WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 08:37 am GMT

PDB ID	:	7NYR
EMDB ID	:	EMD-12653
Title	:	Respiratory complex I from Escherichia coli - conformation 1
Authors	:	Kolata, P.; Efremov, R.G.
Deposited on	:	2021-03-23
Resolution	:	3.30 Å(reported)
Based on initial models	:	4HEA, 3RKO

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:

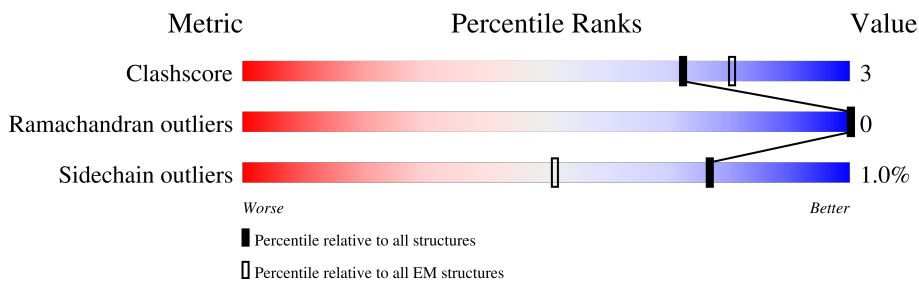|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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.
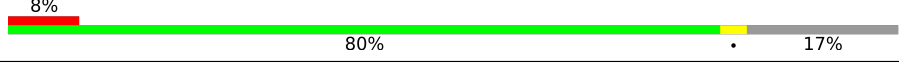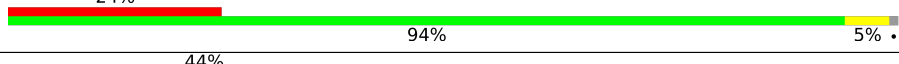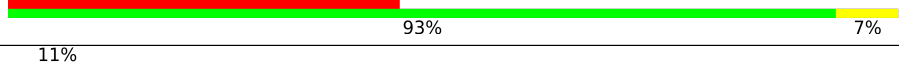
Metric	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.0%

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	220	70% ⋅ 28%
2	D	596	93% 5% ⋅
3	E	166	89% 5% 6%
4	F	445	93% 6% ⋅
5	G	908	96% ⋅
6	I	180	87% ⋅⋅ 12%
7	K	100	12% 89% 11%
8	J	184	9% 75% 14% 11%

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	A	147	12% 50% 13% 37%
10	H	325	8% 80% 17%
11	M	509	24% 94% 5%
12	L	613	44% 93% 7%
13	N	485	11% 85% 11%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 35228 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 NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	159	Total 1222	C 769	N 218	O 222	S 13	0	0

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	588	Total 4725	C 3027	N 825	O 852	S 21	0	0

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	156	Total 1220	C 768	N 215	O 229	S 8	0	0

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	441	Total 3424	C 2171	N 599	O 633	S 21	0	0

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	907	Total 7044	C 4402	N 1272	O 1332	S 38	0	0

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	158	Total 1220	C 771	N 205	O 232	S 12	0	0

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	100	Total 760	C 494	N 132	O 129	S 5	0	0

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	164	Total 1242	C 833	N 193	O 209	S 7	0	0

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	92	Total 668	C 448	N 108	O 111	S 1	0	0

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	270	Total 1985	C 1317	N 317	O 337	S 14	0	0

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	504	Total 3953	C 2661	N 617	O 646	S 29	0	0

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	612	Total 4126	C 2671	N 698	O 733	S 24	0	0

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	467	Total 3543	C 2370	N 559	O 596	S 18	0	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	Fe	S	0
			8	4	4	
14	F	1	Total	Fe	S	0
			8	4	4	
14	G	1	Total	Fe	S	0
			24	12	12	
14	G	1	Total	Fe	S	0
			24	12	12	
14	G	1	Total	Fe	S	0
			24	12	12	
14	I	1	Total	Fe	S	0
			16	8	8	
14	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

FES

Mol	Chain	Residues	Atoms			AltConf
15	E	1	Total 4	Fe 2	S 2	0
15	G	1	Total 4	Fe 2	S 2	0

- Molecule 16 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

FMN
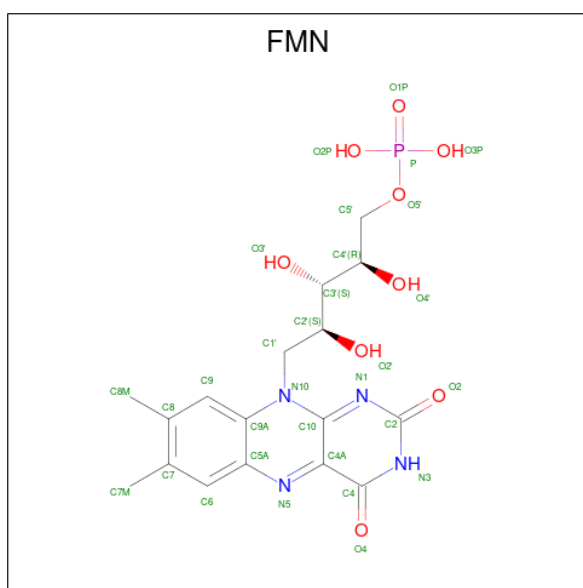
| Mol	Chain	Residues	Atoms					AltConf
16	F	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 17 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol	Chain	Residues	Atoms		AltConf
17	G	1	Total	Ca	0
			1	1	

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.
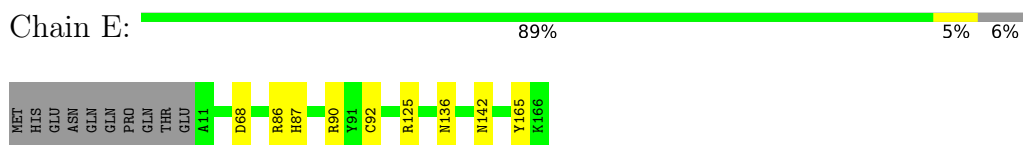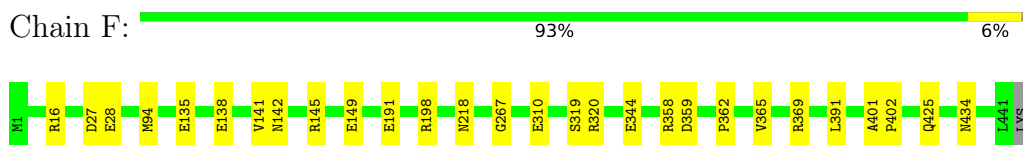
• Molecule 1: NADH-quinone oxidoreductase subunit B
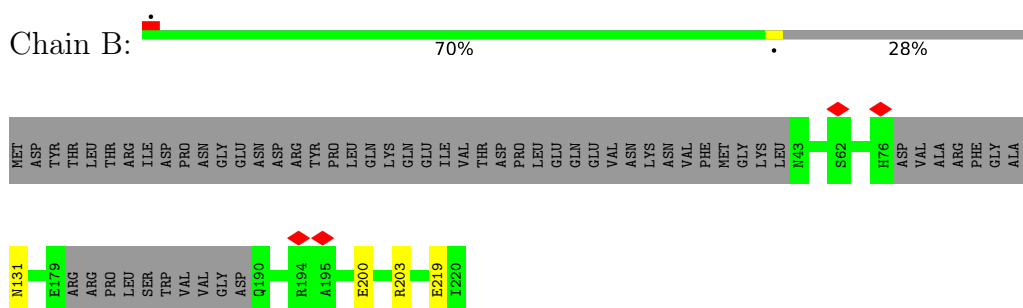
Chain B:

• Molecule 2: NADH-quinone oxidoreductase subunit C/D
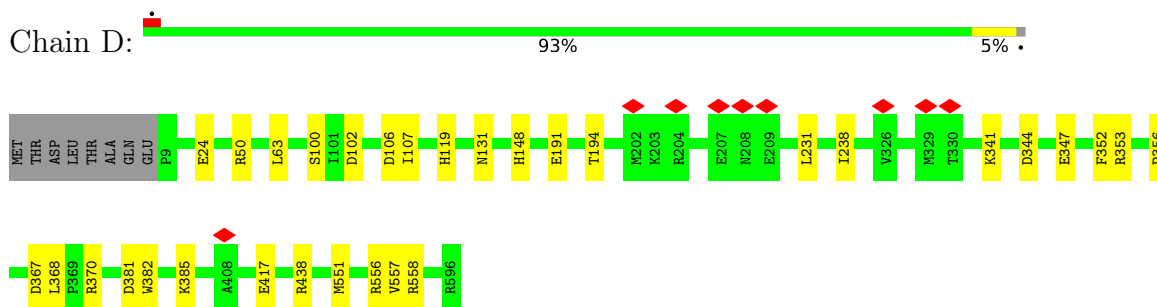
Chain D:

• Molecule 3: NADH-quinone oxidoreductase subunit E

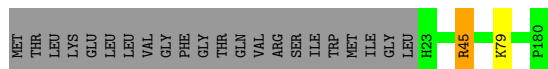Chain E:

• Molecule 4: NADH-quinone oxidoreductase subunit F

Chain F:

• Molecule 5: NADH-quinone oxidoreductase subunit G

Chain G:

96%

M1 F33 N55 S145 R156 K162 D186 T207 S212 C235 R242 R247 L429 D436 A444 Q511 V527 N537 L549 T558 G559 R560 H572 D617 N623 E624 Q632 Q668 P681 H707 I730 W755
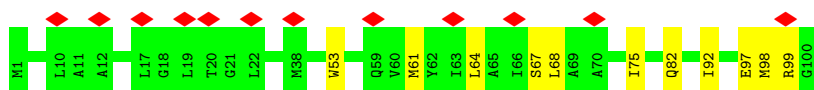
N760 R784 S798 N843 L877 K904 Q907 GLN

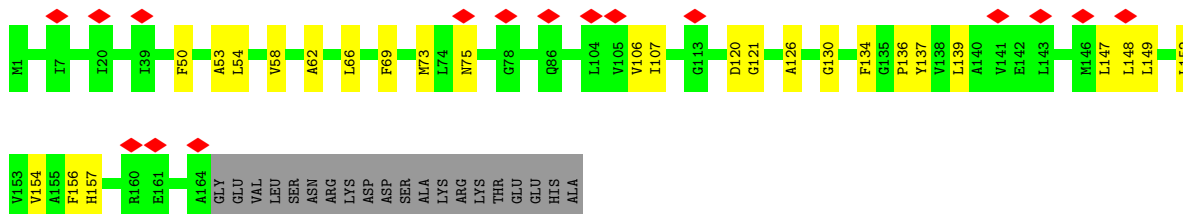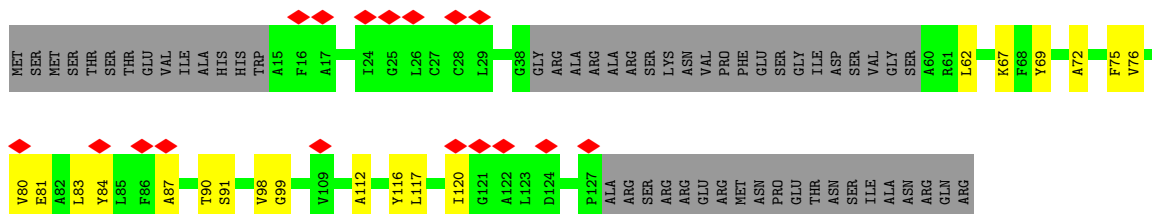• Molecule 6: NADH-quinone oxidoreductase subunit I

Chain I:

87% •• 12%

MET THR LEU LYS GLU LEU LEU VAL GLY PHE GLY THR GLN VAL ARG SER ILE TRP MET ILE GLY LEU H23 R45 K79 P180

• Molecule 7: NADH-quinone oxidoreductase subunit K

12%

Chain K:

89% 11%

M1 L10 A11 A12 L17 G18 L19 T20 G21 L22 M38 W53 Q59 V60 M61 Y62 I63 L64 A65 I66 S67 L68 A69 A70 I75 Q82 I92 E97 M98 R99 G100

• Molecule 8: NADH-quinone oxidoreductase subunit J

9%

Chain J:

75% 14% 11%

M1 I7 I20 I39 F50 A53 L54 V58 A62 L66 F69 M73 L74 N75 G78 Q86 L104 V105 V106 I107 G113 D120 G121 A126 G130 F134 G135 P136 Y137 V138 L139 A140 V141 E142 L143 M146 L147 L148 L149 L152

V153 V154 A155 F156 H157 R160 E161 A164 GLY GLU VAL LEU SER ASN ARG LYS ASP ASP SER ALA LYS ARG LYS THR GLU GLU HIS ALA
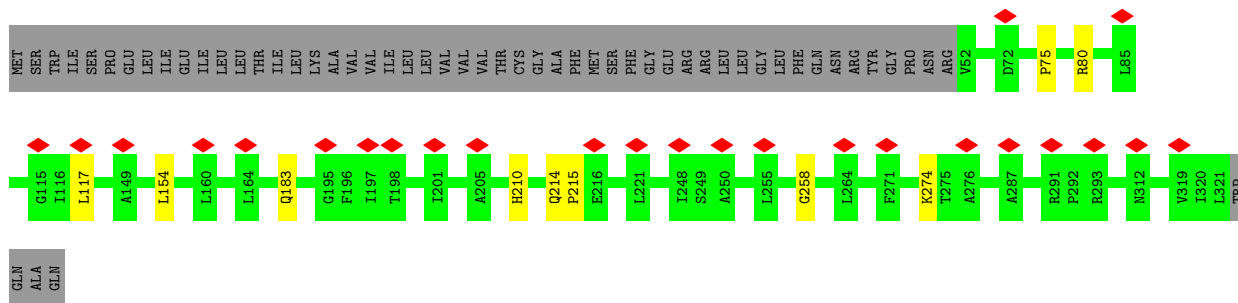
• Molecule 9: NADH-quinone oxidoreductase subunit A

12%

Chain A:

50% 13% 37%

MET SER MET SER THR SER THR GLU VAL ILE ALA HIS HIS TRP A15 F16 A17 I24 G25 L26 C27 C28 L29 G38 GLY ARG ALA ARG ALA ARG SER LYS ASN VAL PRO PHE GLU SER GLY ILE ASP SER VAL GLY SER A60 R61 L62 K67 F68 Y69 A72 F75 V76

V80 E81 A82 L83 Y84 L85 F86 A87 T90 S91 V98 G99 V109 A112 Y116 L117 I120 G121 A122 L123 D124 P127 ALA ARG SER ARG ARG GLU ARG MET ASN PRO GLU THR ASN SER ILE ALA ASN ARG GLN ARG
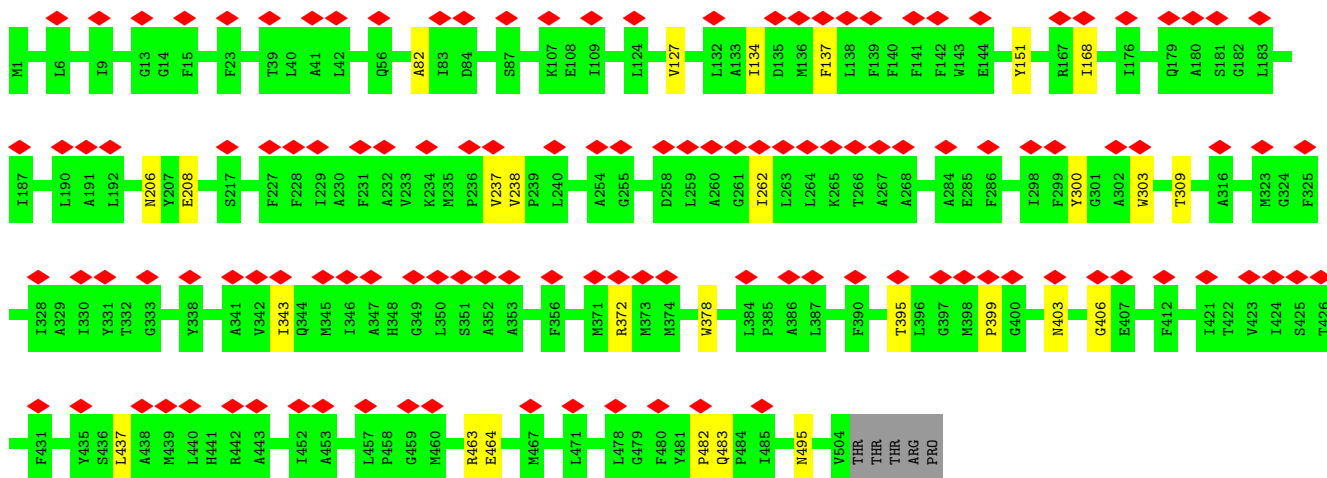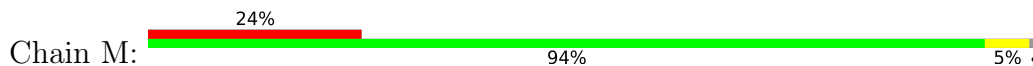
• Molecule 10: NADH-quinone oxidoreductase subunit H

8%

Chain H:

80% • 17%

MET SER TRP ILE SER PRO GLU GLU LEU ILE GLU ILE LEU LEU THR ILE LEU LYS ALA VAL VAL ILE LEU LEU VAL VAL VAL THR CYS GLY ALA PHE MET SER PHE GLY GLU ARG ARG LEU LEU GLY LEU PHE GLN ASN ARG TYR GLY PRO ASN ARG V52 D72 P75 R80 L85

G115 I116 L117 A149 L154 L160 L164 Q183 G195 F196 I197 T198 I201 A205 H210 Q214 P215 E216 L221 I248 S249 A250 L255 G258 L264 F271 K274 T275 A276 A287 R291 P292 R293 N312 V319 I320 L321 TRP

GLN ALA GLN

● Molecule 11: NADH-quinone oxidoreductase subunit M

Chain M:

24%

94% 5% ·

M1 L6 I9 G13 G14 F15 F23 T39 L40 A41 L42 Q56 A82 I83 D84 S87 K107 E108 I109 L124 V127 L132 A133 I134 D135 M136 F137 L138 F139 F140 F141 F142 W143 E144 Y151 R167 I168 I176 Q180 A180 S181 G182 L183

I187 L190 A191 L192 N206 Y207 E208 S217 F227 F228 I229 A230 F231 A232 V233 K234 M235 P236 V237 V238 P239 L240 A254 G255 D258 L259 A260 G261 I262 L263 L264 K265 T266 A267 A268 A284 E285 F286 I298 F299 Y300 G301 A302 W303 T309 A316 M323 G324 F325

I328 A329 I330 Y331 T332 G333 Y338 A341 V342 I343 Q344 M345 I346 A347 H348 G349 L350 S351 A352 A353 F356 M371 R372 M373 M374 W378 L384 P385 A386 L387 F390 T395 L396 G397 M398 P399 G400 N403 G406 E407 F412 I421 T422 V423 I424 S425 T426

F431 Y435 S436 L437 A438 M439 L440 H441 R442 A443 I452 A453 L457 P458 G459 M460 R463 E464 M467 L471 L478 G479 L479 F480 Y481 P482 Q483 P484 I485 N495 V504 THR THR THR ARG PRO
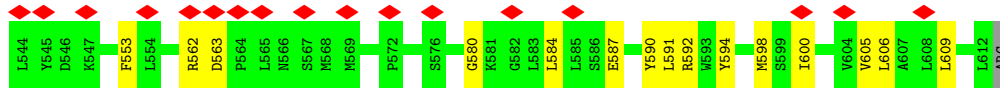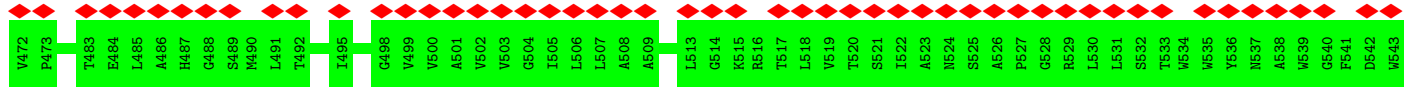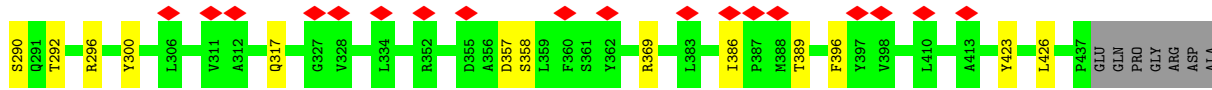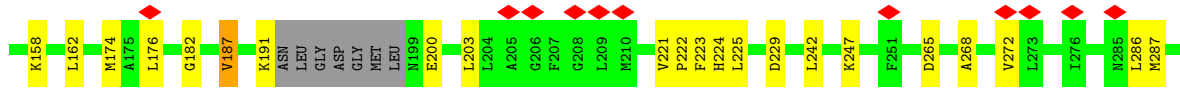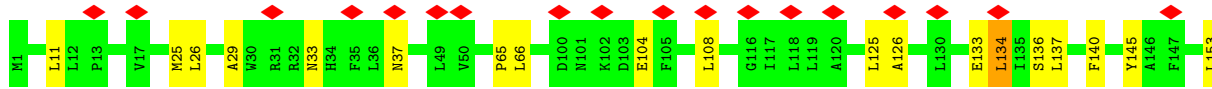
● Molecule 12: NADH-quinone oxidoreductase subunit L

Chain L:

44%

93% 7%

M1 N2 M3 L4 A5 L6 T7 L10 P11 F20 S21 R22 L43 D51 N55 Q58 W67 M68 S69 V70 G71 D72 N78 L79 V80 L81 D82 G83 L84 S85 M88 L89 V92 M101 Y102 A103 S104 W105 R108 G109 E110 E111 G112 Y113 F117 N121

S126 V129 A133 D134 N135 L136 L137 L138 M139 Y140 L141 G142 W143 E144 G145 V146 G147 L148 Y158 T159 A165 M168 F171 V172 V173 T174 R175 V176 G177 D178 V179 F180 F183 F186 R198 A209 N212 N213 M214 L215 M216 T219 L220 M221 L222 L223 G224

G225 A226 V227 G228 K229 S230 A231 Q232 L233 P234 W238 L239 A240 D241 A242 V249 S250 A251 L252 I253 H254 A255 A256 T257 M258 V263 A267 R268 L274 M275 L280 H281 L282 V283 G284 I285 L291 G295 F296 L299 D303 I304 K305 R306 M313 I316 M319

F320 L323 G324 V325 Q326 A330 F333 M336 T337 H338 A339 F340 F341 K342 A343 L344 L347 A348 S349 G350 S351 V352 I353 L354 A355 C356 H357 H358 I362 F363 K364 M365 R369 K370 P373 L374 V375 C378 F379 L380 V381 G382 G383 A384 A385 L386 S387 A388 L389 P390 I391

V392 F396 F397 S398 K399 D400 E401 I402 L403 A404 G405 A406 M407 A408 N409 G410 H411 I412 N413 L414 M415 V416 A417 G421 M424 T425 S426 L427 Y428 R431 M432 E441 Q442 I443 H444 A447 V448 K449 G450 V451 T452 H453 S454 L455 P456 I462 L463 V467 G468 A469 L470 I471

V472 P473 T483 E484 L485 A486 H487 G488 S489 M490 L491 T492 I495 G498 V499 V500 A501 V502 V503 G504 I505 L506 L507 A508 A509 L513 G514 K515 R516 T517 L518 V519 T520 S521 I522 A523 N524 S525 A526 P527 G528 R529 L530 L531 S532 T533 W534 W535 Y536 N537 A538 W539 G540 F541 D542 W543

L544 Y545 D546 K547 F553 L554 R562 D563 P564 L565 N566 S567 M568 M569 P572 S576 G580 K581 G582 L583 L584 L585 S586 E587 Y590 L591 R592 W593 Y594 M598 S599 I600 V604 V605 L606 A607 L608 L609 L612 ARG

• Molecule 13: NADH-quinone oxidoreductase subunit N

Chain N:

11%

85%

11%

M1 L11 L12 P13 V17 M25 L26 A29 W30 R31 R32 N33 H34 F35 L36 N37 L49 V50 P65 L66 D100 N101 K102 D103 E104 F105 L108 G116 I117 I118 I119 A120 L125 A126 L130 E133 L134 I135 S136 L137 F140 Y145 A146 F147 L153

K158 L162 M174 A175 L176 G182 V187 K191 ASN LEU GLY ASP GLY MET LEU N199 E200 L203 L204 A205 G206 F207 G208 L209 M210 V221 P222 F223 H224 L225 D229 L242 K247 F251 D265 A268 V272 L273 I276 N285 L286 M287

S290 Q291 T292 R296 Y300 L306 V311 A312 Q317 G327 V328 L334 R352 D355 A356 D357 S358 L359 F360 S361 Y362 R369 L383 I386 P387 M388 T389 F396 Y397 V398 L410 A413 Y423 L426 P437 GLU GLN PRO GLY ARG ASP ALA

PRO SER N447 W448 L465 V469 W470 P471 L474 P483 LEU MET

4   Experimental information   ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	64.7	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	177.750	Depositor
Minimum map value	-51.739	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.19	Depositor
Map size (Å)	370.17603, 370.17603, 370.17603	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1568, 1.1568, 1.1568	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SF4, FMN, CSX, FES

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	0.30	0/1238	0.64	0/1674
2	D	0.29	0/4856	0.61	0/6593
3	E	0.29	0/1240	0.60	0/1680
4	F	0.31	0/3495	0.63	0/4723
5	G	0.29	0/7195	0.62	0/9755
6	I	0.31	0/1248	0.61	0/1691
7	K	0.27	0/769	0.64	0/1040
8	J	0.28	0/1268	0.56	0/1729
9	A	0.27	0/684	0.59	0/932
10	H	0.28	0/2037	0.57	0/2780
11	M	0.35	0/4074	0.61	0/5546
12	L	0.33	0/4205	0.58	0/5754
13	N	0.37	0/3630	0.61	0/4954
All	All	0.31	0/35939	0.61	0/48851

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1222	0	1182	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4725	0	4619	16	0
3	E	1220	0	1187	5	0
4	F	3424	0	3391	16	0
5	G	7044	0	6849	18	0
6	I	1220	0	1155	3	0
7	K	760	0	817	24	0
8	J	1242	0	1315	65	0
9	A	668	0	623	37	0
10	H	1985	0	1921	5	0
11	M	3953	0	4053	23	0
12	L	4126	0	3691	73	0
13	N	3543	0	3709	101	0
14	B	8	0	0	0	0
14	F	8	0	0	0	0
14	G	24	0	0	1	0
14	I	16	0	0	0	0
15	E	4	0	0	1	0
15	G	4	0	0	0	0
16	F	31	0	19	1	0
17	G	1	0	0	0	0
All	All	35228	0	34531	237	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 3.

All (237) 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)
8:J:149:LEU:HD11	13:N:25:MET:CE	1.63	1.28
12:L:594:TYR:CE2	13:N:225:LEU:HB3	1.75	1.21
8:J:149:LEU:CD1	13:N:25:MET:HE1	1.76	1.14
11:M:378:TRP:HE1	12:L:22:ARG:NH1	1.45	1.13
12:L:598:MET:HE1	13:N:223:PHE:HB3	1.31	1.12
12:L:594:TYR:CZ	13:N:225:LEU:HB3	1.93	1.04
8:J:149:LEU:HD11	13:N:25:MET:HE1	1.04	1.00
8:J:156:PHE:CE2	13:N:104:GLU:OE2	2.20	0.95
12:L:598:MET:CE	13:N:223:PHE:HB3	1.97	0.94
8:J:136:PRO:HB3	13:N:65:PRO:HD2	1.48	0.93
11:M:378:TRP:HE1	12:L:22:ARG:HH12	1.17	0.93
12:L:594:TYR:CE1	13:N:225:LEU:HD12	2.05	0.91
12:L:594:TYR:CD1	13:N:225:LEU:HG	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:605:VAL:HG13	13:N:272:VAL:HG11	1.56	0.88
8:J:106:VAL:HG11	12:L:606:LEU:HD12	1.57	0.85
11:M:378:TRP:NE1	12:L:22:ARG:NH1	2.24	0.84
7:K:98:MET:HE2	13:N:158:LYS:NZ	1.94	0.82
8:J:149:LEU:HD11	13:N:25:MET:SD	2.19	0.82
12:L:598:MET:HE1	13:N:223:PHE:CB	2.09	0.81
9:A:116:TYR:HA	13:N:29:ALA:HB2	1.62	0.80
8:J:149:LEU:CD1	13:N:25:MET:CE	2.46	0.80
7:K:92:ILE:CG2	12:L:592:ARG:HH22	1.96	0.79
5:G:624:GLU:OE2	5:G:784:ARG:NH2	2.16	0.78
8:J:107:ILE:HD11	13:N:176:LEU:CD1	2.15	0.77
7:K:92:ILE:HG21	12:L:592:ARG:HH22	1.48	0.76
12:L:594:TYR:CD2	13:N:225:LEU:HB3	2.22	0.75
7:K:98:MET:CE	13:N:158:LYS:HZ3	1.99	0.75
12:L:594:TYR:CE1	13:N:225:LEU:CD1	2.70	0.74
2:D:347:GLU:OE2	2:D:353:ARG:NH1	2.20	0.74
11:M:378:TRP:HE1	12:L:22:ARG:CZ	2.01	0.74
8:J:106:VAL:CG1	12:L:606:LEU:CD1	2.66	0.73
12:L:580:GLY:HA2	13:N:286:LEU:HB3	1.70	0.73
13:N:265:ASP:OD1	13:N:317:GLN:NE2	2.22	0.73
7:K:98:MET:CE	13:N:158:LYS:NZ	2.52	0.73
12:L:594:TYR:CZ	13:N:225:LEU:HD12	2.24	0.72
11:M:395:THR:O	11:M:403:ASN:ND2	2.23	0.72
8:J:154:VAL:HG13	13:N:108:LEU:HD21	1.70	0.71
8:J:154:VAL:CG1	13:N:108:LEU:HD21	2.21	0.71
8:J:106:VAL:CG1	12:L:606:LEU:HD12	2.20	0.71
12:L:594:TYR:CE1	13:N:225:LEU:HG	2.25	0.71
12:L:609:LEU:HD23	13:N:268:ALA:O	1.90	0.71
12:L:594:TYR:CE1	13:N:225:LEU:CG	2.74	0.70
7:K:82:GLN:OE1	13:N:153:LEU:HD13	1.90	0.70
7:K:99:ARG:CZ	12:L:590:TYR:OH	2.40	0.70
5:G:242:ARG:O	5:G:247:ARG:NH1	2.25	0.69
13:N:136:SER:O	13:N:140:PHE:N	2.25	0.69
8:J:106:VAL:HG11	12:L:606:LEU:CD1	2.21	0.69
12:L:605:VAL:HG22	13:N:272:VAL:CG1	2.23	0.68
4:F:344:GLU:OE2	4:F:369:ARG:NH1	2.27	0.68
12:L:587:GLU:OE2	13:N:287:MET:HE1	1.95	0.67
12:L:609:LEU:HG	13:N:272:VAL:HG21	1.77	0.67
12:L:55:ASN:ND2	12:L:58:GLN:O	2.29	0.66
12:L:584:LEU:HD22	13:N:290:SER:OG	1.95	0.65
8:J:156:PHE:CD2	13:N:104:GLU:OE2	2.48	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:82:GLN:OE1	13:N:153:LEU:HD22	1.96	0.65
4:F:138:GLU:O	4:F:142:ASN:ND2	2.29	0.64
8:J:157:HIS:NE2	13:N:145:TYR:HA	2.12	0.64
8:J:54:LEU:HG	9:A:83:LEU:HD11	1.79	0.64
8:J:69:PHE:HE2	9:A:72:ALA:HB1	1.61	0.64
12:L:587:GLU:CD	13:N:287:MET:HE3	2.19	0.63
2:D:356:PRO:O	6:I:45:ARG:NH2	2.32	0.63
8:J:107:ILE:HD11	13:N:176:LEU:HD13	1.79	0.63
7:K:82:GLN:OE1	13:N:153:LEU:CD1	2.46	0.63
12:L:594:TYR:CE2	13:N:225:LEU:CB	2.69	0.62
12:L:82:ASP:OD2	12:L:268:ARG:NH1	2.32	0.62
7:K:92:ILE:HG21	12:L:592:ARG:NH2	2.13	0.62
1:B:200:GLU:OE2	1:B:203:ARG:NH2	2.33	0.62
12:L:587:GLU:CD	13:N:287:MET:CE	2.67	0.62
8:J:136:PRO:HB3	13:N:65:PRO:CD	2.27	0.62
8:J:126:ALA:HB3	9:A:90:THR:HG21	1.82	0.61
12:L:598:MET:CE	13:N:223:PHE:CB	2.73	0.61
7:K:98:MET:HE2	13:N:158:LYS:HZ1	1.65	0.61
12:L:591:LEU:HD11	13:N:162:LEU:HG	1.82	0.61
8:J:106:VAL:CG1	12:L:606:LEU:HD13	2.29	0.61
8:J:136:PRO:CB	13:N:65:PRO:HD2	2.29	0.61
11:M:206:ASN:ND2	11:M:208:GLU:OE1	2.34	0.61
12:L:594:TYR:CZ	13:N:225:LEU:CB	2.80	0.61
9:A:116:TYR:HA	13:N:29:ALA:CB	2.30	0.60
1:B:127:GLY:O	1:B:131:ASN:ND2	2.35	0.60
10:H:75:PRO:O	10:H:80:ARG:NH2	2.34	0.60
12:L:598:MET:CE	13:N:223:PHE:CD1	2.85	0.59
3:E:125:ARG:NH2	3:E:165:TYR:O	2.35	0.59
7:K:67:SER:HA	9:A:80:VAL:HG11	1.84	0.59
8:J:148:LEU:HB3	9:A:81:GLU:OE2	2.03	0.59
7:K:82:GLN:OE1	13:N:153:LEU:CD2	2.51	0.59
8:J:156:PHE:HE2	13:N:104:GLU:OE2	1.81	0.59
8:J:66:LEU:HB2	9:A:76:VAL:HG21	1.86	0.58
11:M:437:LEU:HD13	12:L:168:MET:HG2	1.84	0.58
8:J:69:PHE:HE2	9:A:72:ALA:CB	2.16	0.58
2:D:100:SER:OG	2:D:102:ASP:OD1	2.22	0.58
3:E:68:ASP:OD1	5:G:162:LYS:NZ	2.34	0.58
4:F:319:SER:OG	4:F:320:ARG:N	2.36	0.58
12:L:609:LEU:CD2	13:N:268:ALA:O	2.51	0.58
13:N:386:ILE:O	13:N:389:THR:OG1	2.22	0.57
2:D:106:ASP:OD2	2:D:438:ARG:NH1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ASN:OD1	2:D:148:HIS:NE2	2.38	0.57
13:N:296:ARG:NH1	13:N:300:TYR:OH	2.37	0.57
8:J:147:LEU:HD13	13:N:134:LEU:HD12	1.87	0.57
12:L:591:LEU:HD11	13:N:162:LEU:CG	2.34	0.57
11:M:151:TYR:CE2	13:N:426:LEU:HD13	2.40	0.57
5:G:668:GLN:NE2	5:G:730:ILE:O	2.38	0.57
2:D:367:ASP:OD1	2:D:368:LEU:N	2.37	0.56
8:J:106:VAL:HG12	12:L:606:LEU:CD1	2.34	0.56
13:N:187:VAL:O	13:N:191:LYS:NZ	2.38	0.56
8:J:54:LEU:HD21	9:A:83:LEU:HD21	1.87	0.56
12:L:594:TYR:CD2	13:N:225:LEU:CB	2.88	0.56
12:L:587:GLU:OE2	13:N:287:MET:CE	2.52	0.56
8:J:152:LEU:HD11	9:A:117:LEU:HD11	1.88	0.56
4:F:401:ALA:HB3	4:F:402:PRO:HD3	1.87	0.55
8:J:73:MET:HE1	9:A:69:TYR:HD1	1.71	0.55
3:E:136:ASN:O	3:E:142:ASN:ND2	2.39	0.55
7:K:98:MET:HE3	13:N:158:LYS:HZ3	1.69	0.55
8:J:75:ASN:HB2	9:A:62:LEU:HD11	1.89	0.55
8:J:134:PHE:HZ	9:A:98:VAL:HG13	1.72	0.54
11:M:399:PRO:HG2	12:L:141:LEU:HG	1.89	0.54
12:L:598:MET:HE1	13:N:223:PHE:CG	2.42	0.54
12:L:605:VAL:HG22	13:N:272:VAL:HG13	1.89	0.54
11:M:151:TYR:CZ	13:N:426:LEU:HD13	2.42	0.54
4:F:358:ARG:NH1	4:F:359:ASP:OD1	2.40	0.54
3:E:90:ARG:NH2	4:F:135:GLU:OE1	2.37	0.54
2:D:191:GLU:O	2:D:194:THR:OG1	2.26	0.54
8:J:149:LEU:CG	13:N:25:MET:CE	2.86	0.54
8:J:137:TYR:CD1	13:N:66:LEU:HD11	2.43	0.53
4:F:145:ARG:NH1	4:F:149:GLU:OE2	2.42	0.53
12:L:598:MET:SD	13:N:223:PHE:CD1	3.01	0.53
8:J:73:MET:SD	9:A:67:LYS:HA	2.48	0.53
8:J:154:VAL:HG12	13:N:108:LEU:HD11	1.90	0.52
5:G:617:ASP:OD1	5:G:632:GLN:N	2.42	0.52
8:J:148:LEU:HD12	9:A:81:GLU:OE1	2.09	0.52
11:M:309:THR:OG1	11:M:372:ARG:NH1	2.41	0.52
5:G:843:ASN:ND2	5:G:877:LEU:O	2.42	0.51
8:J:134:PHE:CE1	9:A:99:GLY:HA2	2.45	0.51
12:L:117:PHE:O	12:L:121:ASN:ND2	2.43	0.51
11:M:343:ILE:HG23	11:M:406:GLY:HA2	1.92	0.51
1:B:219:GLU:OE1	2:D:370:ARG:NH2	2.44	0.51
4:F:191:GLU:OE2	4:F:198:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:27:ASP:OD1	4:F:28:GLU:N	2.43	0.51
5:G:145:SER:OG	5:G:207:THR:OG1	2.29	0.51
5:G:212:SER:O	6:I:79:LYS:NZ	2.43	0.51
8:J:50:PHE:CZ	9:A:87:ALA:HA	2.46	0.51
12:L:137:LEU:O	12:L:140:TYR:N	2.44	0.51
7:K:98:MET:HE3	13:N:229:ASP:HB3	1.92	0.51
8:J:120:ASP:OD1	8:J:121:GLY:N	2.42	0.50
12:L:591:LEU:HD11	13:N:162:LEU:CD2	2.41	0.50
8:J:149:LEU:HD21	13:N:25:MET:HE3	1.93	0.50
7:K:64:LEU:CD2	9:A:84:TYR:HE1	2.25	0.50
12:L:591:LEU:HD11	13:N:162:LEU:HD21	1.94	0.50
5:G:429:LEU:O	5:G:444:ALA:N	2.44	0.49
7:K:64:LEU:CD2	9:A:84:TYR:CE1	2.95	0.49
8:J:69:PHE:CE2	9:A:72:ALA:CB	2.95	0.49
8:J:50:PHE:HZ	9:A:87:ALA:HA	1.77	0.49
10:H:258:GLY:O	10:H:274:LYS:NZ	2.46	0.49
5:G:755:TRP:NE1	5:G:760:ASN:OD1	2.45	0.48
8:J:62:ALA:HB1	9:A:76:VAL:HA	1.96	0.48
11:M:463:ARG:NH2	11:M:464:GLU:OE2	2.47	0.48
8:J:54:LEU:CD2	9:A:83:LEU:HD21	2.44	0.48
8:J:156:PHE:CZ	9:A:120:ILE:HD12	2.49	0.47
8:J:134:PHE:CZ	9:A:98:VAL:HG13	2.48	0.47
8:J:139:LEU:HD11	13:N:11:LEU:HD11	1.97	0.47
8:J:149:LEU:CG	13:N:25:MET:HE3	2.45	0.47
12:L:324:GLY:O	12:L:326:GLN:NE2	2.48	0.47
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.97	0.47
2:D:231:LEU:CD1	2:D:238:ILE:HG23	2.44	0.46
8:J:106:VAL:HG12	12:L:606:LEU:HD13	1.95	0.46
9:A:75:PHE:CD2	10:H:154:LEU:HD12	2.49	0.46
8:J:130:GLY:HA3	9:A:91:SER:HB2	1.97	0.46
2:D:381:ASP:OD1	2:D:382:TRP:N	2.47	0.46
4:F:267:GLY:N	4:F:310:GLU:OE2	2.48	0.46
2:D:50:ARG:NH1	2:D:119:HIS:O	2.43	0.46
12:L:212:ASN:O	12:L:212:ASN:ND2	2.39	0.46
12:L:587:GLU:CD	13:N:287:MET:HE1	2.34	0.46
5:G:558:THR:OG1	5:G:560:ARG:NH2	2.47	0.46
7:K:75:ILE:HD13	13:N:140:PHE:HB3	1.97	0.46
4:F:362:PRO:HA	4:F:365:VAL:HG12	1.98	0.45
9:A:69:TYR:O	9:A:72:ALA:N	2.49	0.45
4:F:391:LEU:HD22	4:F:401:ALA:HB1	1.98	0.45
7:K:61:MET:SD	13:N:126:ALA:HB1	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:482:PRO:HD2	12:L:67:TRP:O	2.16	0.45
4:F:218:ASN:ND2	16:F:502:FMN:O2	2.44	0.45
10:H:214:GLN:HB2	10:H:215:PRO:HD3	1.99	0.45
12:L:126:SER:OG	12:L:146:VAL:N	2.49	0.45
2:D:551:MET:SD	5:G:707:HIS:ND1	2.88	0.45
8:J:148:LEU:CD1	9:A:81:GLU:OE1	2.65	0.45
13:N:357:ASP:OD1	13:N:357:ASP:N	2.46	0.45
8:J:62:ALA:O	9:A:76:VAL:HG22	2.17	0.44
7:K:53:TRP:CH2	13:N:182:GLY:HA2	2.52	0.44
2:D:231:LEU:HD11	2:D:238:ILE:HG23	1.99	0.44
12:L:580:GLY:CA	13:N:286:LEU:HB3	2.43	0.44
7:K:67:SER:HB3	8:J:148:LEU:HD21	2.00	0.44
11:M:399:PRO:CG	12:L:141:LEU:HG	2.48	0.44
12:L:609:LEU:CD2	13:N:268:ALA:C	2.86	0.44
8:J:58:VAL:CG1	9:A:80:VAL:HG22	2.48	0.44
7:K:53:TRP:CZ2	13:N:182:GLY:HA2	2.53	0.43
8:J:154:VAL:CG1	13:N:108:LEU:CD2	2.95	0.43
12:L:605:VAL:CG1	13:N:272:VAL:HG11	2.38	0.43
3:E:92:CYS:CB	15:E:201:FES:S2	3.03	0.43
8:J:148:LEU:HD13	9:A:81:GLU:CD	2.39	0.43
4:F:138:GLU:HA	4:F:141:VAL:HG12	2.00	0.43
11:M:237:VAL:HG12	11:M:238:VAL:H	1.83	0.43
5:G:436:ASP:N	5:G:436:ASP:OD1	2.51	0.43
12:L:609:LEU:HD23	13:N:268:ALA:C	2.38	0.43
13:N:33:ASN:O	13:N:37:ASN:ND2	2.52	0.43
7:K:97:GLU:HG2	7:K:98:MET:H	1.83	0.42
13:N:200:GLU:OE2	13:N:203:LEU:N	2.51	0.42
13:N:242:LEU:O	13:N:247:LYS:NZ	2.53	0.42
8:J:54:LEU:CG	9:A:83:LEU:HD21	2.49	0.42
5:G:623:ASN:OD1	5:G:624:GLU:N	2.52	0.42
2:D:556:ARG:NH1	2:D:557:VAL:O	2.53	0.42
11:M:82:ALA:HB3	11:M:134:ILE:HG13	2.01	0.42
8:J:134:PHE:HE1	9:A:99:GLY:HA2	1.84	0.41
9:A:112:ALA:HB1	13:N:26:LEU:CD2	2.50	0.41
2:D:341:LYS:O	2:D:344:ASP:OD1	2.38	0.41
7:K:68:LEU:HD22	13:N:133:GLU:HG3	2.03	0.41
8:J:69:PHE:CE2	9:A:72:ALA:HB1	2.48	0.41
11:M:127:VAL:HG11	11:M:262:ILE:HG13	2.03	0.41
2:D:352:PHE:HB2	6:I:45:ARG:HE	1.85	0.41
5:G:235:CYS:CB	14:G:1004:SF4:S1	2.99	0.41
4:F:94:MET:O	4:F:94:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:483:GLN:CD	12:L:69:SER:HG	2.23	0.41
5:G:33:PHE:O	5:G:156:ARG:NE	2.52	0.41
11:M:137:PHE:HE1	13:N:396:PHE:CE1	2.39	0.41
8:J:149:LEU:HD21	13:N:25:MET:CE	2.50	0.41
11:M:168:ILE:HD11	13:N:423:TYR:OH	2.20	0.41
11:M:300:TYR:OH	12:L:563:ASP:OD1	2.28	0.41
13:N:221:VAL:O	13:N:224:HIS:ND1	2.54	0.41
12:L:51:ASP:O	12:L:55:ASN:N	2.53	0.41
8:J:53:ALA:HB1	10:H:117:LEU:HB3	2.02	0.40
5:G:55:ASN:OD1	5:G:55:ASN:N	2.54	0.40
12:L:78:ASN:HB2	12:L:134:ASP:HB3	2.03	0.40
13:N:137:LEU:HA	13:N:140:PHE:HD2	1.86	0.40
4:F:425:GLN:OE1	4:F:425:GLN:N	2.54	0.40
5:G:511:GLN:OE1	5:G:798:SER:OG	2.40	0.40
8:J:149:LEU:HD21	13:N:25:MET:SD	2.61	0.40
11:M:303:TRP:CD1	12:L:553:PHE:HE1	2.40	0.40
12:L:232:GLN:HG3	12:L:233:LEU:H	1.86	0.40
13:N:221:VAL:CG1	13:N:222:PRO:HD3	2.51	0.40
13:N:292:THR:O	13:N:358:SER:OG	2.34	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	152/220 (69%)	142 (93%)	10 (7%)	0	100	100
2	D	586/596 (98%)	569 (97%)	17 (3%)	0	100	100
3	E	153/166 (92%)	150 (98%)	3 (2%)	0	100	100
4	F	438/445 (98%)	430 (98%)	8 (2%)	0	100	100
5	G	905/908 (100%)	886 (98%)	19 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	I	156/180 (87%)	154 (99%)	2 (1%)	0	100	100
7	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
8	J	162/184 (88%)	154 (95%)	8 (5%)	0	100	100
9	A	88/147 (60%)	84 (96%)	4 (4%)	0	100	100
10	H	268/325 (82%)	252 (94%)	16 (6%)	0	100	100
11	M	502/509 (99%)	485 (97%)	17 (3%)	0	100	100
12	L	610/613 (100%)	576 (94%)	34 (6%)	0	100	100
13	N	461/485 (95%)	447 (97%)	14 (3%)	0	100	100
All	All	4579/4878 (94%)	4425 (97%)	154 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	126/191 (66%)	126 (100%)	0	100	100
2	D	500/515 (97%)	494 (99%)	6 (1%)	71	83
3	E	128/138 (93%)	126 (98%)	2 (2%)	62	79
4	F	354/358 (99%)	352 (99%)	2 (1%)	86	91
5	G	735/736 (100%)	728 (99%)	7 (1%)	76	86
6	I	126/154 (82%)	125 (99%)	1 (1%)	81	89
7	K	79/79 (100%)	79 (100%)	0	100	100
8	J	129/146 (88%)	129 (100%)	0	100	100
9	A	55/119 (46%)	55 (100%)	0	100	100
10	H	190/269 (71%)	188 (99%)	2 (1%)	73	85
11	M	413/418 (99%)	412 (100%)	1 (0%)	93	97
12	L	322/486 (66%)	314 (98%)	8 (2%)	47	72
13	N	371/385 (96%)	366 (99%)	5 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3528/3994 (88%)	3494 (99%)	34 (1%)	77 86

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	24	GLU
2	D	63	LEU
2	D	107	ILE
2	D	385	LYS
2	D	417	GLU
2	D	558	ARG
3	E	86	ARG
3	E	87	HIS
4	F	16	ARG
4	F	434	ASN
5	G	186	ASP
5	G	527	VAL
5	G	537	ASN
5	G	549	LEU
5	G	572	HIS
5	G	681	PRO
5	G	904	LYS
6	I	45	ARG
10	H	183	GLN
10	H	210	HIS
11	M	495	ASN
12	L	80	VAL
12	L	137	LEU
12	L	198	ARG
12	L	212	ASN
12	L	258	MET
12	L	342	LYS
12	L	562	ARG
12	L	600	ILE
13	N	125	LEU
13	N	134	LEU
13	N	174	MET
13	N	187	VAL
13	N	369	ARG

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

Mol	Chain	Res	Type
11	M	206	ASN
11	M	416	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	CSX	B	102	1	3,6,7	0.91	0	1,6,8	0.66	0
4	CSX	F	215	4	3,6,7	0.62	0	1,6,8	0.40	0
3	CSX	E	132	3	3,6,7	0.89	0	1,6,8	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSX	B	102	1	-	0/1/5/7	-
4	CSX	F	215	4	-	1/1/5/7	-
3	CSX	E	132	3	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	132	CSX	N-CA-CB-SG
4	F	215	CSX	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
15	FES	G	1001	5	0,4,4	-	-	-		
14	SF4	G	1002	5	0,12,12	-	-	-		
14	SF4	B	301	1	0,12,12	-	-	-		
14	SF4	F	501	4	0,12,12	-	-	-		
14	SF4	G	1004	5	0,12,12	-	-	-		
16	FMN	F	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.36	8 (16%)
14	SF4	I	202	6	0,12,12	-	-	-		
14	SF4	I	201	6	0,12,12	-	-	-		
15	FES	E	201	3	0,4,4	-	-	-		
14	SF4	G	1003	5	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FES	G	1001	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	G	1002	5	-	-	0/6/5/5
14	SF4	B	301	1	-	-	0/6/5/5
14	SF4	F	501	4	-	-	0/6/5/5
14	SF4	G	1004	5	-	-	0/6/5/5
14	SF4	I	202	6	-	-	0/6/5/5
14	SF4	I	201	6	-	-	0/6/5/5
16	FMN	F	502	-	-	1/18/18/18	0/3/3/3
15	FES	E	201	3	-	-	0/1/1/1
14	SF4	G	1003	5	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	F	502	FMN	C4A-N5	3.54	1.37	1.30
16	F	502	FMN	C10-N1	2.41	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	F	502	FMN	C4-N3-C2	-3.34	119.46	125.64
16	F	502	FMN	C4A-C10-N10	2.92	120.76	116.48
16	F	502	FMN	C4A-C4-N3	2.72	120.10	113.19
16	F	502	FMN	C4A-C10-N1	-2.71	118.45	124.73
16	F	502	FMN	O4-C4-C4A	-2.50	119.97	126.60
16	F	502	FMN	C10-C4A-N5	-2.25	120.09	124.86
16	F	502	FMN	C4-C4A-C10	2.24	120.56	116.79
16	F	502	FMN	C10-N1-C2	2.05	121.00	116.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	F	502	FMN	C4'-C5'-O5'-P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1004	SF4	1	0
16	F	502	FMN	1	0
15	E	201	FES	1	0

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

Ligand FMN F 502

Bond lengths

Bond angles

Torsions

Rings
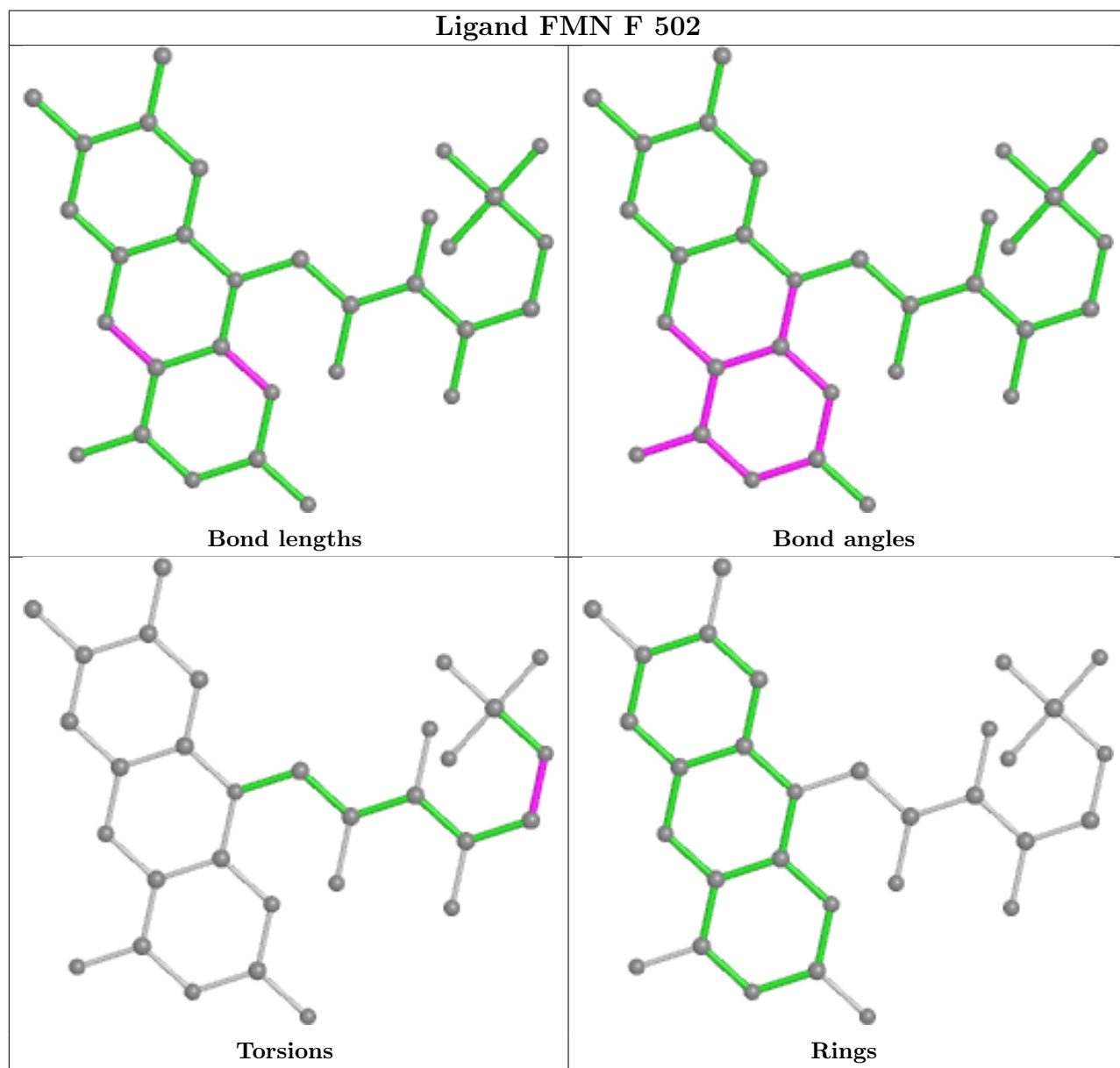
5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-12653. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

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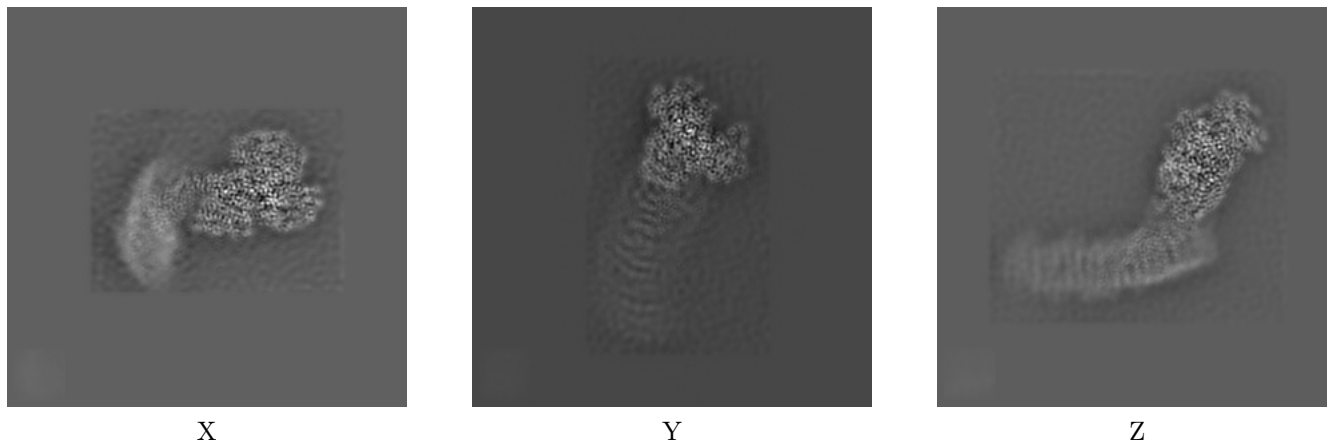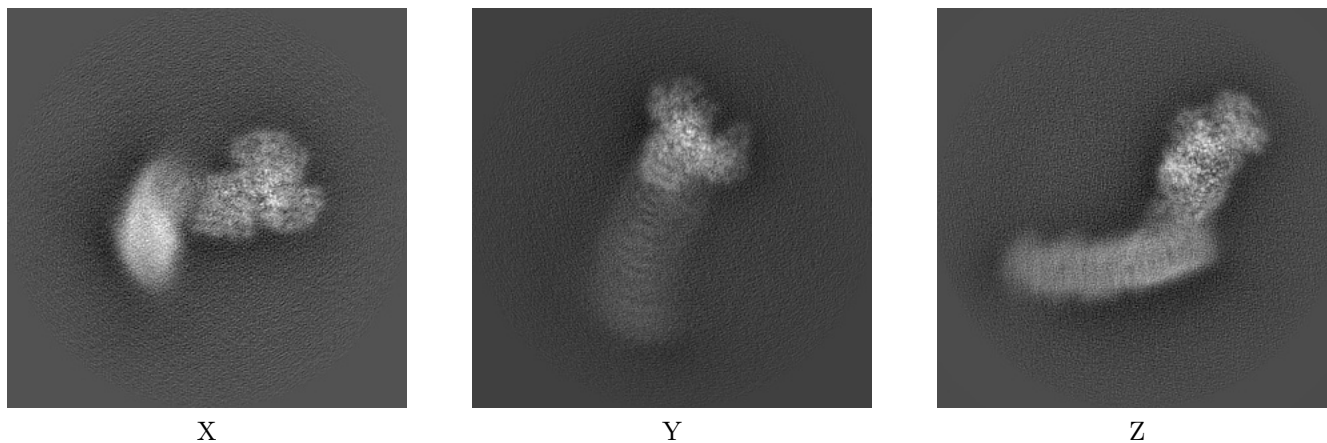
The images above show the map projected in three orthogonal directions.

6.2　Central slices　ⓘ
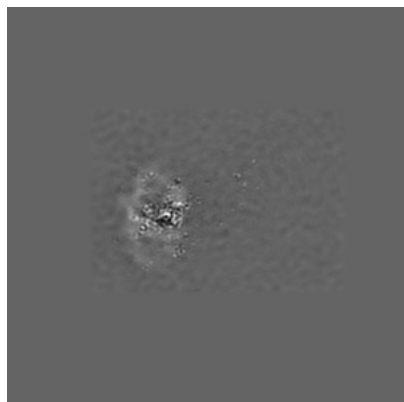
6.2.1　Primary map
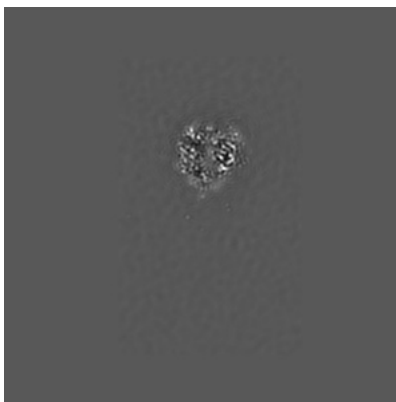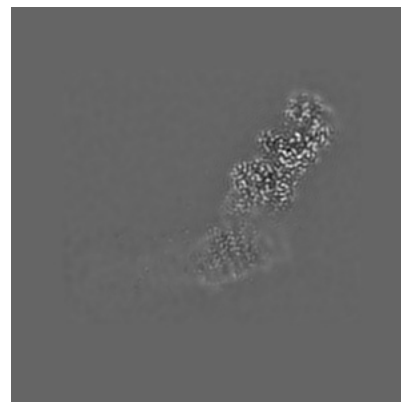
X Index: 160　　　　　　　Y Index: 160　　　　　　　Z Index: 160

6.2.2　Raw map
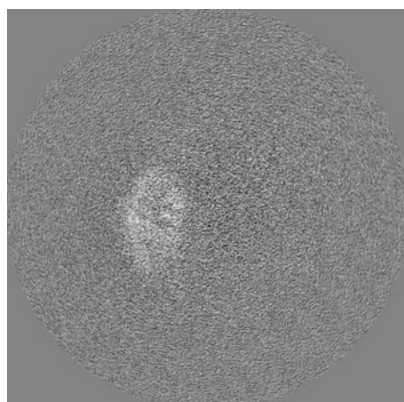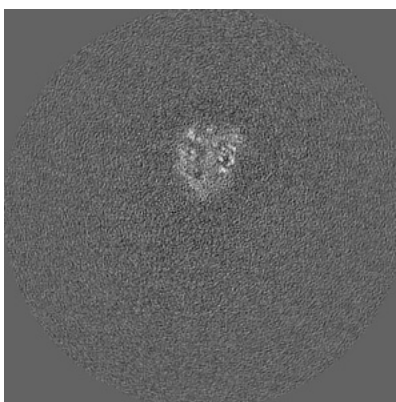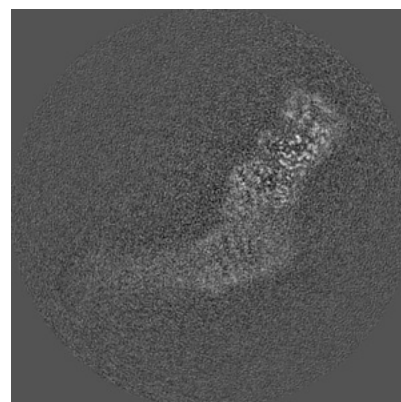
X Index: 160　　　　　　　Y Index: 160　　　　　　　Z Index: 160

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
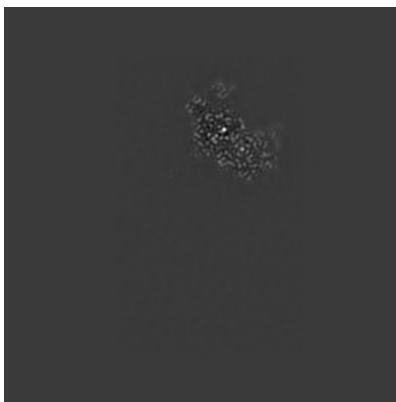
| X Index: 221 | Y Index: 206 | Z Index: 175 |
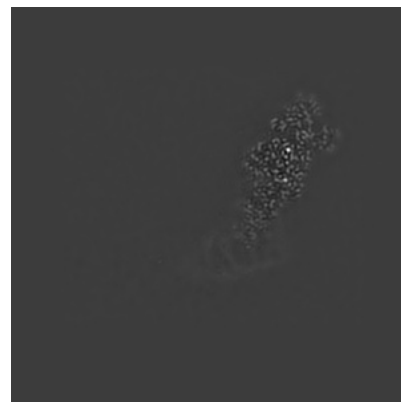
6.3.2 Raw map
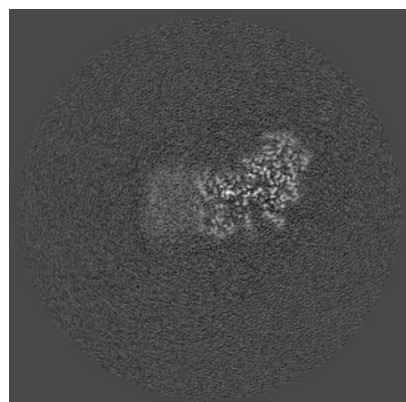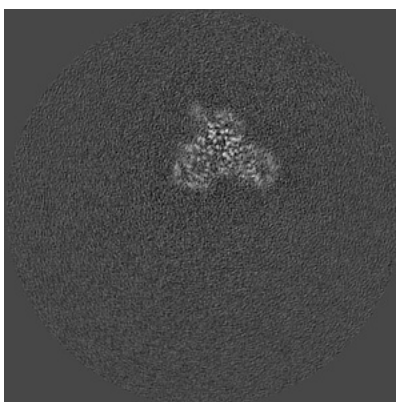
| X Index: 210 | Y Index: 190 | Z Index: 172 |
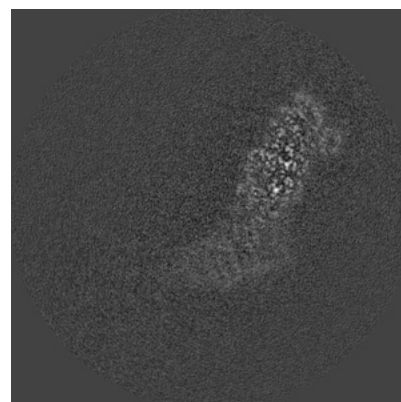
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
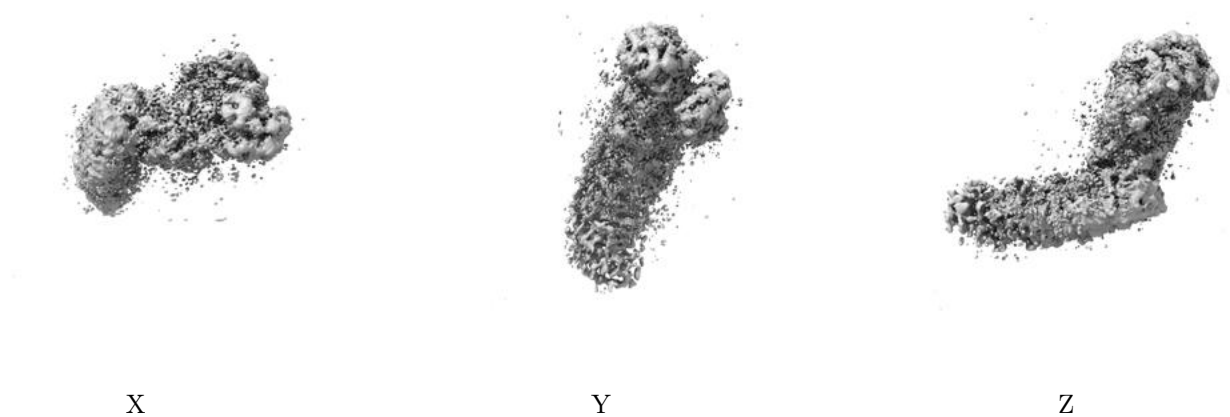
The images above show the 3D surface view of the map at the recommended contour level 1.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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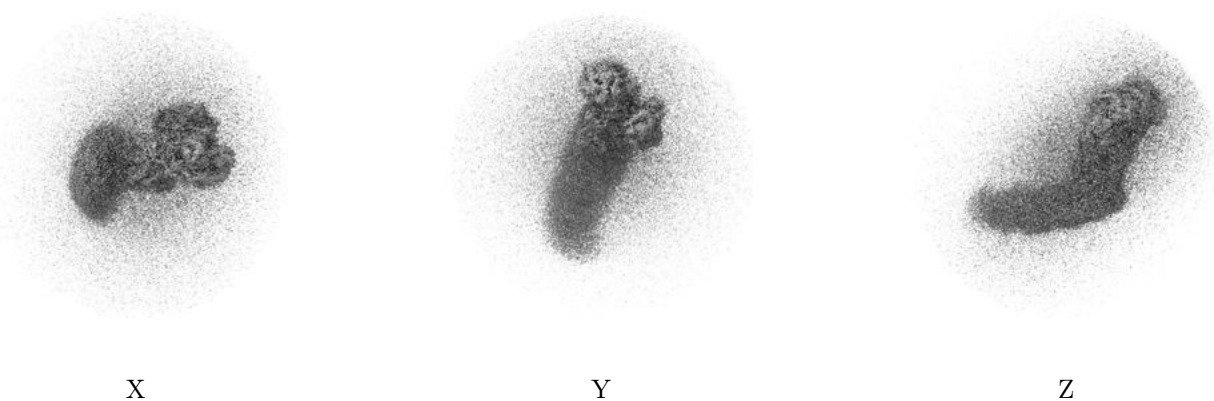
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

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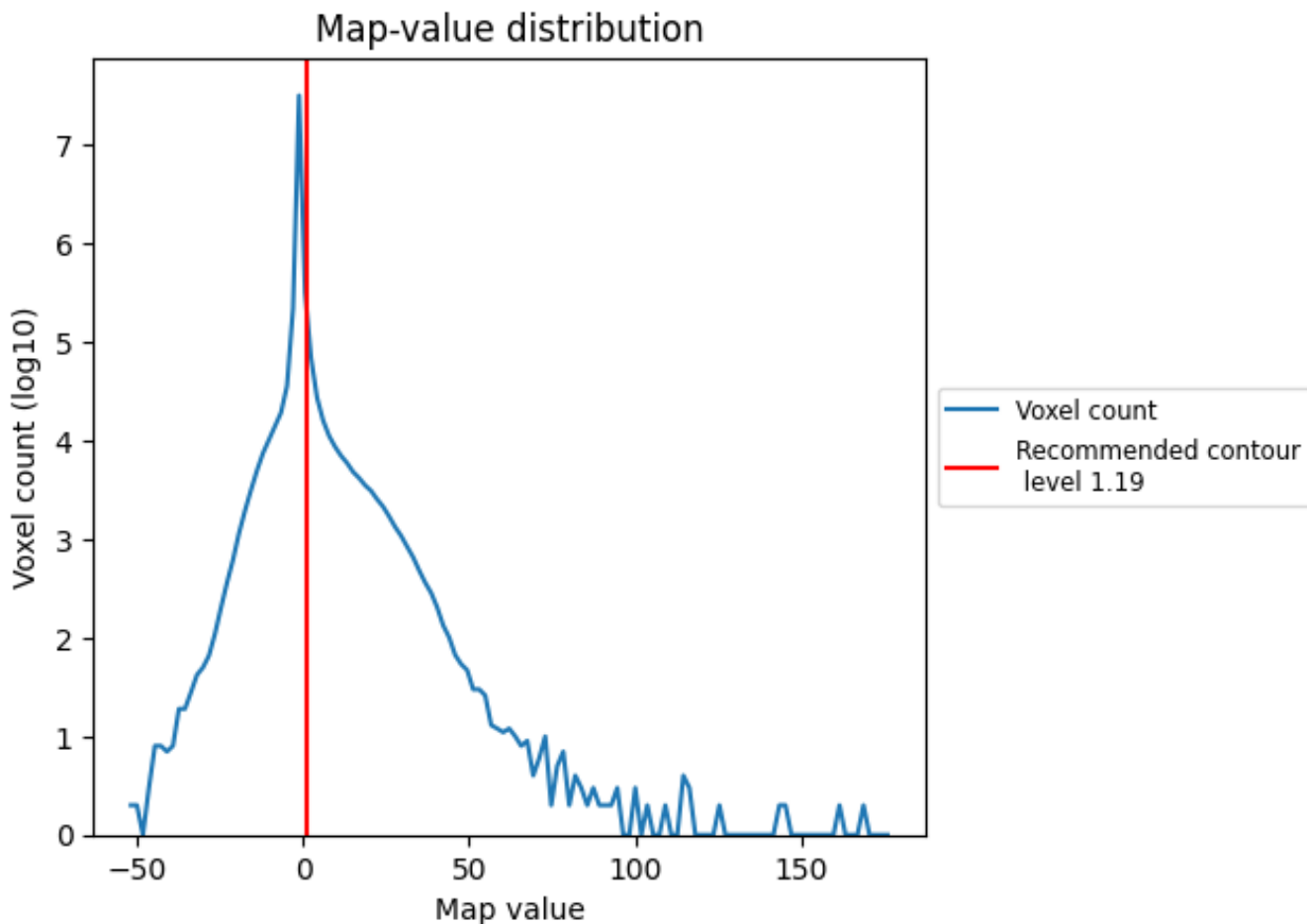
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
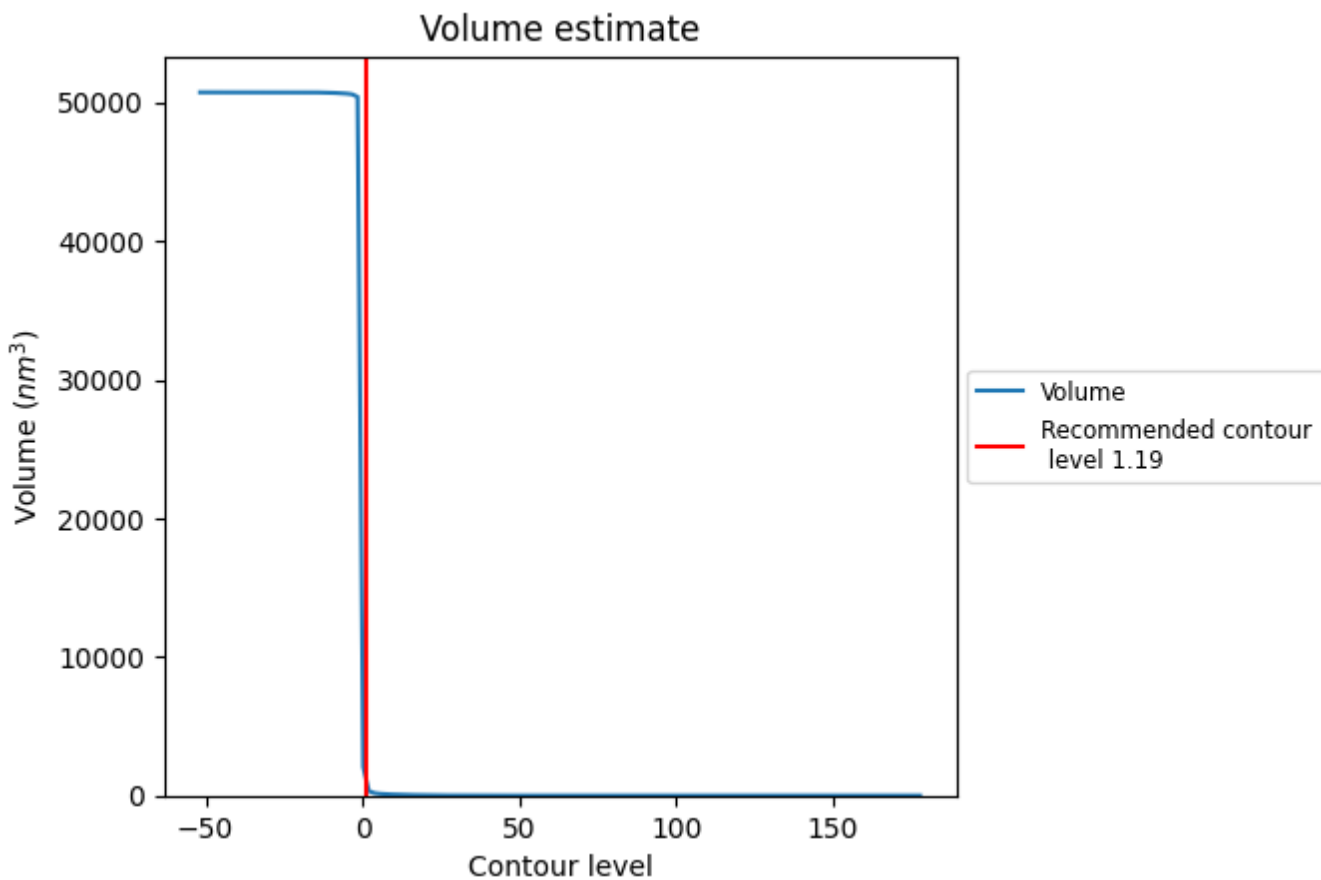
The volume at the recommended contour level is 1164 nm^3; this corresponds to an approximate mass of 1052 kDa.

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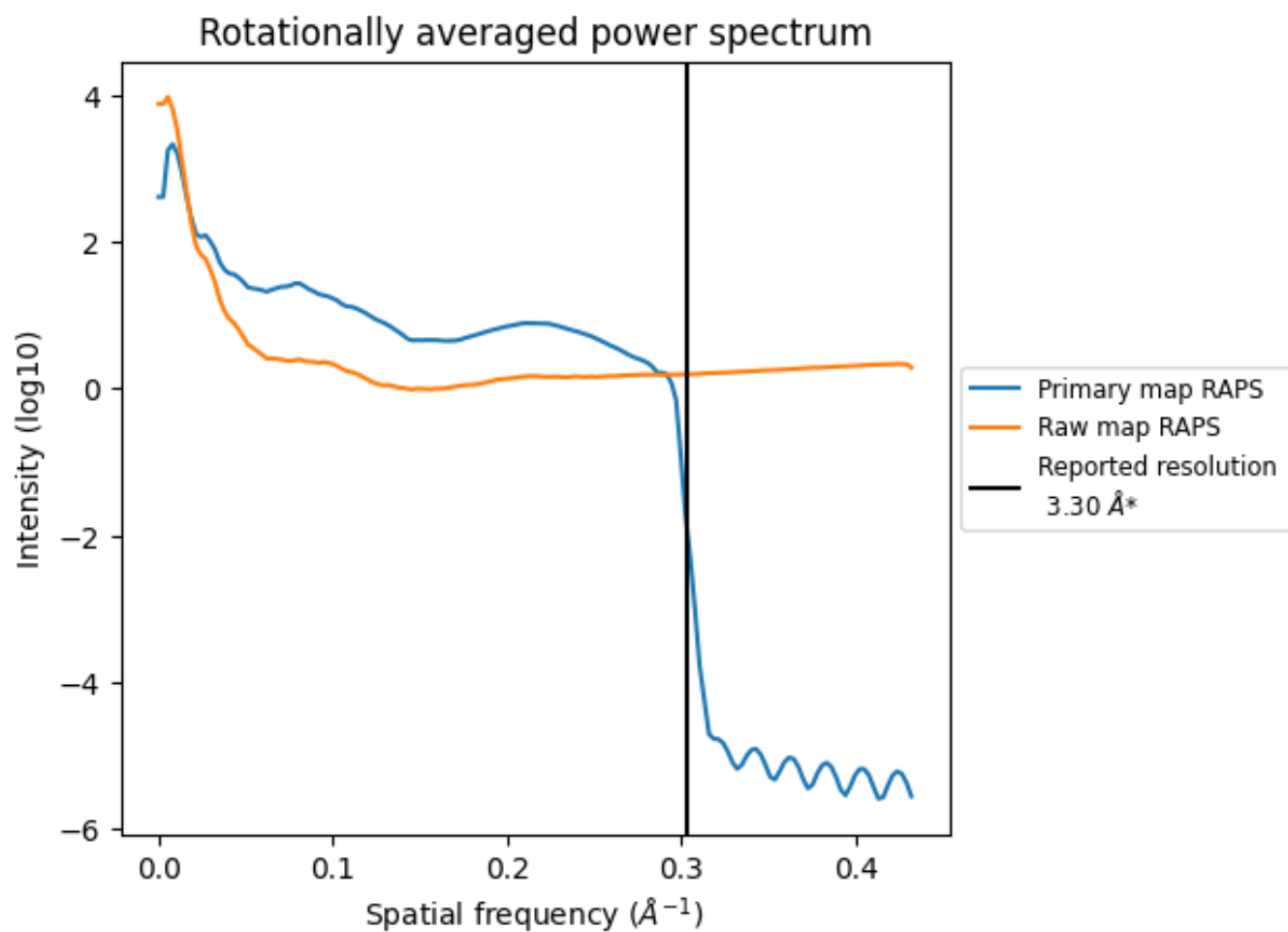
*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation ⓘ

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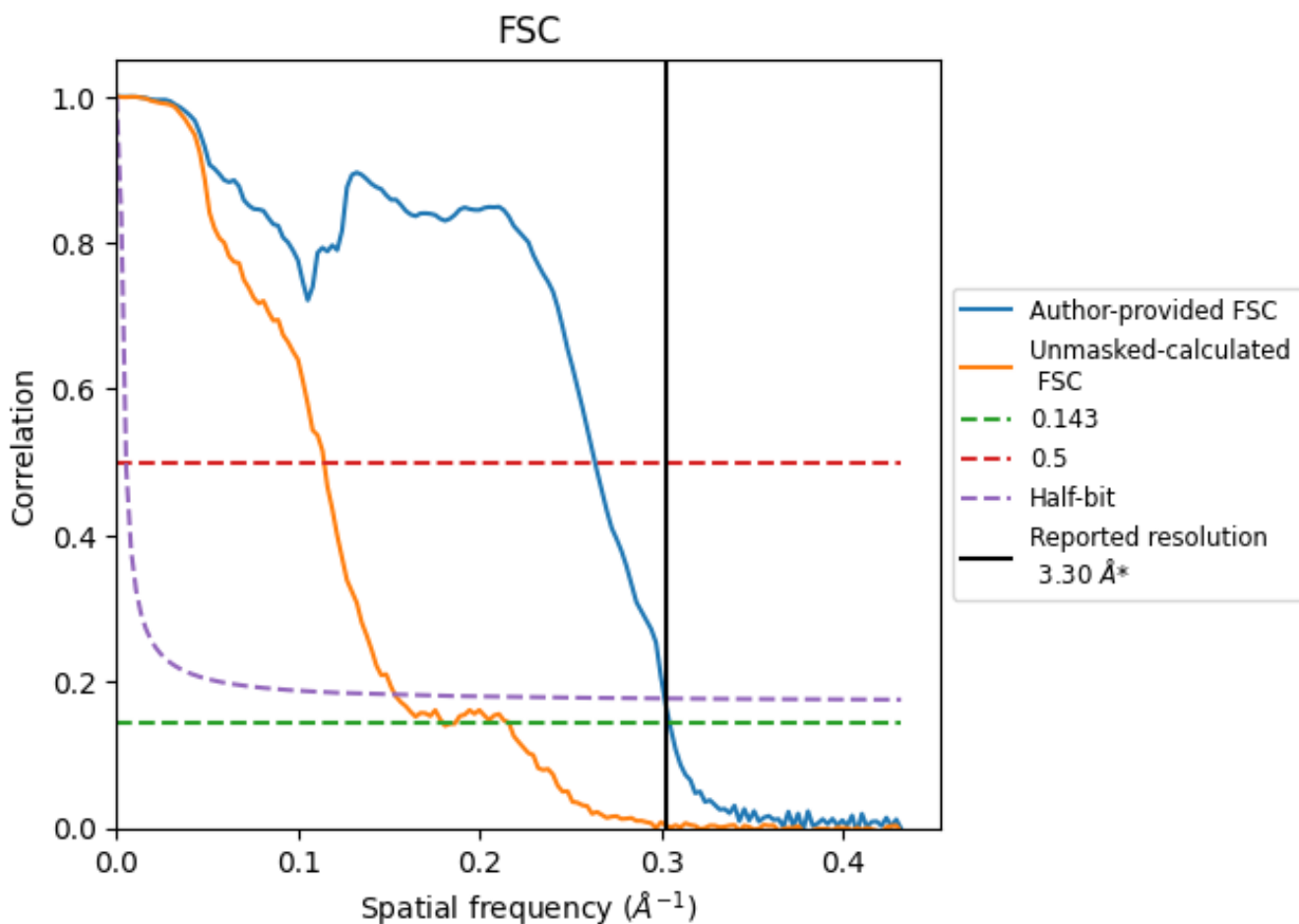
*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.79	3.31
Unmasked-calculated*	5.56	8.75	6.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.56 differs from the reported value 3.3 by more than 10 %

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-12653 and PDB model 7NYR. Per-residue inclusion information can be found in section 3 on page 9.

9.1　Map-model overlay ⓘ

X　　　　　　　　　　　　　　　Y　　　　　　　　　　　　　　　Z
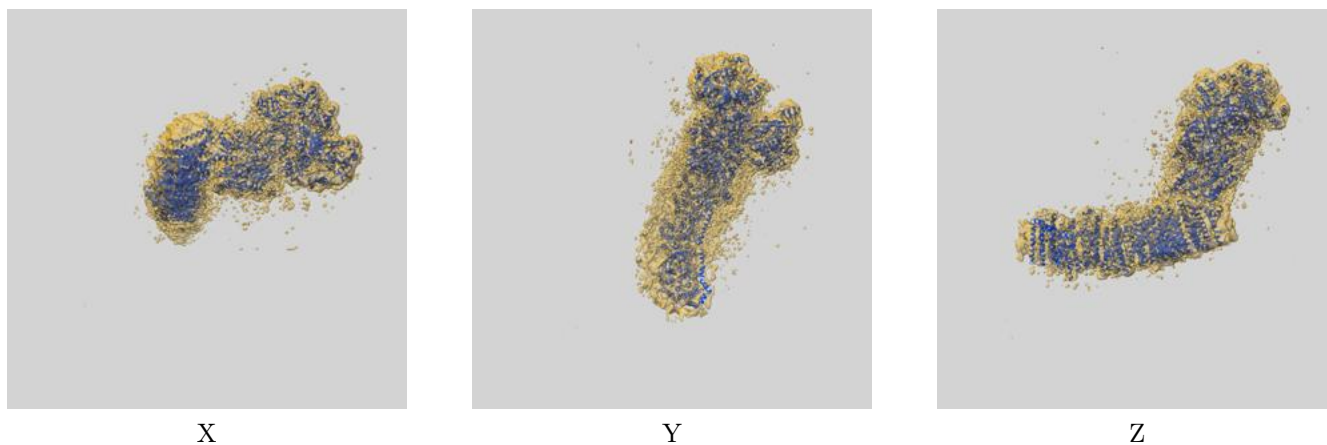
The images above show the 3D surface view of the map at the recommended contour level 1.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
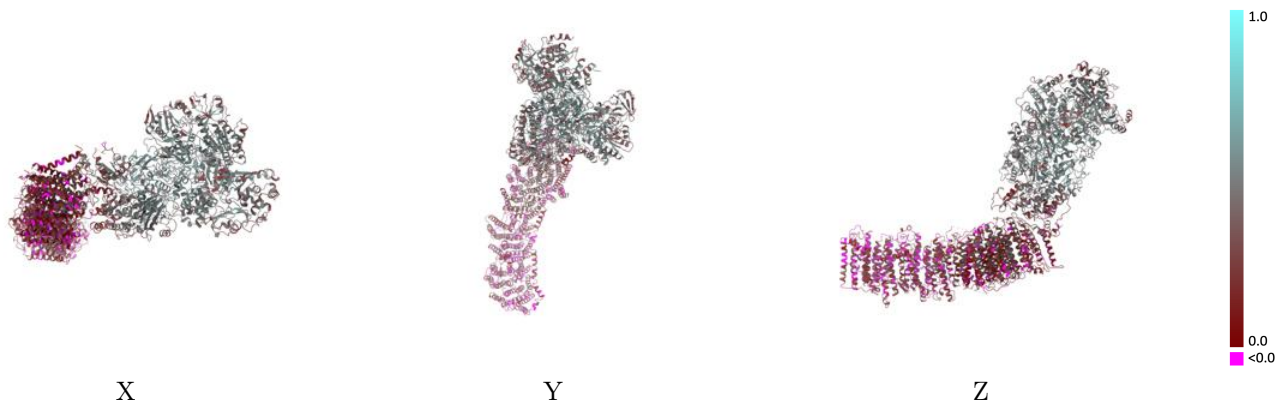
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
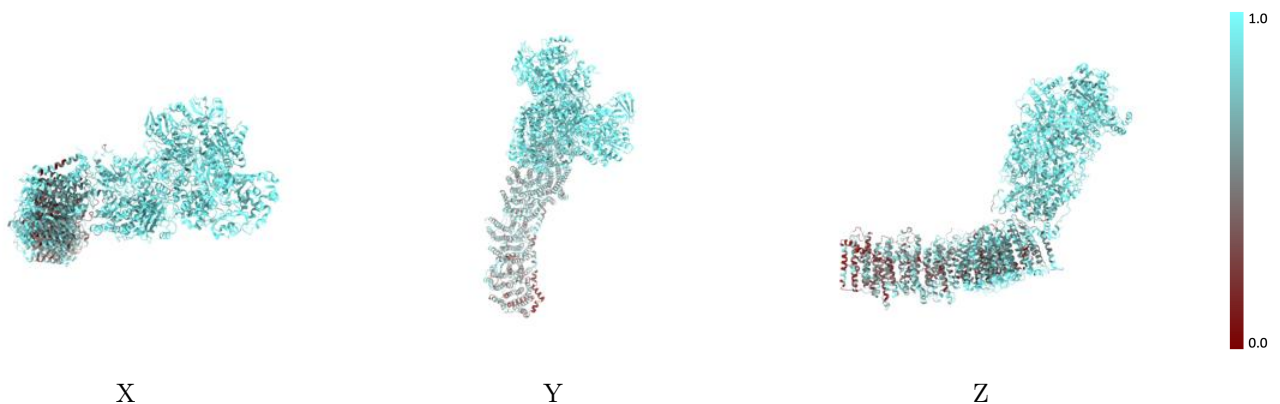
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.19).

9.4 Atom inclusion ⓘ
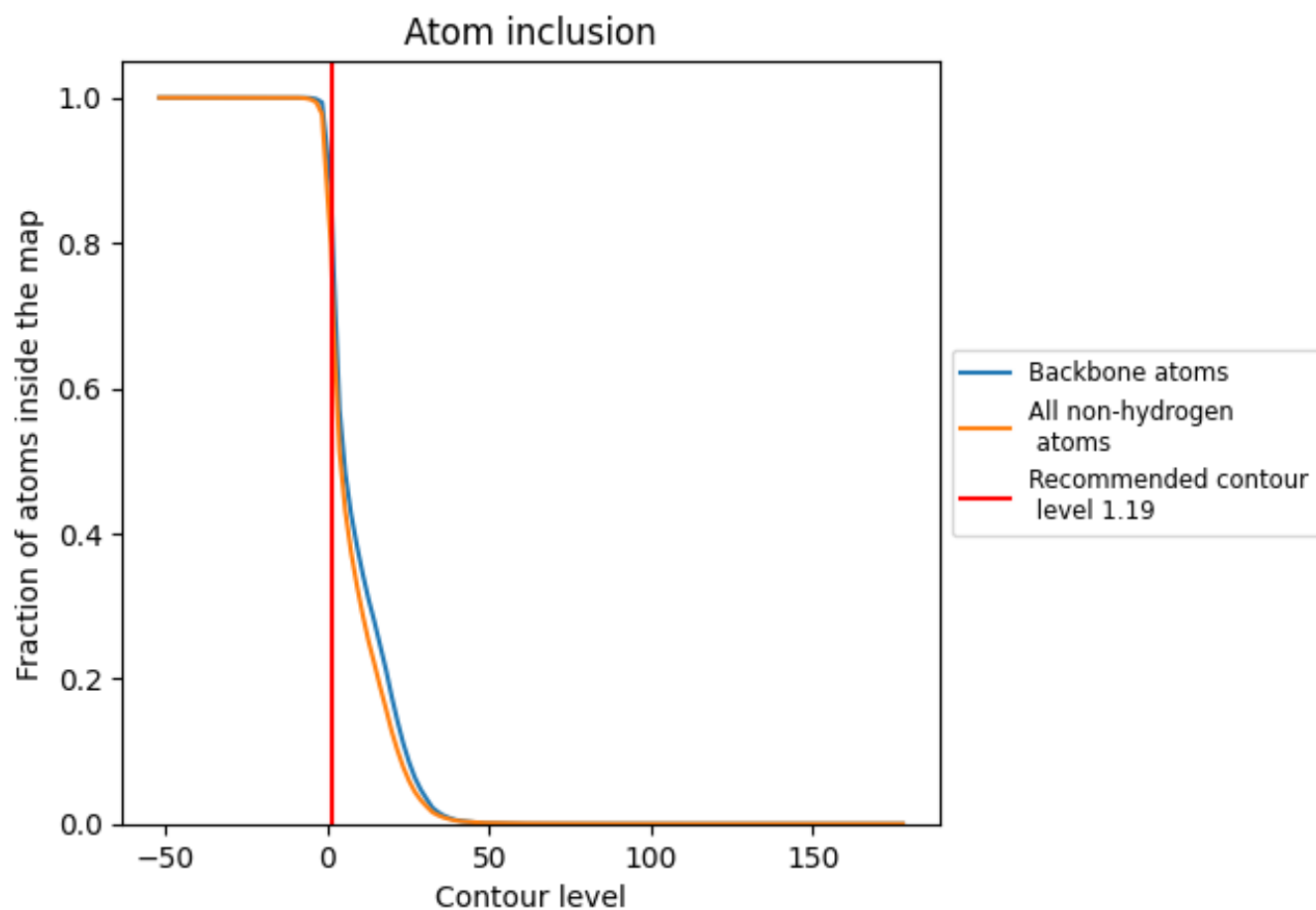
At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7963	0.3080
A	0.6697	0.1690
B	0.8774	0.3820
D	0.9084	0.4240
E	0.9368	0.4480
F	0.9389	0.4580
G	0.9469	0.4910
H	0.7357	0.2140
I	0.9420	0.4850
J	0.7480	0.1940
K	0.7383	0.2050
L	0.5023	0.0790
M	0.6260	0.0920
N	0.7058	0.1520

1.0

0.0
<0.0