRO HIS HIS GLU LEU SER HIS GLN LYS ASP LYS THR GLU GLU ASP ILE HIS

• Molecule 6: Inner kinetochore subunit NKP1

Chain G:

SER ASN ALA MET THR ASP **T4** **S22 D23** **A31 G32 E33 L34 P35 N36** GLU VAL CYS **R40** **I47 E48 K49 R50 K51** **R56** **L62** **N69** **L73 R74** **Q79 Q80 I81 M82 E83** **G86 D87** **K90** **L93** **E96 L97 R98 N99 R100** **E104 P105 Q106 S107**

T108 S109 **R112 L113 I114 E115 D116 V117 L118 K119 L120 P121** GLN MET GLU VAL ALA ASP GLU GLU VAL GLU VAL GLU **N135** **Q170** **L177** THR THR SER ILE LYS GLU ALA SER GLU **D187 D188 D189 I190 S191 E192 Y193 F194 A195 T196 Y197 N198 G199 K200 L201 V202 V203 A204** LEU GLU

GLU MET LYS LEU LEU LEU GLU GLU ALA VAL LYS THR PHE GLY ASN SER PRO GLU LYS ARG GLU ILE LYS LYS ILE LYS LEU SER GLU LYS LYS

• Molecule 7: Inner kinetochore subunit AME1

Chain I:

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

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

PRO ILE ARG **Q124** **S127** **N144** **I150** ILE PRO GLN ALA LEU LEU LYS ASP PHE ASN LYS SER ASP ASP GLN PHE ARG ARG LYS LEU **L170 Y171 K172** **R176 L177 F178** **I181 S182 D183** **R187** **D191 I192** **I195 N196** **N200 E201** **Q205** **Q208** **R224** **I227**

D235 W236 H237 D238 L239 Q240 N241 E242 **L246** **K249 V250** **R255** **L259 T260** **S261 T262 L263 L264** **G265 K266 Y267 E268 G269 D270 R271 K272 I273 M274** **D277** SER GLU ASP ASP SER ILE ARG ASP ASP SER ASN **I289 L290 D291 I292 A293 H294 F295** **D300 P301 Y302 N303 G304 L305 L306**

K307 K308 I309 **N310 K311 I312** **N315 L316 S317 N318 E319 L320 Q321** PRO SER LEU HIS HIS HIS HIS HIS HIS

• Molecule 8: Inner kinetochore subunit CTF3,Inner kinetochore subunit CTF3

Chain H:

33% 6% 61%

SER ASN ALA MET SER LEU ILE LEU ASP ASP ILE ILE LEU LEU SER LEU THR ASN ALA ASN GLU ARG THR PRO ALA GLN ALA LEU LYS THR LEU SER LEU LEU TYR GLU GLU LYS SER GLN TYR GLY LEU SER **P43** **Q44** **A47** **L48** **V49** **R50** **L51** **K63** **I66** VAL GLU ASN

CYS PHE LEU PRO ASP GLY TYR LEU THR LYS GLU LEU **L82** **L83** **E84** **I85** **I86** **N87** **H88** LEU GLY THR PRO THR VAL PHE SER ARG ARG ILE GLN THR PRO **P104** GLN **L120** PHE PRO VAL HIS SER GLU ARG GLU **H129** **N130** **I131** **L137** **H138** **L139** **S143** **F144** **L145** **Q146** **K147** **W148**

P151 **P160** **P165** **P178** **P184** **S202** **E206** **I209** **C213** **T217** **A228** **S232** ILE LEU LYS ARG ILE LEU SER ARG ALA HIS PRO ALA ASN PHE PRO ALA ASP THR VAL GLN ASN THR ILE ASP MET TYR LEU SER GLU ILE HIS GLN LEU GLY ALA ASP SER

ILE TYR PRO ARG LEU ARG LEU GLN SER LEU PRO GLU TYR VAL PRO SER ASP SER THR VAL SER LEU TRP ASP VAL THR SER LEU **E297** **Q298** **Q301** **P304** **P309** **P318** **S319** **L320** **V324** **P327** **M331** **S335** **P356** **P375** **P380** **S387** **K391** **I396** **I397**

GLN THR PHE CYS ASN LEU LYS TYR LEU LEU ASP GLU **L411** **P422** **P426** **S430** **S459** GLU THR CYS PHE TYR VAL LEU GLN MET ILE THR ASN TRP VAL LEU ASP ASP LYS LEU ILE ALA LEU GLY LEU THR LEU LEU HIS ASP SER MET GLN SER LEU LEU THR LEU ASP LYS

ILE PHE ASN ASN ALA THR SER ASN ARG PHE SER THR MET ALA PHE ILE SER SER LEU ASP ILE LEU THR GLN LEU SER LYS GLN THR LYS SER ASP TYR ALA ILE GLN THR ILE LYS VAL GLY PRO ASP ILE MET ASN LYS VAL PHE SER ASP PRO LEU LYS GLN ILE LEU LEU SER ALA ALA

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

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

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

UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

• Molecule 8: Inner kinetochore subunit CTF3,Inner kinetochore subunit CTF3

Chain Y:

19% 81%

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

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

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

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

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

GLN LEU ALA GLN ASN TRP PRO GLN LEU HIS ILE PRO ASN ASP VAL D313 P318 L326 PRO R328 S335 L336 K337 P356 A369 HIS GLN ILE GLU THR PRO GLN GLU VAL ILE PRO ILE ILE SER VAL SER SER MET ASP ASN LYS SER LEU SER ARG ILE ILE GLN THR

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

GLU THR CYS PHE TYR VAL GLN MET THR ASN VAL LEU ASP LYS LEU I479 Q490 SER LEU LEU THR LEU ASP LYS ILE PHE ASN ALA THR SER ASN ARG PHE SER THR ALA PHE ILE PHE SER SER LEU ASP ILE LEU THR GLN LEU SER LYS GLN THR LYS SER

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

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

ARG LEU GLU THR A653 H678 ASP GLU ILE GLY Q683 L701 MET HIS LEU SER ASN THR ALA ASN PRO TYR ARG ASP ILE ALA ALA PHE LEU PHE THR TYR LEU LYS SER LEU SER LYS TYR SER VAL GLN ASN SER X1196 X1201 X1206 X1677 X1681 X1685

• Molecule 9: Inner kinetochore subunit NKP2

Chain J:

24%
75%   20%

MET N2 Q5 L6 L7 H8 L16 T17 S21 F22 Q23 E24 F25 K26 Q27 Q28 L29 Q30 S31 Y32 Q40 H41 W42 Y43 L46 Q47 A48 R49 D50 A51 R52 V53 T54 S55 E56 K62 F65 S70 L73 R74 F75 L76 E77 S78 GLU GLN LEU SER HIS S84 L85

S86 L87 E88 I97 F122 E123 V126 R127 S128 P129 S130 A131 A135 I136 P137 G138 L139 I142 I143 Q144 S145 Y146 I147 N148 L149 L150 E151 E152 N153

• Molecule 10: Inner kinetochore subunit Mcm22

Chain X:

95%   5%

X71 X72 X105 X109 X119 X123 X124 X125 X129 X208

• Molecule 11: Inner kinetochore subunit Mcm16

Chain M:

95%   5%

X70 X71 X72 X73 X77 X164

• Molecule 12: Unknown (unassigned)

Chain U:

87%
100%

X1 X2 X3 X4 X5 X6 X7 X8 X9 X10 X11 X12 X13 X14 X15 X16 X17 X20 X21 X22 X23

4　Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	119469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	373.92, 373.92, 373.92	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	B	0.76	1/2002 (0.0%)	0.83	2/2713 (0.1%)
2	C	0.79	0/1630	0.87	1/2190 (0.0%)
3	D	0.52	0/1598	0.77	1/2146 (0.0%)
4	E	0.74	1/2912 (0.0%)	0.88	6/3943 (0.2%)
5	F	0.36	0/1367	0.65	2/1845 (0.1%)
6	G	0.36	0/1115	0.62	2/1513 (0.1%)
7	I	0.37	0/1303	0.76	1/1754 (0.1%)
8	H	0.46	0/1674	0.74	16/2316 (0.7%)
8	Y	0.37	0/556	0.51	2/768 (0.3%)
9	J	0.36	0/1006	0.65	3/1371 (0.2%)
All	All	0.59	2/15163 (0.0%)	0.77	36/20559 (0.2%)

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	C	0	1
3	D	0	6
4	E	0	8
6	G	0	1
8	H	0	2
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	106	TRP	CB-CG	-7.07	1.37	1.50
1	B	5	TRP	CB-CG	-5.75	1.39	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	260	PRO	CA-N-CD	-8.54	99.54	111.50
9	J	129	PRO	N-CA-CB	7.12	111.85	103.30
9	J	46	LEU	CA-CB-CG	6.74	130.81	115.30
8	H	184	PRO	N-CA-CB	6.51	111.11	103.30
5	F	340	ILE	CG1-CB-CG2	-6.17	97.82	111.40
8	H	422	PRO	N-CA-CB	6.04	110.55	103.30
8	H	104	PRO	N-CA-CB	6.03	110.54	103.30
8	H	151	PRO	N-CA-CB	6.02	110.53	103.30
4	E	193	PRO	N-CA-CB	6.00	110.50	103.30
3	D	317	PRO	N-CA-CB	5.88	110.36	103.30
8	H	86	ILE	CG1-CB-CG2	-5.88	98.47	111.40
6	G	62	LEU	CA-CB-CG	5.83	128.71	115.30
8	H	178	PRO	N-CA-CB	5.83	110.30	103.30
2	C	297	LEU	CA-CB-CG	5.81	128.66	115.30
5	F	224	PRO	N-CA-CB	5.80	110.26	103.30
8	H	165	PRO	N-CA-CB	5.78	110.24	103.30
8	H	318	PRO	N-CA-CB	5.75	110.20	103.30
8	H	375	PRO	N-CA-CB	5.70	110.14	103.30
6	G	35	PRO	N-CA-CB	5.68	110.11	103.30
9	J	137	PRO	N-CA-CB	5.53	109.94	103.30
8	H	380	PRO	N-CA-CB	5.48	109.88	103.30
8	Y	318	PRO	N-CA-CB	5.47	109.86	103.30
8	H	304	PRO	N-CA-CB	5.46	109.85	103.30
4	E	76	LEU	CA-CB-CG	5.44	127.82	115.30
4	E	402	LEU	CB-CG-CD2	-5.42	101.78	111.00
8	H	160	PRO	N-CA-CB	5.42	109.80	103.30
8	H	309	PRO	N-CA-CB	5.41	109.80	103.30
8	Y	356	PRO	N-CA-CB	5.40	109.78	103.30
8	H	356	PRO	N-CA-CB	5.29	109.64	103.30
1	B	90	CYS	C-N-CA	5.28	133.39	122.30
7	I	191	ASP	CB-CG-OD2	5.22	123.00	118.30
8	H	327	PRO	N-CA-CB	5.13	109.45	103.30
4	E	259	GLY	C-N-CD	5.07	139.05	128.40
1	B	173	LEU	CA-CB-CG	-5.05	103.69	115.30
4	E	106	TRP	CA-CB-CG	-5.04	104.13	113.70
8	H	426	PRO	N-CA-CB	5.03	109.34	103.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	310	VAL	Peptide
3	D	147	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	D	149	ASN	Peptide
3	D	167	VAL	Peptide
3	D	197	PHE	Peptide
3	D	213	LEU	Peptide
3	D	304	MET	Peptide
4	E	140	TYR	Peptide
4	E	149	HIS	Peptide
4	E	152	LEU	Peptide
4	E	153	PRO	Peptide
4	E	235	ARG	Peptide
4	E	29	VAL	Peptide
4	E	422	ILE	Peptide
4	E	423	ASN	Peptide
6	G	90	LYS	Peptide
8	H	138	HIS	Peptide
8	H	143	SER	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	B	1962	0	1968	54	0
2	C	1601	0	1618	88	0
3	D	1578	0	1614	125	0
4	E	2851	0	2789	94	0
5	F	1360	0	1181	14	0
6	G	1114	0	867	13	0
7	I	1295	0	1241	20	0
8	H	1668	0	945	18	0
8	Y	746	0	274	2	0
9	J	997	0	792	20	0
10	X	630	0	133	3	0
11	M	375	0	80	3	0
12	U	115	0	25	0	0
All	All	16292	0	13527	399	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 13.

All (399) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:234:THR:HA	3:D:235:ARG:CZ	1.41	1.47
3:D:134:LEU:CD2	3:D:150:MET:HE2	1.46	1.45
2:C:297:LEU:CD1	2:C:299:LEU:HD21	1.51	1.40
3:D:234:THR:HA	3:D:235:ARG:NH2	1.30	1.39
3:D:134:LEU:CD2	3:D:150:MET:CE	2.01	1.39
2:C:297:LEU:CD1	2:C:299:LEU:CD2	2.00	1.39
3:D:234:THR:C	3:D:235:ARG:NH1	1.90	1.25
2:C:302:GLU:OE2	4:E:207:ASN:CG	1.76	1.24
2:C:297:LEU:HD13	2:C:299:LEU:CD2	1.62	1.22
3:D:234:THR:CA	3:D:235:ARG:CZ	2.17	1.22
2:C:297:LEU:HD11	2:C:299:LEU:CD2	1.68	1.16
2:C:298:ASP:C	2:C:299:LEU:HD23	1.65	1.16
3:D:234:THR:CA	3:D:235:ARG:NH1	2.10	1.15
3:D:134:LEU:HD21	3:D:150:MET:CE	1.70	1.12
2:C:209:PHE:N	3:D:238:GLN:HE22	1.47	1.11
3:D:134:LEU:HD22	3:D:150:MET:HE3	1.30	1.09
2:C:300:ASP:OD2	2:C:305:MET:N	1.85	1.07
2:C:302:GLU:OE2	4:E:207:ASN:CB	2.04	1.03
3:D:233:ALA:C	3:D:235:ARG:HH12	1.60	1.03
2:C:297:LEU:CD1	2:C:299:LEU:HD22	1.88	1.02
2:C:297:LEU:HD11	2:C:299:LEU:HD22	1.37	1.02
3:D:234:THR:CA	3:D:235:ARG:NH2	2.23	1.01
3:D:233:ALA:O	3:D:235:ARG:NH1	1.92	1.01
2:C:302:GLU:OE2	4:E:207:ASN:ND2	1.93	1.00
2:C:219:PRO:O	4:E:262:ARG:NH2	1.96	0.99
3:D:132:THR:HG22	3:D:150:MET:HG3	1.45	0.98
2:C:300:ASP:OD1	2:C:305:MET:O	1.84	0.95
3:D:134:LEU:CD2	3:D:150:MET:HE3	1.85	0.94
2:C:209:PHE:H	3:D:238:GLN:HE22	1.13	0.90
2:C:209:PHE:N	3:D:238:GLN:NE2	2.21	0.89
3:D:239:LYS:HG3	3:D:310:LYS:NZ	1.89	0.87
2:C:302:GLU:CD	4:E:207:ASN:ND2	2.28	0.87
3:D:241:LEU:O	3:D:241:LEU:HD12	1.76	0.85
2:C:302:GLU:OE1	2:C:302:GLU:N	2.11	0.84
3:D:134:LEU:HD21	3:D:150:MET:HE2	0.86	0.83
3:D:234:THR:HA	3:D:235:ARG:HH22	1.45	0.82
2:C:302:GLU:OE2	4:E:207:ASN:HB3	1.79	0.82
3:D:215:TRP:CH2	3:D:232:LEU:HD22	2.14	0.82
2:C:209:PHE:H	3:D:238:GLN:NE2	1.76	0.80
2:C:297:LEU:HD13	2:C:299:LEU:HD23	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:LEU:HD11	3:D:131:LEU:CD2	2.13	0.78
3:D:135:GLN:HA	3:D:135:GLN:NE2	1.97	0.78
2:C:297:LEU:HD13	2:C:299:LEU:HD21	1.36	0.78
3:D:233:ALA:O	3:D:235:ARG:CZ	2.32	0.78
2:C:160:LEU:HD11	3:D:131:LEU:HD21	1.66	0.77
2:C:239:THR:OG1	4:E:262:ARG:CG	2.31	0.77
3:D:239:LYS:HD2	3:D:310:LYS:HZ2	1.49	0.77
2:C:298:ASP:C	2:C:299:LEU:CD2	2.51	0.76
2:C:239:THR:OG1	4:E:262:ARG:HG3	1.84	0.76
3:D:234:THR:C	3:D:235:ARG:CZ	2.47	0.76
2:C:297:LEU:HD11	2:C:299:LEU:HD21	1.37	0.75
3:D:239:LYS:CG	3:D:310:LYS:NZ	2.49	0.75
2:C:302:GLU:OE1	4:E:207:ASN:ND2	2.20	0.74
3:D:215:TRP:HH2	3:D:232:LEU:HD22	1.50	0.74
2:C:299:LEU:HD23	2:C:299:LEU:N	2.02	0.72
3:D:233:ALA:O	3:D:235:ARG:NH2	2.23	0.71
4:E:267:MET:SD	4:E:267:MET:N	2.63	0.71
2:C:220:HIS:HA	4:E:262:ARG:NH2	2.04	0.71
2:C:299:LEU:HB3	2:C:306:VAL:HG12	1.72	0.70
3:D:239:LYS:HG3	3:D:310:LYS:HZ1	1.56	0.69
2:C:208:VAL:C	3:D:238:GLN:HE22	1.94	0.69
3:D:150:MET:SD	3:D:150:MET:N	2.62	0.69
3:D:234:THR:O	3:D:235:ARG:NH1	2.26	0.69
3:D:234:THR:N	3:D:235:ARG:HH12	1.89	0.69
1:B:34:ASP:HB3	1:B:57:GLU:HB2	1.74	0.69
2:C:298:ASP:CA	2:C:299:LEU:HD23	2.23	0.69
2:C:301:LEU:HD13	2:C:301:LEU:C	2.14	0.68
3:D:168:SER:OG	3:D:170:GLN:NE2	2.27	0.68
3:D:215:TRP:HZ2	3:D:235:ARG:HA	1.57	0.67
3:D:170:GLN:HE22	3:D:181:GLU:HG2	1.59	0.67
4:E:32:LEU:HD22	4:E:100:LYS:NZ	2.10	0.67
3:D:131:LEU:HD12	3:D:131:LEU:O	1.95	0.67
5:F:327:ASN:O	5:F:331:GLU:HB2	1.95	0.67
3:D:239:LYS:CD	3:D:310:LYS:HZ2	2.07	0.67
2:C:239:THR:OG1	4:E:262:ARG:HG2	1.97	0.65
3:D:231:LEU:HD21	3:D:304:MET:HG2	1.78	0.65
3:D:239:LYS:HG3	3:D:310:LYS:CE	2.27	0.65
2:C:237:LYS:HG2	4:E:265:GLU:HB3	1.77	0.65
3:D:182:VAL:HG12	3:D:196:PRO:HD3	1.78	0.65
3:D:239:LYS:CD	3:D:310:LYS:NZ	2.59	0.65
2:C:263:ASP:OD1	2:C:263:ASP:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:243:SER:O	3:D:247:PHE:CB	2.45	0.65
8:H:48:LEU:HD13	8:H:51:LEU:HD12	1.79	0.64
4:E:19:VAL:O	4:E:23:GLN:NE2	2.30	0.64
3:D:134:LEU:HD22	3:D:150:MET:CE	1.88	0.64
3:D:272:TYR:C	3:D:279:SER:HA	2.17	0.64
1:B:68:GLY:O	1:B:95:ARG:NH2	2.31	0.63
2:C:243:PHE:CE1	2:C:301:LEU:HD11	2.33	0.63
1:B:143:PHE:HB3	1:B:211:ALA:HB3	1.80	0.63
3:D:134:LEU:HD23	3:D:150:MET:CE	2.20	0.63
3:D:234:THR:C	3:D:235:ARG:HH11	1.97	0.63
9:J:76:LEU:HG	9:J:77:GLU:HG3	1.81	0.63
4:E:263:PHE:HA	4:E:266:SER:OG	1.99	0.62
3:D:239:LYS:HD2	3:D:310:LYS:NZ	2.14	0.62
4:E:93:ASP:HA	4:E:96:LEU:HB2	1.82	0.62
3:D:239:LYS:CG	3:D:310:LYS:HZ2	2.12	0.62
3:D:271:CYS:SG	3:D:272:TYR:N	2.73	0.61
7:I:246:LEU:O	7:I:250:VAL:HB	2.00	0.61
3:D:127:ARG:HH21	3:D:127:ARG:HG3	1.65	0.61
7:I:290:LEU:O	7:I:294:HIS:ND1	2.30	0.61
8:H:63:LYS:NZ	8:H:84:GLU:OE1	2.33	0.61
1:B:172:GLY:HA2	4:E:396:ARG:HE	1.65	0.60
2:C:182:ASP:N	2:C:182:ASP:OD1	2.32	0.60
4:E:333:PHE:HD2	4:E:414:HIS:HB3	1.66	0.60
3:D:243:SER:O	3:D:247:PHE:N	2.30	0.60
4:E:263:PHE:CD2	4:E:266:SER:OG	2.54	0.60
4:E:263:PHE:CE2	4:E:274:ALA:HB1	2.36	0.60
2:C:302:GLU:CD	4:E:207:ASN:HD22	2.05	0.60
6:G:51:LYS:HB3	9:J:22:PHE:HE1	1.65	0.60
4:E:106:TRP:H	4:E:248:VAL:HG11	1.67	0.60
1:B:24:ASN:ND2	1:B:30:GLU:OE1	2.35	0.60
3:D:127:ARG:HH21	3:D:127:ARG:CG	2.15	0.60
3:D:234:THR:CA	3:D:235:ARG:HH12	2.00	0.59
2:C:300:ASP:OD1	2:C:300:ASP:N	2.35	0.59
4:E:329:ASN:ND2	4:E:418:ASP:OD1	2.35	0.59
2:C:300:ASP:CG	2:C:305:MET:H	1.98	0.59
3:D:194:MET:HG2	3:D:217:ILE:HD13	1.85	0.59
4:E:218:ASP:H	4:E:221:ALA:HB3	1.68	0.59
2:C:224:LEU:HD13	2:C:233:TRP:HB3	1.85	0.58
2:C:187:LYS:NZ	4:E:300:ARG:O	2.34	0.58
6:G:40:ARG:NH2	9:J:31:SER:OG	2.36	0.58
1:B:56:TYR:HB2	1:B:75:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:TYR:HB3	1:B:76:LEU:HD21	1.84	0.58
7:I:260:THR:O	7:I:264:LEU:HB2	2.04	0.58
3:D:339:GLU:OE2	7:I:255:ARG:NH2	2.37	0.58
1:B:154:GLN:O	1:B:157:ASN:ND2	2.37	0.57
4:E:262:ARG:HG2	4:E:262:ARG:O	2.04	0.57
2:C:185:ASP:OD1	2:C:185:ASP:N	2.37	0.57
9:J:40:GLN:HA	9:J:43:TYR:HD2	1.69	0.57
3:D:166:GLN:O	3:D:183:LEU:N	2.33	0.57
3:D:177:ASN:N	3:D:199:ILE:O	2.38	0.57
5:F:246:ASN:O	5:F:250:GLN:NE2	2.38	0.57
1:B:181:MET:SD	1:B:181:MET:N	2.78	0.57
3:D:241:LEU:HD12	3:D:241:LEU:C	2.23	0.57
6:G:90:LYS:HB3	6:G:93:LEU:HD21	1.86	0.57
6:G:119:LYS:NZ	9:J:86:SER:O	2.38	0.57
3:D:134:LEU:HD23	3:D:150:MET:HE2	1.72	0.57
4:E:97:MET:O	4:E:100:LYS:HB2	2.04	0.57
4:E:263:PHE:O	4:E:264:ALA:C	2.43	0.57
4:E:272:CYS:SG	4:E:277:ASN:ND2	2.78	0.56
1:B:-1:ASN:HB3	1:B:215:LYS:HZ2	1.70	0.56
2:C:208:VAL:HA	3:D:238:GLN:HE22	1.71	0.56
3:D:186:ASN:HD22	3:D:192:ASN:HB3	1.71	0.56
3:D:215:TRP:CZ3	3:D:232:LEU:HD22	2.40	0.56
3:D:243:SER:O	3:D:247:PHE:HB2	2.06	0.56
1:B:182:HIS:O	1:B:186:ASP:HB2	2.05	0.56
1:B:203:LEU:HD13	1:B:204:PRO:HD2	1.88	0.56
2:C:301:LEU:HD22	2:C:301:LEU:O	2.05	0.56
3:D:239:LYS:HG3	3:D:310:LYS:HE3	1.88	0.56
1:B:97:GLU:OE1	1:B:97:GLU:N	2.39	0.56
1:B:60:LEU:HD13	1:B:71:SER:HB3	1.89	0.55
1:B:133:THR:H	1:B:138:GLU:HG2	1.71	0.55
3:D:226:LEU:HD23	3:D:229:LYS:HD2	1.88	0.55
4:E:209:PRO:HG2	4:E:210:ILE:HG12	1.89	0.55
2:C:208:VAL:CA	3:D:238:GLN:HE22	2.19	0.55
4:E:99:SER:O	4:E:148:LYS:NZ	2.40	0.55
1:B:83:VAL:O	1:B:241:GLN:NE2	2.39	0.55
1:B:128:SER:O	1:B:229:ARG:NH1	2.40	0.55
4:E:120:VAL:HG12	4:E:208:SER:H	1.71	0.55
8:Y:1677:UNK:O	8:Y:1681:UNK:N	2.39	0.55
1:B:36:GLN:NE2	1:B:57:GLU:OE2	2.39	0.55
2:C:168:ASN:OD1	2:C:171:ARG:NH2	2.40	0.55
3:D:134:LEU:O	3:D:138:LEU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:N	1:B:185:ASN:OD1	2.38	0.54
2:C:301:LEU:HD12	2:C:302:GLU:HG3	1.89	0.54
3:D:267:ARG:NH1	7:I:270:ASP:OD1	2.40	0.54
4:E:263:PHE:CE2	4:E:274:ALA:CB	2.91	0.54
2:C:260:SER:OG	2:C:261:HIS:N	2.41	0.54
8:H:147:LYS:HD2	8:H:148:TRP:HB2	1.89	0.54
3:D:134:LEU:HD23	3:D:134:LEU:N	2.23	0.54
7:I:268:GLU:O	7:I:272:LYS:N	2.40	0.54
1:B:208:VAL:HG13	1:B:216:ILE:HB	1.90	0.54
4:E:263:PHE:CZ	4:E:274:ALA:HB1	2.43	0.54
5:F:273:ARG:NH1	5:F:276:CYS:SG	2.81	0.54
1:B:157:ASN:O	4:E:407:ASN:N	2.36	0.53
7:I:178:PHE:HA	7:I:181:ILE:HD12	1.89	0.53
2:C:239:THR:HG1	4:E:262:ARG:CG	2.20	0.53
1:B:195:GLU:OE2	4:E:391:ASN:ND2	2.41	0.53
4:E:28:PRO:HG2	4:E:32:LEU:HD21	1.91	0.53
6:G:47:ILE:HA	6:G:50:ARG:HD2	1.89	0.53
8:H:50:ARG:HH22	11:M:71:UNK:HA	1.74	0.53
2:C:324:ILE:HD13	2:C:346:ILE:HG13	1.90	0.53
3:D:301:ILE:HD13	3:D:303:THR:HG23	1.91	0.53
4:E:409:ILE:O	4:E:412:GLY:N	2.42	0.53
1:B:32:ASP:HB3	1:B:59:ARG:HB3	1.92	0.52
9:J:50:ASP:N	9:J:50:ASP:OD1	2.41	0.52
1:B:187:ALA:O	1:B:191:TYR:N	2.39	0.52
4:E:37:LEU:HD11	4:E:75:ILE:HD13	1.91	0.52
3:D:235:ARG:CZ	3:D:235:ARG:N	2.73	0.52
4:E:94:CYS:SG	4:E:95:HIS:N	2.82	0.52
4:E:318:GLU:HG2	4:E:320:GLU:H	1.75	0.52
1:B:153:THR:OG1	1:B:154:GLN:N	2.44	0.51
4:E:235:ARG:HB2	4:E:237:THR:HG23	1.91	0.51
4:E:233:SER:O	4:E:237:THR:OG1	2.27	0.51
3:D:195:ASN:OD1	3:D:195:ASN:N	2.42	0.51
3:D:267:ARG:HH12	7:I:274:MET:HG3	1.76	0.51
4:E:68:ARG:H	4:E:68:ARG:HD3	1.75	0.51
2:C:300:ASP:OD2	2:C:304:SER:N	2.41	0.51
2:C:208:VAL:HA	3:D:238:GLN:NE2	2.26	0.51
5:F:350:LYS:HA	5:F:353:VAL:HB	1.93	0.51
3:D:211:THR:HG21	4:E:282:PRO:HB2	1.93	0.51
3:D:127:ARG:HD2	3:D:127:ARG:N	2.26	0.51
7:I:201:GLU:O	7:I:205:GLN:NE2	2.44	0.51
10:X:105:UNK:O	10:X:109:UNK:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:307:GLU:HB3	3:D:308:ARG:HH11	1.75	0.51
8:Y:1201:UNK:O	8:Y:1206:UNK:N	2.44	0.51
2:C:220:HIS:HA	4:E:262:ARG:HH21	1.75	0.50
3:D:164:HIS:HB2	3:D:185:VAL:HB	1.92	0.50
3:D:235:ARG:N	3:D:235:ARG:CD	2.73	0.50
2:C:343:LYS:HE2	2:C:358:LYS:HB2	1.92	0.50
8:H:213:CYS:O	8:H:217:THR:CB	2.59	0.50
4:E:20:VAL:HG22	4:E:24:LEU:HD13	1.94	0.50
3:D:127:ARG:N	3:D:127:ARG:CD	2.74	0.50
4:E:51:ILE:HA	4:E:54:LEU:HB2	1.93	0.49
4:E:100:LYS:CB	4:E:101:PRO:CD	2.90	0.49
4:E:263:PHE:O	4:E:265:GLU:N	2.46	0.49
3:D:127:ARG:CG	3:D:127:ARG:NH2	2.74	0.49
5:F:279:LEU:HA	5:F:282:ASN:HD22	1.76	0.49
11:M:73:UNK:O	11:M:77:UNK:N	2.44	0.49
2:C:207:GLU:HG3	2:C:219:PRO:HB3	1.93	0.49
3:D:215:TRP:CZ2	3:D:235:ARG:HA	2.45	0.49
8:H:331:MET:O	8:H:335:SER:CB	2.60	0.49
1:B:161:PHE:HB2	4:E:404:PHE:CD1	2.48	0.49
1:B:214:THR:OG1	1:B:215:LYS:N	2.44	0.49
3:D:233:ALA:C	3:D:235:ARG:HH22	2.15	0.49
8:H:144:PHE:O	8:H:148:TRP:N	2.44	0.49
10:X:125:UNK:O	10:X:129:UNK:CB	2.61	0.49
1:B:11:SER:OG	1:B:12:LYS:N	2.46	0.49
2:C:208:VAL:HG23	2:C:276:VAL:HG23	1.93	0.49
2:C:210:SER:HG	2:C:215:GLN:H	1.60	0.49
4:E:32:LEU:HD22	4:E:100:LYS:HZ2	1.76	0.49
4:E:72:VAL:O	4:E:76:LEU:HB2	2.12	0.49
1:B:83:VAL:N	1:B:241:GLN:OE1	2.39	0.48
4:E:268:GLY:N	4:E:271:GLU:OE2	2.37	0.48
1:B:33:LEU:HD11	1:B:56:TYR:HB3	1.95	0.48
1:B:209:ILE:HG13	1:B:215:LYS:HG3	1.94	0.48
8:H:63:LYS:HA	8:H:66:ILE:HG22	1.95	0.48
6:G:108:THR:O	6:G:112:ARG:HB2	2.12	0.48
8:H:387:SER:O	8:H:391:LYS:CB	2.61	0.48
2:C:161:GLU:HB2	4:E:284:HIS:CE1	2.48	0.48
3:D:188:LYS:HE2	3:D:252:SER:HB2	1.96	0.48
1:B:8:LEU:HD11	1:B:111:MET:HB3	1.95	0.48
3:D:197:PHE:HB3	3:D:215:TRP:HA	1.96	0.48
6:G:93:LEU:HA	6:G:96:GLU:HB3	1.96	0.48
3:D:149:ASN:HA	3:D:153:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:261:LEU:HB3	3:D:354:LEU:HD22	1.95	0.48
8:H:44:GLN:HA	8:H:47:ALA:HB3	1.94	0.48
1:B:117:GLU:OE1	1:B:119:LYS:N	2.45	0.48
4:E:235:ARG:NH1	6:G:104:GLU:OE1	2.45	0.48
2:C:265:TYR:OH	3:D:242:LEU:HD11	2.14	0.48
2:C:327:CYS:O	6:G:100:ARG:NH2	2.46	0.47
2:C:199:ARG:HH11	2:C:228:ILE:HD11	1.79	0.47
2:C:225:LYS:HD2	2:C:236:PHE:HB2	1.96	0.47
3:D:195:ASN:OD1	3:D:219:ARG:N	2.47	0.47
4:E:388:THR:HB	4:E:441:THR:HA	1.95	0.47
2:C:338:GLN:HA	2:C:341:LYS:HG2	1.96	0.47
8:H:426:PRO:O	8:H:430:SER:CB	2.61	0.47
4:E:205:PRO:HB2	4:E:260:PRO:HG3	1.96	0.47
5:F:332:LEU:HD11	5:F:334:LEU:HD23	1.97	0.47
9:J:5:GLN:HA	9:J:8:HIS:CD2	2.48	0.47
9:J:7:LEU:HD13	9:J:62:LYS:HE2	1.96	0.47
3:D:131:LEU:HB2	4:E:291:GLY:O	2.14	0.47
4:E:277:ASN:N	4:E:277:ASN:OD1	2.44	0.47
7:I:242:GLU:O	7:I:246:LEU:HB2	2.15	0.47
3:D:135:GLN:NE2	3:D:135:GLN:CA	2.73	0.47
5:F:252:LEU:HA	5:F:255:ASN:HD22	1.79	0.47
1:B:146:LYS:O	1:B:148:TYR:N	2.44	0.47
4:E:17:THR:HA	4:E:20:VAL:HG12	1.97	0.47
4:E:425:ASP:OD1	4:E:425:ASP:N	2.45	0.47
1:B:29:LEU:HD21	1:B:62:ILE:HG21	1.96	0.46
2:C:212:ARG:HH22	2:C:282:ARG:HG2	1.80	0.46
7:I:195:ILE:HD13	7:I:195:ILE:HA	1.84	0.46
7:I:196:ASN:O	7:I:200:ASN:ND2	2.48	0.46
8:H:137:LEU:HD12	8:H:137:LEU:HA	1.76	0.46
2:C:301:LEU:CD1	2:C:302:GLU:HG3	2.46	0.46
3:D:151:ASN:O	3:D:155:SER:N	2.33	0.46
3:D:314:CYS:HB3	5:F:335:MET:HB2	1.97	0.46
4:E:73:ASN:HA	4:E:76:LEU:HB3	1.96	0.46
9:J:123:GLU:O	9:J:127:ARG:CB	2.63	0.46
2:C:211:GLU:OE1	2:C:283:GLN:NE2	2.48	0.46
2:C:301:LEU:HD13	2:C:301:LEU:O	2.16	0.46
4:E:214:SER:OG	4:E:215:VAL:N	2.49	0.46
2:C:160:LEU:CD2	3:D:131:LEU:HD11	2.45	0.46
2:C:169:VAL:HA	2:C:172:MET:SD	2.56	0.46
3:D:225:ARG:HH22	7:I:306:LEU:HB3	1.81	0.46
4:E:379:LEU:HG	4:E:380:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASP:H	1:B:69:THR:HG1	1.63	0.46
4:E:442:ILE:HG22	4:E:447:PHE:HD1	1.81	0.46
3:D:143:ASP:OD1	3:D:143:ASP:N	2.46	0.45
8:H:297:GLU:O	8:H:301:GLN:CB	2.64	0.45
1:B:68:GLY:HA2	1:B:93:ASP:HB2	1.97	0.45
3:D:244:LEU:HD23	3:D:244:LEU:N	2.31	0.45
7:I:260:THR:HA	7:I:263:LEU:HD23	1.97	0.45
1:B:50:ALA:O	1:B:78:ASN:ND2	2.49	0.45
1:B:198:MET:HA	4:E:422:ILE:HG22	1.98	0.45
8:H:228:ALA:O	8:H:232:SER:N	2.44	0.45
1:B:200:VAL:HA	1:B:203:LEU:HB2	1.99	0.45
3:D:301:ILE:H	3:D:301:ILE:HG13	1.54	0.45
4:E:155:LEU:HA	4:E:203:ALA:HA	1.97	0.45
1:B:129:ILE:O	1:B:141:THR:OG1	2.32	0.45
2:C:160:LEU:HD21	3:D:131:LEU:HD11	1.98	0.45
3:D:200:GLN:HG3	3:D:213:LEU:HD13	1.99	0.45
4:E:244:GLN:HB3	4:E:245:LYS:H	1.66	0.45
5:F:365:LYS:HD2	5:F:368:LYS:HD2	1.97	0.45
2:C:240:ILE:HD11	2:C:246:VAL:HG13	1.98	0.45
3:D:186:ASN:HB2	3:D:192:ASN:HB3	1.99	0.45
1:B:155:ASP:HB2	1:B:157:ASN:HD21	1.81	0.45
3:D:163:PRO:HD2	3:D:245:TYR:HE1	1.82	0.45
4:E:158:ARG:NH1	4:E:200:TYR:HB3	2.32	0.45
1:B:65:LEU:HB2	1:B:69:THR:HG21	1.99	0.45
3:D:193:THR:OG1	3:D:194:MET:N	2.40	0.45
4:E:249:LYS:HG3	4:E:250:SER:H	1.82	0.45
5:F:340:ILE:HG22	5:F:341:LYS:H	1.80	0.45
10:X:119:UNK:O	10:X:123:UNK:CB	2.65	0.45
1:B:93:ASP:OD1	1:B:94:ASN:N	2.51	0.44
2:C:160:LEU:HD11	3:D:131:LEU:HD22	1.95	0.44
4:E:146:MET:HB2	4:E:155:LEU:HG	1.98	0.44
7:I:259:LEU:HD13	7:I:263:LEU:HD22	1.99	0.44
8:H:202:SER:O	8:H:206:GLU:CB	2.65	0.44
2:C:251:ASP:O	2:C:256:GLY:N	2.50	0.44
4:E:208:SER:OG	4:E:210:ILE:O	2.32	0.44
3:D:358:CYS:O	3:D:362:LEU:N	2.49	0.44
4:E:29:VAL:HA	4:E:33:TYR:CD2	2.53	0.44
8:H:320:LEU:O	8:H:324:VAL:N	2.51	0.44
1:B:180:THR:OG1	1:B:181:MET:N	2.50	0.44
3:D:129:ASN:OD1	3:D:129:ASN:N	2.50	0.44
5:F:269:LEU:HA	7:I:227:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:23:GLN:HA	9:J:42:TRP:HZ3	1.82	0.44
3:D:215:TRP:HH2	3:D:232:LEU:CD2	2.25	0.44
4:E:64:LYS:HD2	4:E:64:LYS:HA	1.81	0.44
1:B:14:LEU:HD23	1:B:14:LEU:HA	1.80	0.43
4:E:29:VAL:HA	4:E:33:TYR:HD2	1.82	0.43
2:C:257:LEU:HG	2:C:259:ILE:HD11	2.00	0.43
4:E:141:HIS:NE2	4:E:159:ILE:O	2.52	0.43
9:J:62:LYS:HA	9:J:65:PHE:CE2	2.53	0.43
2:C:212:ARG:HB3	2:C:283:GLN:HE21	1.84	0.43
4:E:60:LEU:O	4:E:64:LYS:N	2.41	0.43
4:E:253:ASN:OD1	4:E:253:ASN:N	2.52	0.43
4:E:389:LEU:HB3	4:E:400:ILE:HG13	2.00	0.43
1:B:10:ILE:HD11	1:B:87:LEU:HB2	2.00	0.43
9:J:7:LEU:HD23	9:J:7:LEU:HA	1.87	0.43
1:B:-1:ASN:OD1	1:B:-1:ASN:N	2.52	0.43
1:B:15:SER:OG	1:B:17:GLU:OE1	2.29	0.43
2:C:273:LEU:HA	2:C:276:VAL:HG12	2.01	0.43
2:C:328:SER:HA	6:G:100:ARG:HH12	1.83	0.43
5:F:280:LYS:HD3	5:F:283:ASN:HD22	1.83	0.43
3:D:234:THR:CA	3:D:235:ARG:HH22	2.14	0.43
5:F:353:VAL:HG13	5:F:357:LEU:HB3	2.01	0.43
9:J:7:LEU:HB3	9:J:62:LYS:NZ	2.34	0.43
1:B:240:ILE:H	1:B:240:ILE:HG13	1.56	0.42
4:E:92:ILE:HD12	4:E:92:ILE:HA	1.78	0.42
6:G:56:ARG:HD3	6:G:56:ARG:HA	1.88	0.42
7:I:224:ARG:HA	7:I:227:ILE:HG22	2.01	0.42
9:J:49:ARG:HA	9:J:54:THR:HG21	2.01	0.42
9:J:53:VAL:O	9:J:56:GLU:HG2	2.19	0.42
2:C:199:ARG:HD2	2:C:228:ILE:HD11	2.02	0.42
2:C:320:LYS:HG3	2:C:321:GLN:H	1.83	0.42
4:E:159:ILE:HG12	4:E:199:PRO:HB3	2.00	0.42
8:H:145:LEU:HD22	8:H:145:LEU:HA	1.85	0.42
3:D:134:LEU:HD23	3:D:134:LEU:H	1.84	0.42
1:B:151:PRO:HB3	1:B:204:PRO:HG2	2.01	0.42
3:D:313:ASN:N	5:F:333:ASN:O	2.53	0.42
1:B:55:ARG:HB3	1:B:76:LEU:HD23	2.02	0.42
2:C:212:ARG:NH2	2:C:282:ARG:HG2	2.35	0.42
3:D:302:ILE:HA	3:D:313:ASN:ND2	2.35	0.42
7:I:306:LEU:HA	7:I:309:ILE:HG12	2.00	0.42
1:B:116:PHE:HB2	1:B:120:THR:HG21	2.01	0.42
4:E:132:LEU:HD13	4:E:132:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:THR:CG2	3:D:150:MET:HG3	2.33	0.41
7:I:292:ILE:HA	7:I:295:PHE:CD1	2.55	0.41
1:B:217:MET:HG2	1:B:218:ARG:H	1.85	0.41
3:D:134:LEU:HA	3:D:137:GLU:OE2	2.21	0.41
4:E:98:ILE:HA	4:E:101:PRO:HD2	2.02	0.41
4:E:205:PRO:HG2	4:E:208:SER:HB3	2.01	0.41
3:D:246:GLU:O	3:D:250:ILE:HG12	2.20	0.41
4:E:37:LEU:HD13	4:E:37:LEU:HA	1.81	0.41
4:E:138:LYS:HA	4:E:138:LYS:HD2	1.88	0.41
9:J:74:ARG:NH2	9:J:78:SER:OG	2.42	0.41
4:E:397:ILE:HD12	4:E:397:ILE:HA	1.94	0.41
7:I:305:LEU:HD11	9:J:139:LEU:HA	2.02	0.41
4:E:32:LEU:HD22	4:E:100:LYS:HZ1	1.85	0.41
6:G:106:GLN:O	6:G:109:SER:OG	2.29	0.41
2:C:298:ASP:O	2:C:299:LEU:CD2	2.67	0.41
3:D:264:LEU:O	3:D:268:LYS:HG2	2.21	0.41
6:G:112:ARG:NH2	9:J:97:ILE:HA	2.36	0.41
3:D:152:LEU:HD22	3:D:152:LEU:HA	1.85	0.41
4:E:107:LEU:HD23	4:E:215:VAL:HB	2.03	0.41
4:E:158:ARG:HH22	4:E:160:GLN:HB2	1.86	0.41
3:D:243:SER:O	3:D:247:PHE:HB3	2.21	0.40
3:D:302:ILE:HA	3:D:313:ASN:HD22	1.86	0.40
4:E:254:ILE:HD12	4:E:254:ILE:HA	1.88	0.40
8:H:50:ARG:NH1	11:M:70:UNK:O	2.36	0.40
2:C:210:SER:HB3	2:C:217:GLU:OE2	2.20	0.40
3:D:244:LEU:N	3:D:244:LEU:CD2	2.83	0.40
9:J:70:SER:HA	9:J:73:LEU:HG	2.03	0.40
3:D:151:ASN:O	3:D:154:LEU:N	2.54	0.40
9:J:16:LEU:HD13	9:J:16:LEU:HA	1.95	0.40
2:C:212:ARG:NE	2:C:287:ASP:OD2	2.54	0.40
2:C:224:LEU:H	2:C:224:LEU:HG	1.42	0.40

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	B	242/248 (98%)	203 (84%)	38 (16%)	1 (0%)	34	72
2	C	188/371 (51%)	160 (85%)	28 (15%)	0	100	100
3	D	184/369 (50%)	139 (76%)	43 (23%)	2 (1%)	14	52
4	E	359/461 (78%)	275 (77%)	78 (22%)	6 (2%)	9	44
5	F	184/406 (45%)	167 (91%)	16 (9%)	1 (0%)	29	68
6	G	168/241 (70%)	151 (90%)	16 (10%)	1 (1%)	25	65
7	I	162/330 (49%)	150 (93%)	12 (7%)	0	100	100
8	H	290/773 (38%)	242 (83%)	45 (16%)	3 (1%)	15	54
8	Y	103/773 (13%)	91 (88%)	12 (12%)	0	100	100
9	J	143/153 (94%)	121 (85%)	20 (14%)	2 (1%)	11	47
All	All	2023/4125 (49%)	1699 (84%)	308 (15%)	16 (1%)	24	60

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	129	PRO
4	E	295	LYS
8	H	209	ILE
4	E	264	ALA
6	G	35	PRO
3	D	280	LEU
4	E	192	LYS
9	J	128	SER
1	B	147	LEU
3	D	267	ARG
4	E	260	PRO
8	H	396	ILE
4	E	150	PRO
5	F	223	PHE
8	H	131	ILE
4	E	149	HIS

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	B	219/223 (98%)	209 (95%)	10 (5%)	27	54
2	C	183/349 (52%)	169 (92%)	14 (8%)	13	39
3	D	176/344 (51%)	154 (88%)	22 (12%)	4	22
4	E	291/418 (70%)	281 (97%)	10 (3%)	37	61
5	F	120/378 (32%)	114 (95%)	6 (5%)	24	51
6	G	72/221 (33%)	68 (94%)	4 (6%)	21	49
7	I	133/314 (42%)	128 (96%)	5 (4%)	33	58
8	H	47/685 (7%)	44 (94%)	3 (6%)	17	44
9	J	73/143 (51%)	72 (99%)	1 (1%)	67	80
All	All	1314/3075 (43%)	1239 (94%)	75 (6%)	24	48

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LEU
1	B	54	ILE
1	B	103	LEU
1	B	106	GLU
1	B	124	LEU
1	B	189	VAL
1	B	194	ASN
1	B	203	LEU
1	B	214	THR
1	B	221	ILE
2	C	170	TYR
2	C	172	MET
2	C	176	THR
2	C	202	LEU
2	C	206	LEU
2	C	224	LEU
2	C	225	LYS
2	C	239	THR
2	C	299	LEU
2	C	300	ASP
2	C	302	GLU
2	C	305	MET
2	C	310	VAL

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Mol	Chain	Res	Type
2	C	348	LEU
3	D	127	ARG
3	D	129	ASN
3	D	131	LEU
3	D	132	THR
3	D	135	GLN
3	D	143	ASP
3	D	148	LEU
3	D	149	ASN
3	D	152	LEU
3	D	156	TYR
3	D	172	ARG
3	D	182	VAL
3	D	192	ASN
3	D	212	LEU
3	D	235	ARG
3	D	237	PHE
3	D	240	CYS
3	D	241	LEU
3	D	243	SER
3	D	244	LEU
3	D	267	ARG
3	D	268	LYS
4	E	68	ARG
4	E	96	LEU
4	E	106	TRP
4	E	204	PHE
4	E	212	PHE
4	E	245	LYS
4	E	258	LEU
4	E	261	SER
4	E	267	MET
4	E	431	LEU
5	F	262	LEU
5	F	286	ARG
5	F	290	LYS
5	F	333	ASN
5	F	356	LEU
5	F	371	LYS
6	G	49	LYS
6	G	69	ASN
6	G	98	ARG

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Mol	Chain	Res	Type
6	G	112	ARG
7	I	176	ARG
7	I	187	ARG
7	I	240	GLN
7	I	263	LEU
7	I	303	ASN
8	H	86	ILE
8	H	139	LEU
8	H	145	LEU
9	J	62	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	ASN
1	B	194	ASN
3	D	149	ASN
3	D	151	ASN
3	D	170	GLN
3	D	186	ASN
3	D	192	ASN
3	D	238	GLN
3	D	313	ASN
4	E	23	GLN
4	E	133	GLN
4	E	149	HIS
4	E	207	ASN
4	E	284	HIS
4	E	391	ASN
4	E	423	ASN
5	F	250	GLN
5	F	255	ASN
5	F	278	ASN
5	F	282	ASN
5	F	283	ASN
5	F	333	ASN
5	F	382	HIS
7	I	200	ASN
7	I	205	GLN
7	I	228	GLN
7	I	303	ASN
9	J	5	GLN

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 ⓘ

There are no ligands in this entry.

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
10	X	2
8	Y	1
11	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	1213:UNK	C	1667:UNK	N	26.06
1	X	129:UNK	C	136:UNK	N	14.95
1	M	128:UNK	C	149:UNK	N	10.69
1	X	168:UNK	C	175:UNK	N	9.72

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-0523. 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 |
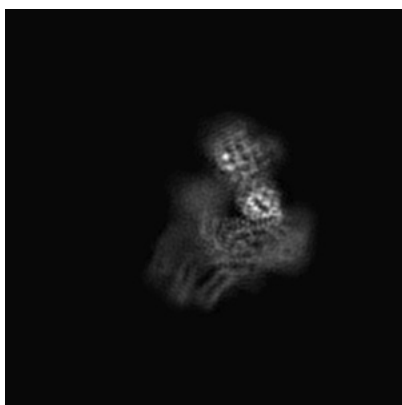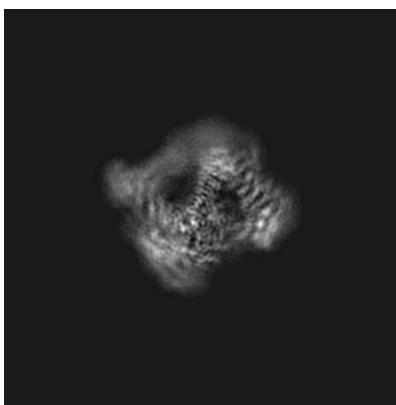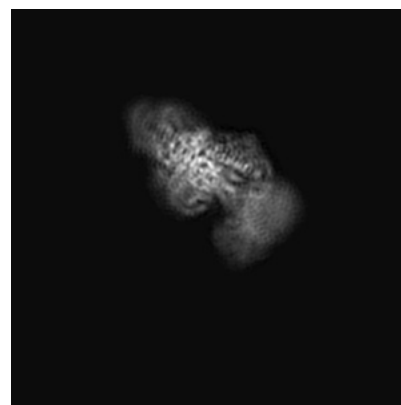
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ
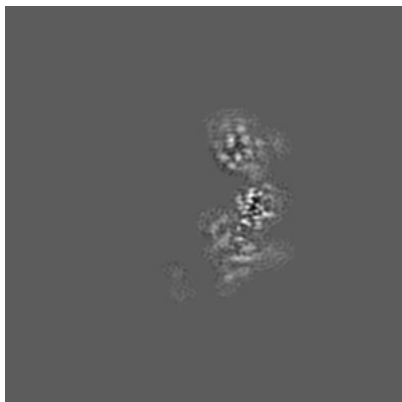
6.2.1　Primary map
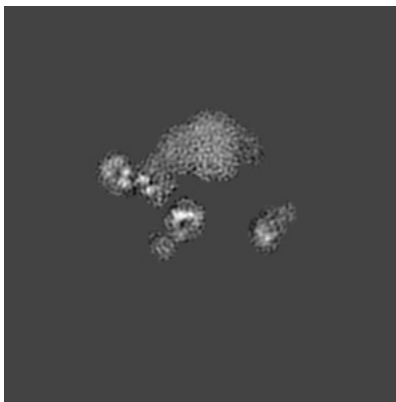
| X Index: 152 | Y Index: 152 | Z Index: 152 |
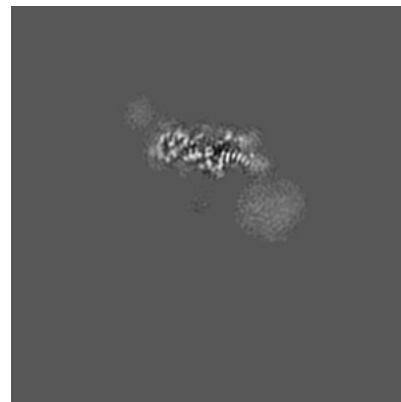
The images above show central slices of the map in three orthogonal directions.

6.3　Largest variance slices ⓘ
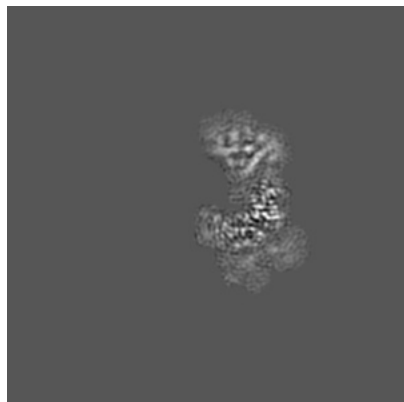
6.3.1　Primary map
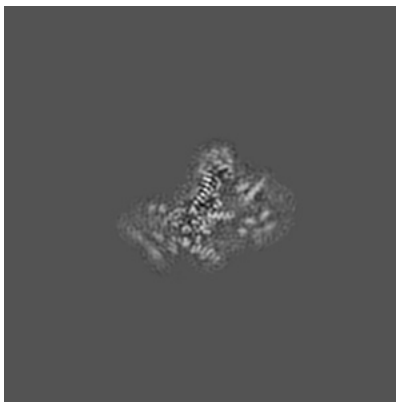
| X Index: 140 | Y Index: 188 | Z Index: 156 |
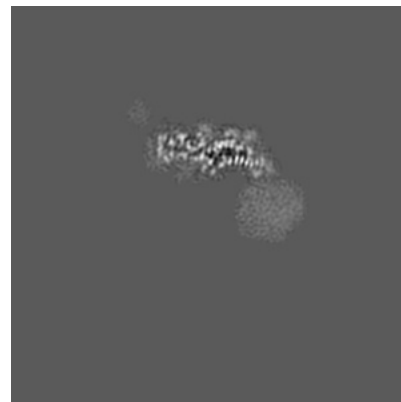
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1　Primary map

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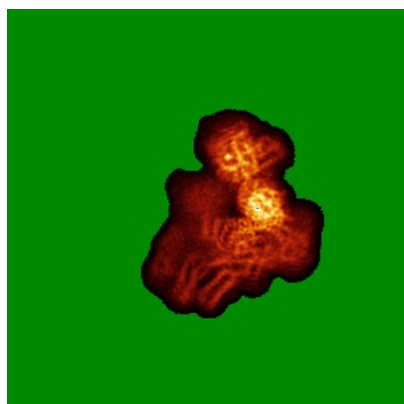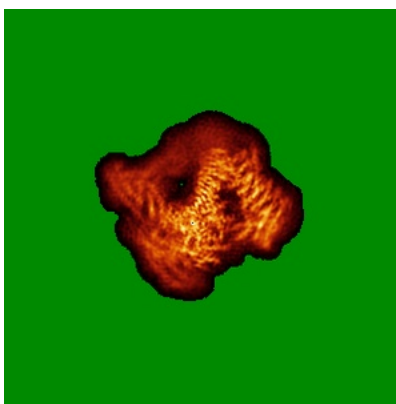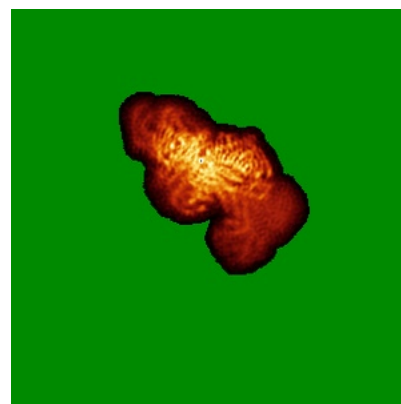
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
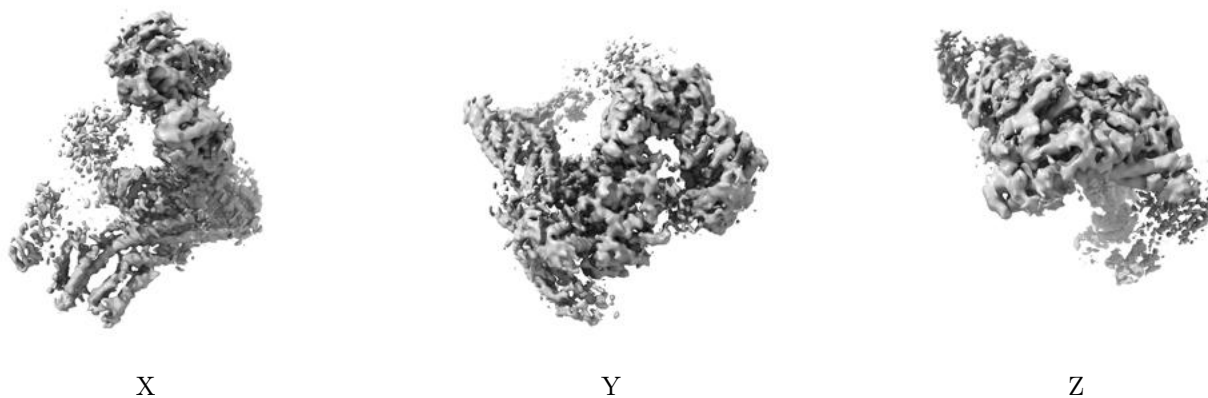
The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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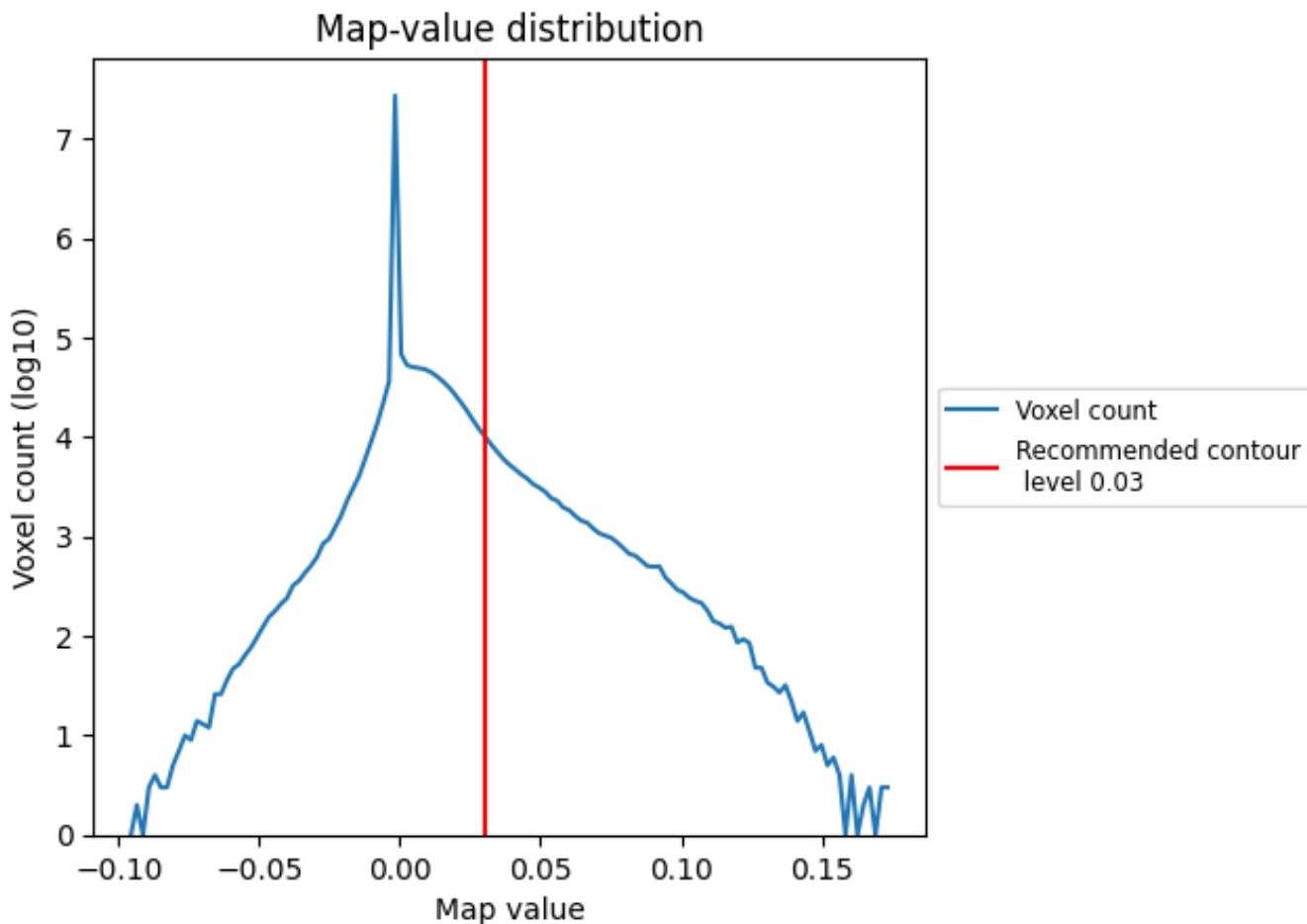
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
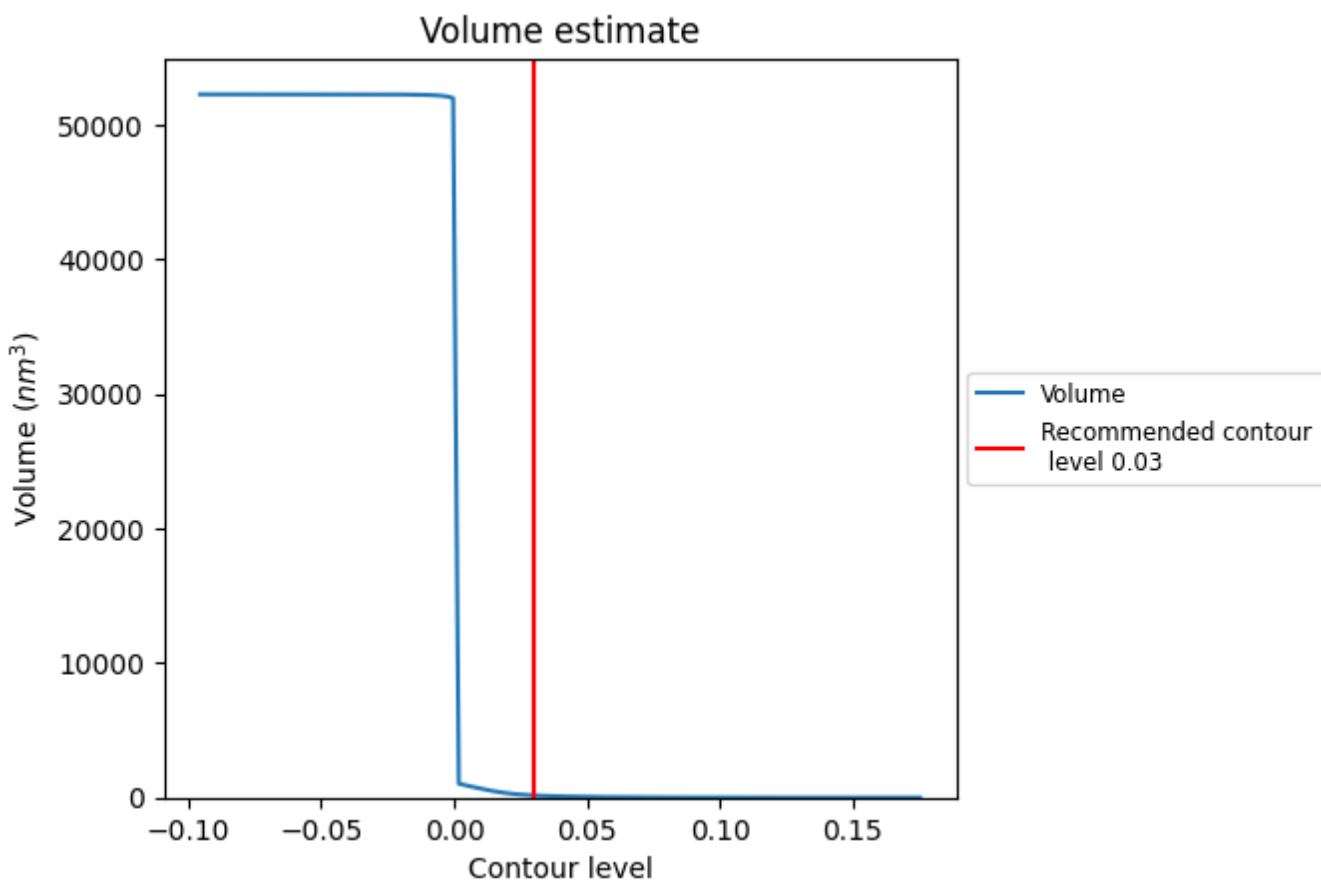
The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 146 kDa.

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 ⓘ
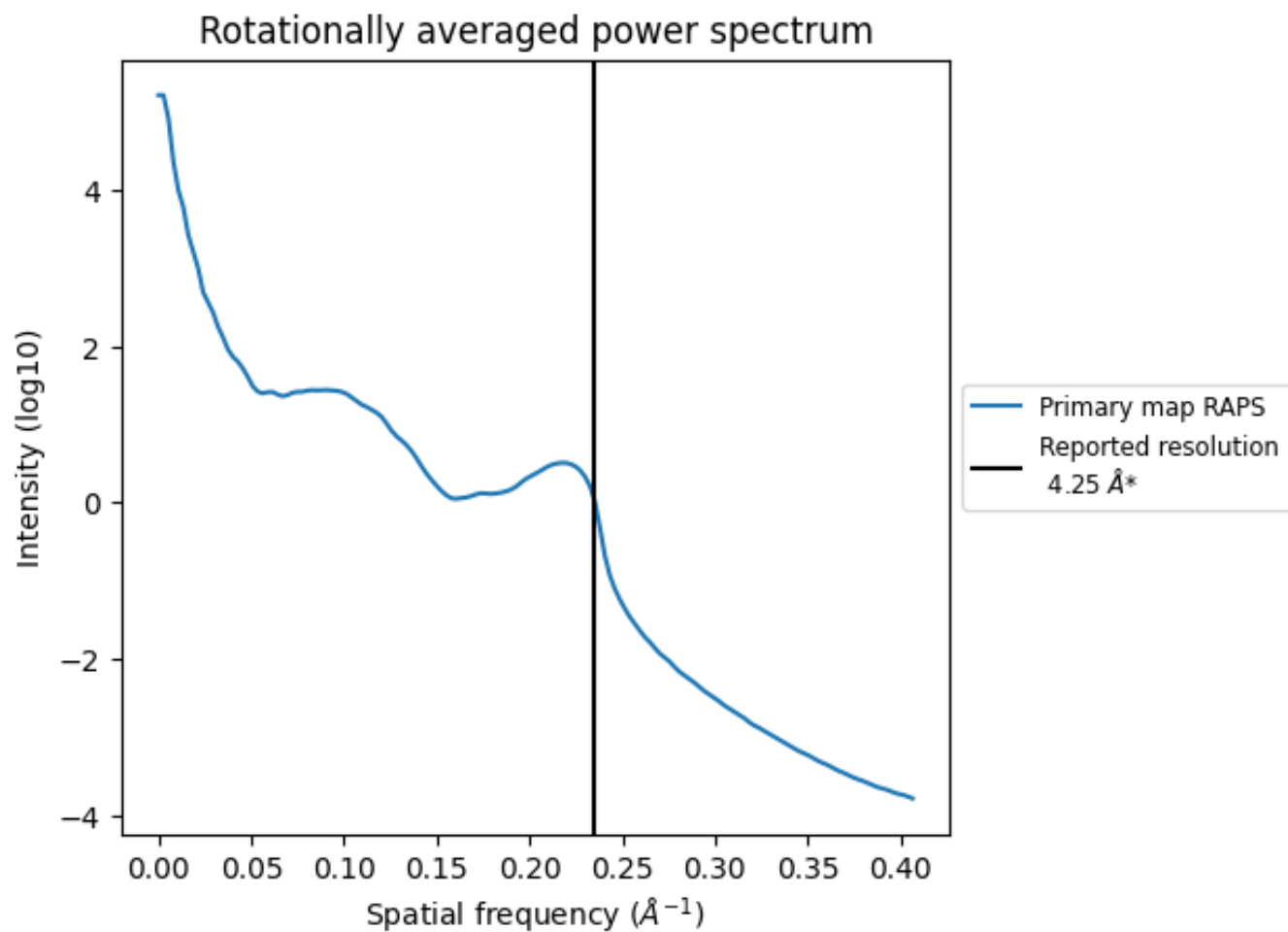
*Reported resolution corresponds to spatial frequency of 0.235 Å^{-1}

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 ⓘ
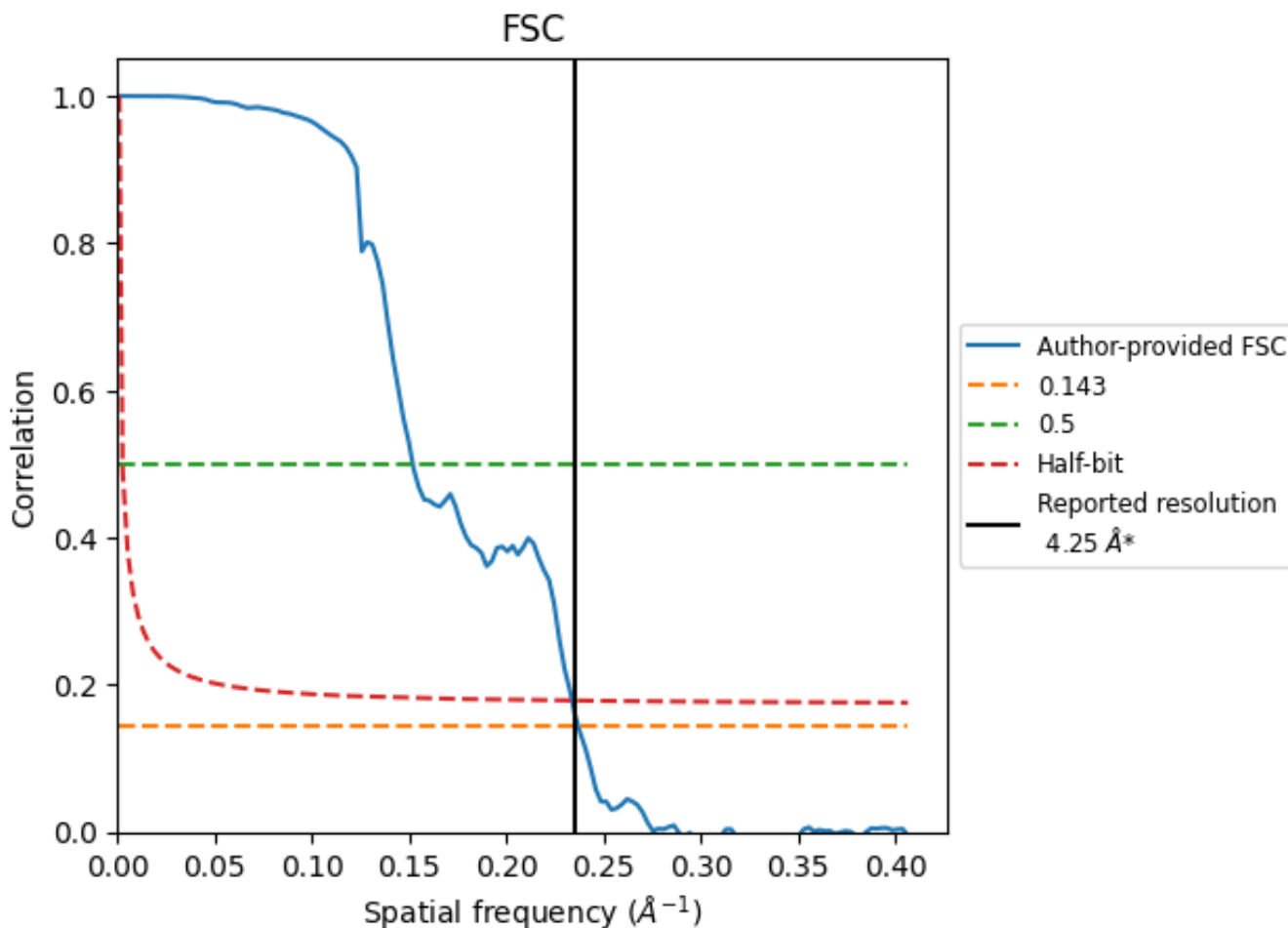
*Reported resolution corresponds to spatial frequency of 0.235 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.22	6.58	4.28
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-0523 and PDB model 6NUW. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ

| X | Y | Z |
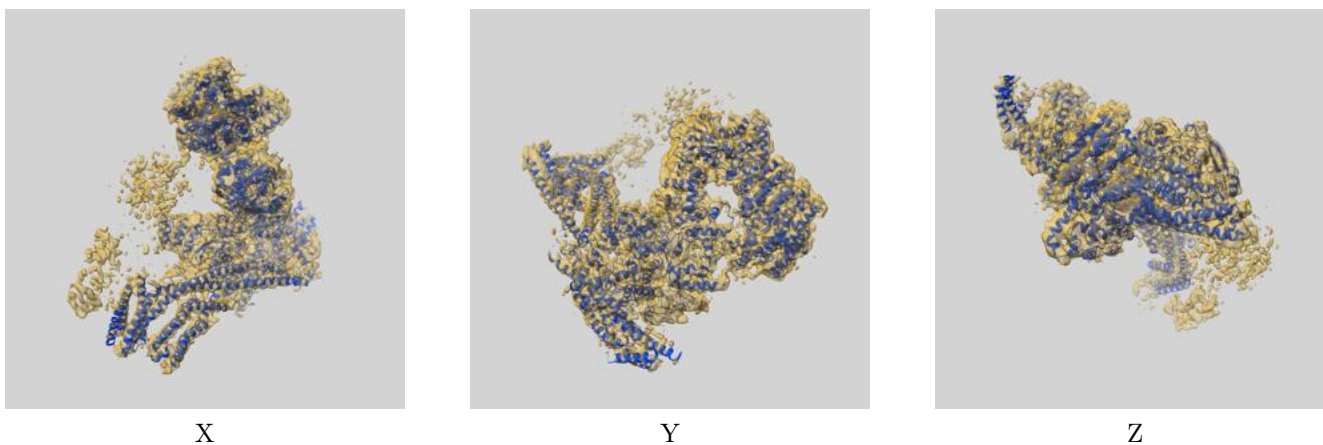
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
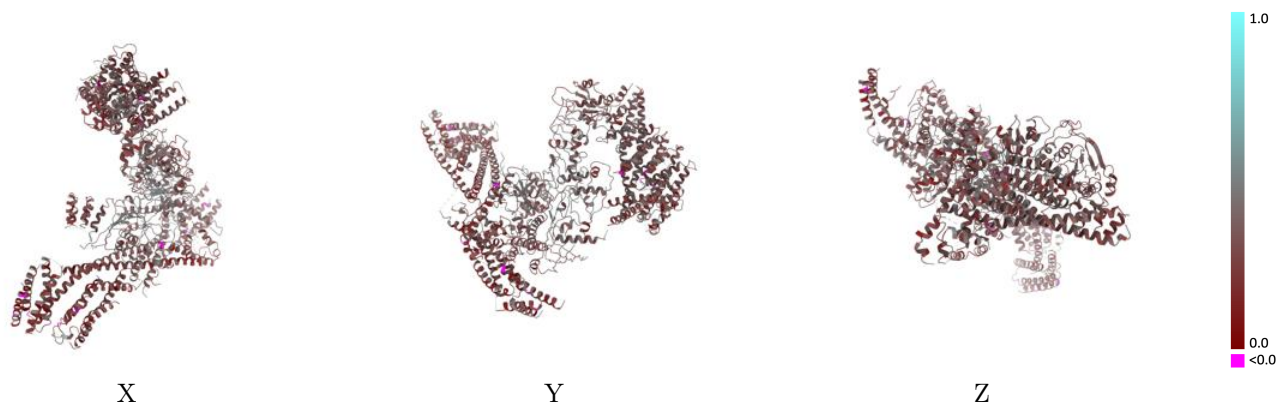
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
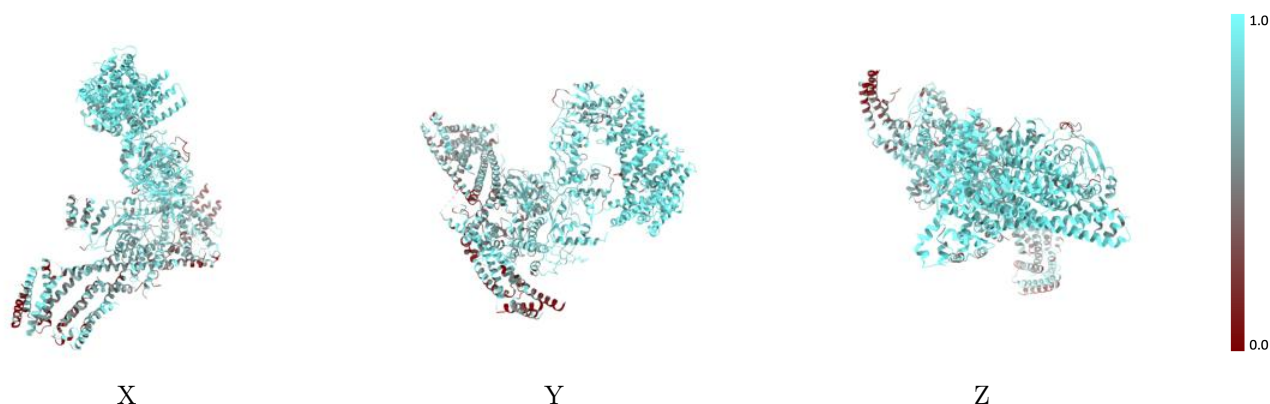
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion ⓘ
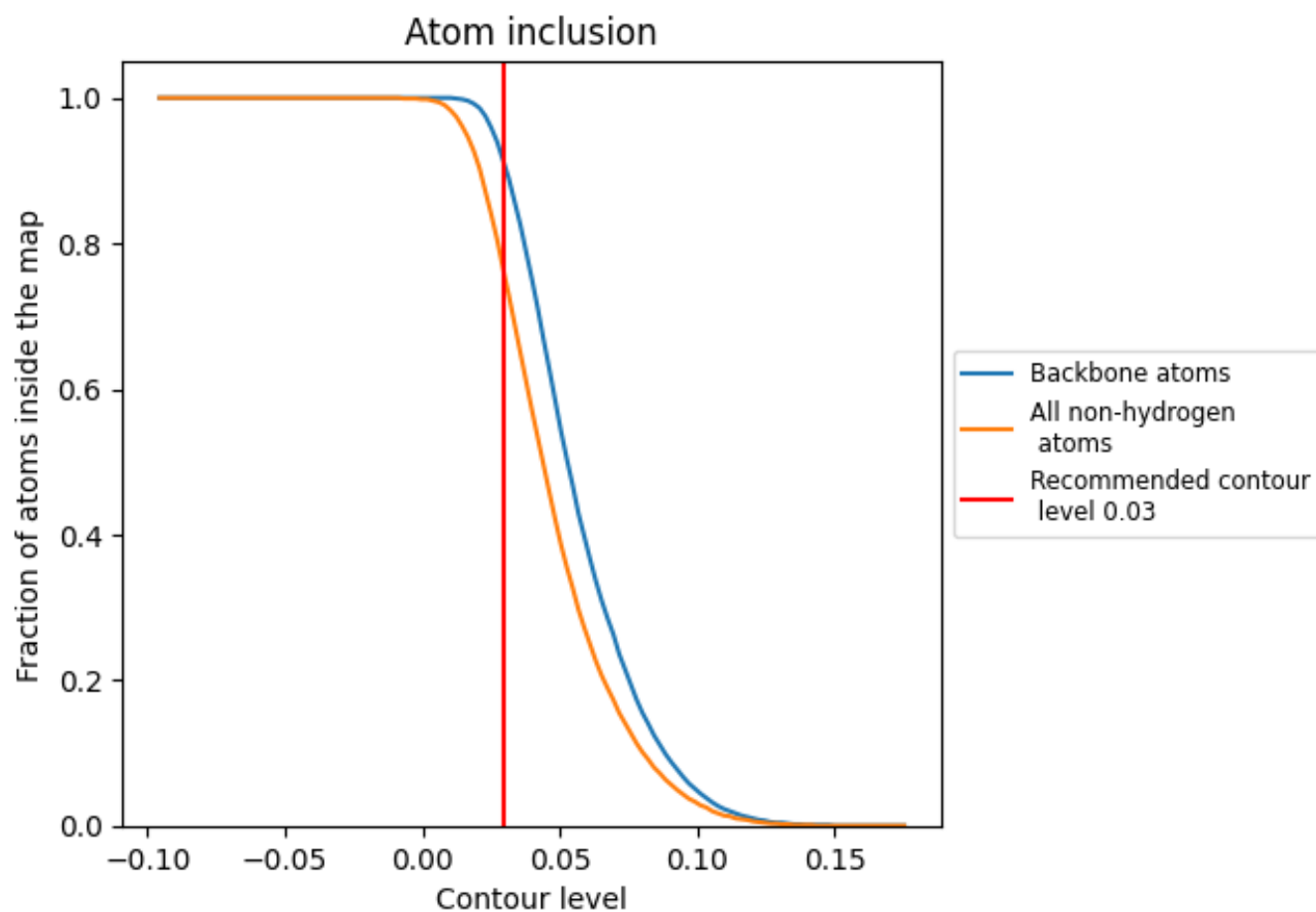
At the recommended contour level, 91% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score
for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.3420
B	0.8130	0.3820
C	0.7930	0.3810
D	0.7960	0.3560
E	0.7690	0.3960
F	0.5650	0.2940
G	0.6330	0.3020
H	0.9000	0.3400
I	0.5740	0.2670
J	0.5930	0.2740
M	0.9570	0.3370
U	0.1390	0.2250
X	0.9430	0.3200
Y	0.9520	0.3310

1.0

0.0
<0.0