Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 07:53 AM EST

PDB ID	:	7JMN
EMDB ID	:	EMD-22397
Title	:	Tail module of Mediator complex
Authors	:	Zhang, H.Q.; Chen, D.C.
Deposited on	:	2020-08-02
Resolution	:	3.58 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

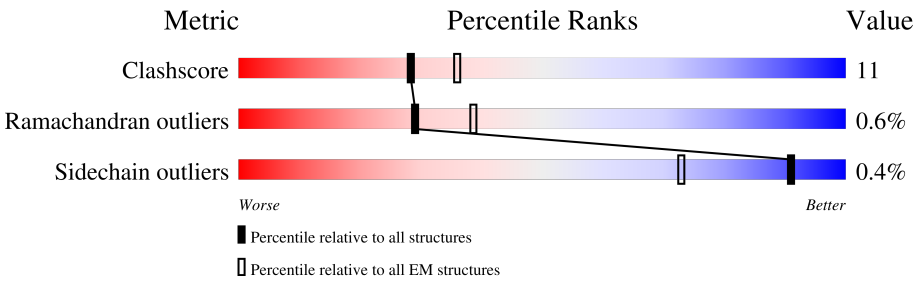
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.58 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	E	1099	42% 11% 47%
2	N	1168	14% • 83%
3	P	1130	52% 19% 28%
4	O	1625	8% • 90%
5	X	52	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13633 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 Mediator of RNA polymerase II transcription subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	584	4467	2851	745	846	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	228	ILE	LEU	conflict	UNP G0SGD2

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	N	198	1439	905	272	260	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	822	ASP	GLN	conflict	UNP G0SCL5
N	908	GLN	GLU	conflict	UNP G0SCL5

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	P	810	6178	3911	1074	1167	26	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	180	PRO	LEU	conflict	UNP G0SEV7
P	327	TRP	GLY	conflict	UNP G0SEV7

- Molecule 4 is a protein called MED15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	164	1290	788	248	245	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	117	LYS	ALA	conflict	UNP G0SHL5
O	308	GLU	GLN	conflict	UNP G0SHL5

- Molecule 5 is a protein called Unknown peptide.

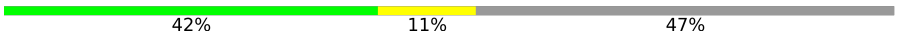
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	X	52	259	155	52	52	0	0

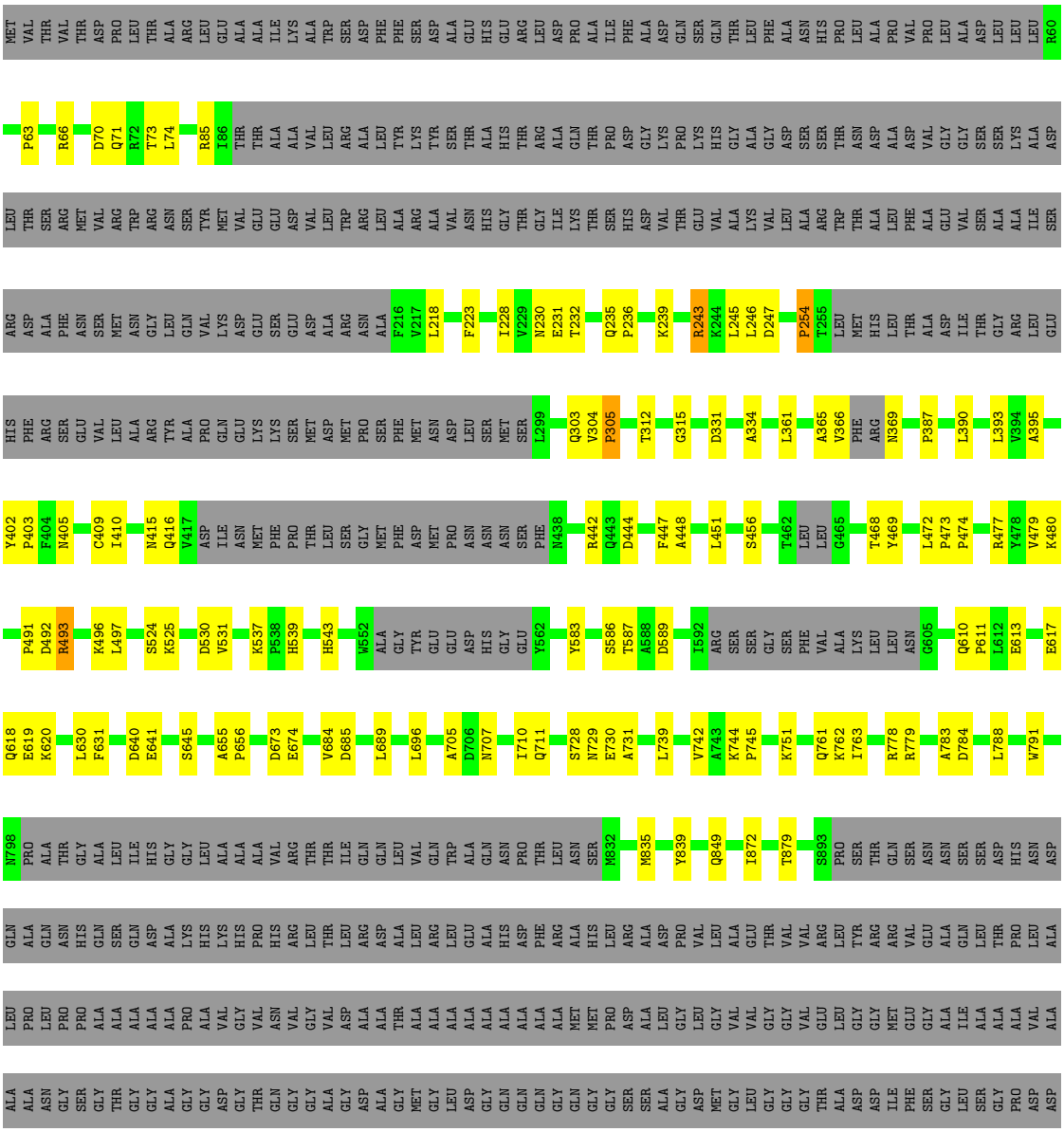
3 Residue-property plots (i)

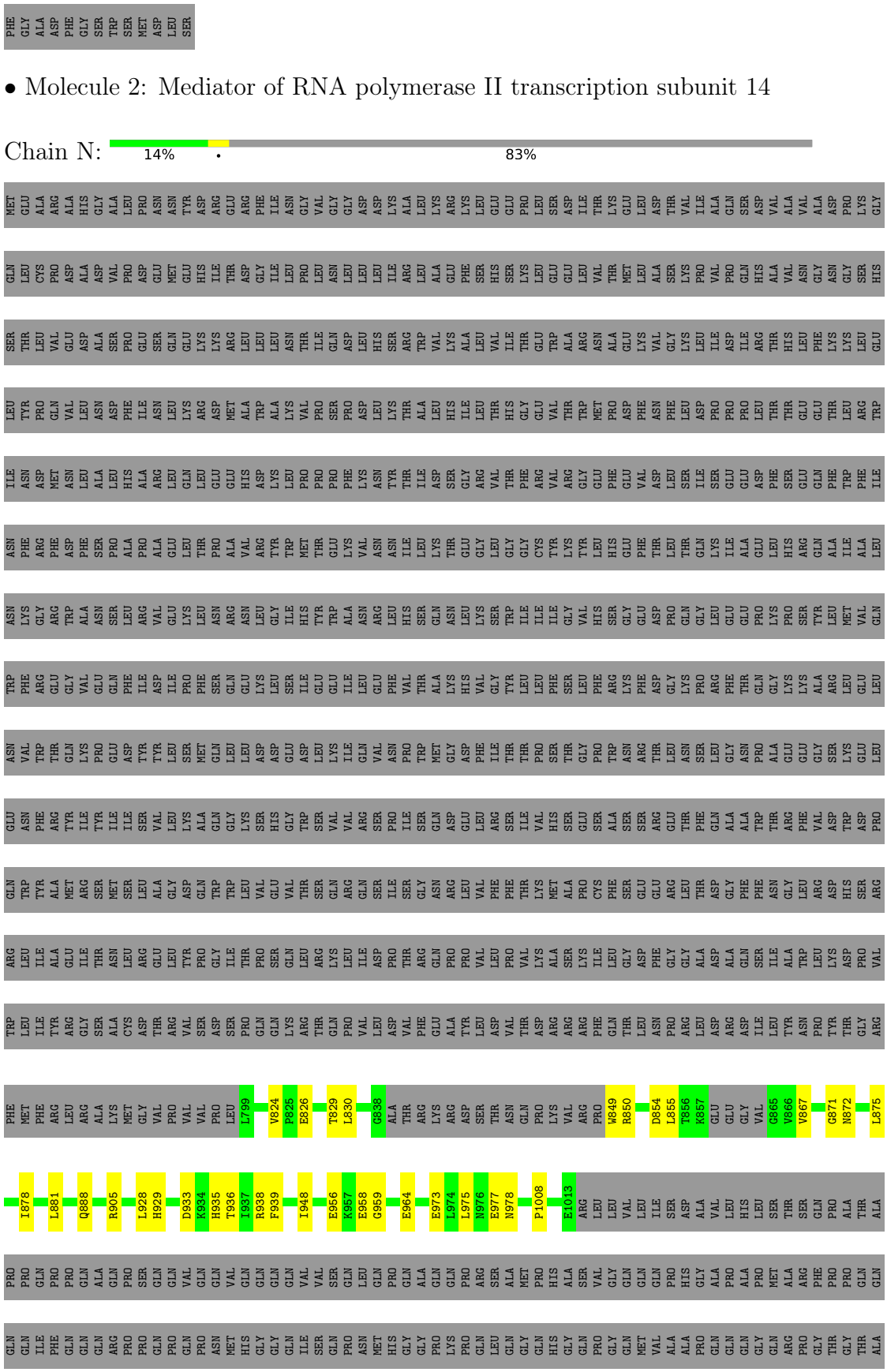
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

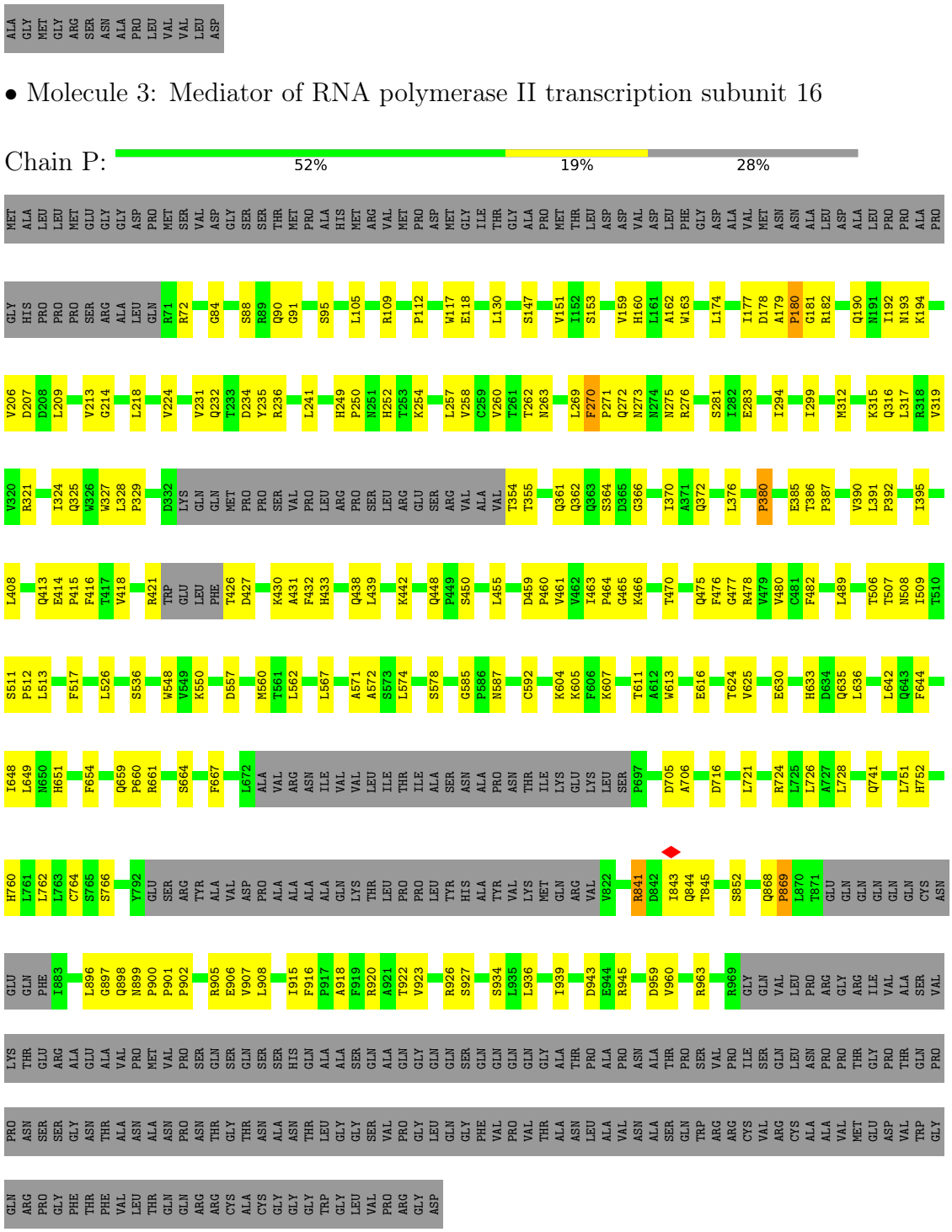
- Molecule 1: Mediator of RNA polymerase II transcription subunit 5

Chain E:






PHE GLY ALA ASP PHE GLY SER TRP SER MET ASP LEU SER
• Molecule 2: Mediator of RNA polymerase II transcription subunit 14
Chain N:
14%
83%
MET GLU ALA ARG ALA HIS GLY ALA LEU PRO ASN ASN TYR ASP ARG GLU ARG PHE ILE ASN GLY VAL GLY GLY ASP ASP LYS ALA LEU LYS ARG LYS LEU GLU GLU PRO LEU SER ASP ILE THR LYS GLU LEU ASP THR VAL ILE ALA GLN SER ASP VAL ALA VAL ALA ASP PRO LYS GLY
GLN LEU CYS PRO ASP ALA ASP VAL PRO ASP GLU MET GLU HIS ILE THR ASP GLY ILE LEU ASN PRO LEU ASN LEU LEU LEU ILE ARG LEU ALA GLU PHE SER HIS SER LYS LEU GLU GLU LEU VAL THR MET LEU ALA SER LYS PRO VAL PRO GLN HIS ALA VAL ASN GLY ASN GLY SER HIS
SER THR LEU VAL GLU ASP ALA SER PRO GLU SER GLN GLU LYS LYS ARG LEU LEU LEU ASN THR ILE GLN ASP LEU HIS SER ARG TRP VAL LYS ALA LEU VAL ILE THR GLU TRP ALA ARG ASN ALA GLU LYS VAL GLY LYS LEU ILE ASP ILE ARG THR HIS LEU PHE LYS LYS LYS LEU GLU
LEU TYR PRO GLN VAL LEU ASN ASP PHE ILE ASN LEU LYS ARG ASP MET ALA TRP ALA LYS VAL PRO SER PRO ASP LEU LYS THR ALA LEU HIS ILE LEU THR HIS GLY GLU VAL THR TRP MET PRO ASP PHE ASN PHE LEU ASP PRO PRO PRO LEU THR THR GLU GLU GLU THR LEU ARG TRP
ILE ASN ASP MET ASN LEU ALA LEU HIS ALA ARG LEU GLN LEU GLU GLU HIS ASP LYS LEU PRO PRO PRO PHE LYS ASN TYR THR ILE ASP SER GLY ARG VAL THR PHE ARG VAL ARG GLY GLU PHE GLU VAL ASP LEU SER ILE SER GLU GLU ASP PHE SER GLU GLN PHE PHE ILE
ASN PHE ARG PHE ASP PHE SER PRO ALA PRO ALA GLU LEU THR PRO ALA VAL ARG TYR TRP MET THR GLU LYS VAL ASN ASN TYR LEU ILE LEU LYS THR GLU GLY LEU GLY GLY CYS TYR LYS TYR LEU HIS GLU PHE THR LEU THR GLN LYS ILE ALA GLU LEU GLN ALA ILE ALA LEU
ASN LYS GLY ARG TRP ALA ASN SER LEU ARG VAL GLU LYS LEU ASN ARG ASN LEU GLY ILE HIS TYR TRP ALA ASN ARG LEU HIS SER GLN ASN LEU LYS SER TRP ILE ILE GLY VAL HIS SER GLY GLU ASP PRO GLN GLY LEU GLU GLU PRO LYS PRO SER TYR LEU MET VAL GLN
TRP PHE ARG GLU GLY VAL GLU GLN PHE ILE ASP ILE PRO PHE SER GLN GLU LYS LEU SER ILE GLU GLU ILE LEU GLU PHE VAL THR ALA LYS HIS VAL GLY TYR LEU LEU PHE SER LEU PHE ARG LYS PHE ASP GLY LYS PRO ARG PHE THR GLN GLY LYS LYS ALA ARG LEU GLU LEU
ASN VAL TRP THR GLN LYS PRO GLU ASP TYR TYR LEU SER MET GLN LEU LEU ASP ASP GLU ASP LEU LYS ILE GLN VAL ASN PRO TRP MET GLY ASP PHE ILE THR THR PRO SER THR GLY PRO TRP ASN ARG THR LEU ASN SER LEU GLY GLN GLU GLU GLY SER LYS GLU LEU
GLU ASN PHE ARG TYR ILE TYR ILE ILE SER VAL LEU LYS ALA GLN GLY LYS SER HIS GLY TRP SER VAL VAL ARG SER PRO ILE SER SER GLN ASP GLU LEU ARG SER ILE VAL HIS SER GLU SER ALA SER SER ARG GLU THR PHE GLN ALA ALA TRP THR ARG PHE VAL ASP PRO
GLN TRP TYR ALA MET ARG SER MET SER LEU ALA GLY ASP GLN TRP TRP LEU VAL GLU VAL THR SER GLN ARG GLN SER ILE SER GLY ASN ARG LEU VAL PHE PHE THR LYS MET ALA PRO CYS PHE SER GLU GLU ARG LEU THR ASP GLY PHE PHE ASN GLY LEU ARG ASP
ARG LEU ILE ALA GLU ILE THR ASN LEU ARG GLU LEU TYR PRO GLY ILE THR PRO SER GLN LYS LEU ILE ASP PRO THR ARG GLN PRO PRO VAL LEU PRO VAL LYS ALA SER LYS ILE LEU GLY ASP PHE GLY GLY ALA ASP ALA GLN SER ILE ALA TRP THR LEU ARG ASP PRO VAL
TRP LEU ILE TYR ARG GLY SER ALA CYS ASP THR ARG VAL SER ASP SER PRO GLN GLN LYS ARG THR GLN PRO VAL LEU ASP VAL PHE GLU ALA TYR LEU ASP VAL THR ASP ARG ASP ARG ARG ARG PHE GLN THR LEU ASN PRO ARG LEU ASP ARG ASP TYR LEU ILE LEU TYR ASN PRO TYR THR GLY ARG
PHE MET PHE ARG LEU ARG ALA LYS MET GLY VAL PRO VAL VAL PRO LEU L799 V824 P825 E826 T829 L830 G838 ALA THR ARG LYS ARG ASP SER THR ASN GLN PRO LYS VAL ARG PRO W849 R850 D854 L855 T856 K857 GLU GLU GLY VAL G865 V866 V867 G871 N872 L875
I878 L881 Q888 R905 L928 H929 D933 K934 H935 T936 I937 R938 F939 I948 E956 K957 E958 G959 E964 E973 L974 L975 N976 E977 N978 P1008 E1013 ARG LEU LEU VAL LEU ILE SER ASP ALA VAL LEU HIS LEU SER THR SER GLN PRO ALA THR ALA
PRO PRO GLN PRO PRO GLN ALA GLN PRO SER GLN GLN VAL GLN GLN VAL SER GLN GLN GLN GLN VAL VAL SER GLN LEU GLN PRO GLN ALA GLN GLN PRO ARG SER ALA MET PRO HIS ALA SER VAL GLY GLN GLN GLN PRO GLY ALA ALA PRO MET ALA ARG PHE PRO PRO GLN GLN
GLN GLN ILE PHE GLN GLN GLN ARG PRO PRO GLN PRO GLN PRO ASN MET HIS GLY GLY GLN ILE SER GLN PRO ASN MET HIS GLY GLY PRO LYS PRO GLN LEU GLN GLY GLN HIS GLY GLN PRO GLY GLN MET VAL ALA ALA PRO GLN GLN GLN GLY GLN ARG PRO GLY THR GLY THR ALA


ALA GLY MET GLY ARG SER ASN ALA PRO LEU VAL VAL LEU ASP
• Molecule 3: Mediator of RNA polymerase II transcription subunit 16
Chain P:
52%
19%
28%
MET ALA LEU LEU MET GLU GLY GLY GLY ASP PRO MET SER VAL ASP GLY SER SER THR MET PRO ALA HIS MET ARG VAL MET PRO ASP MET GLY ILE THR GLY ALA PRO MET THR LEU ASP ASP VAL ASP LEU PHE GLY ASP ALA VAL MET ASN ASN ALA LEU ASP ALA LEU PRO PRO ALA PRO
GLY HIS PRO PRO PRO SER ARG ALA LEU GLN R71 R72 G84 S88 R89 Q90 G91 S95 L105 R109 P112 W117 E118 L130 S147 V151 I152 S153 V159 H160 L161 A162 W163 L174 I177 D178 A179 P180 G181 R182 Q190 N191 I192 N193 K194
V206 D207 D208 L209 V213 G214 L218 V224 V231 Q232 T233 D234 Y235 R236 L241 H249 P250 N251 H252 T253 K254 L257 V258 C259 V260 T261 T262 N263 L269 F270 P271 Q272 N273 N274 N275 R276 S281 I282 E283 I294 I299 M312 K315 Q316 L317 R318 V319
V320 R321 I324 Q325 W326 W327 L328 P329 D332 LYS GLN GLN MET PRO PRO SER VAL PRO LEU ARG PRO SER LEU ARG GLU SER ARG VAL ALA VAL T354 T355 Q361 Q362 Q363 S364 D365 G366 I370 A371 Q372 L376 P380 E385 T386 P387 V390 L391 P392 I395
L408 Q413 E414 P415 F416 T417 V418 R421 TRP GLU LEU PHE T426 D427 K430 A431 F432 H433 Q438 L439 K442 Q448 P449 S450 L455 D459 P460 V461 V462 I463 P464 G465 K466 T470 Q475 F476 G477 R478 V479 V480 C481 F482 L489 T506 T507 N508 I509 T510
S511 P512 L513 F517 L526 S536 W548 V549 K550 D557 M560 T561 L562 L567 A571 A572 S573 L574 S578 G585 P586 N587 C592 K604 K605 F606 K607 T611 A612 W613 E616 T624 V625 E630 H633 D634 Q635 L636 L642 Q643 F644
I648 L649 N650 H651 F654 Q659 P660 R661 S664 F667 L672 ALA VAL ARG ASN ILE VAL VAL LEU ILE THR ILE ALA SER ASN ALA PRO ASN THR ILE LYS GLU LYS LEU SER P697 D705 A706 D716 L721 R724 L725 L726 A727 L728 Q741 L751 H752
H760 L761 L762 L763 C764 S765 S766 V792 GLU SER ARG TYR ALA VAL ASP PRO ALA ALA ALA ALA GLN LYS THR LEU PRO PRO LEU TYR HIS ALA TYR VAL LYS MET GLN ARG VAL V922 R841 D842 I843 Q844 T845 S852 Q868 P869 L870 T871 GLU GLN GLN GLN GLN GLN CYS ASN
GLU GLN PHE I883 L896 G897 Q898 N899 P900 P901 P902 R905 E906 V907 L908 I915 F916 P917 A918 F919 R920 A921 T922 V923 R926 S927 S934 L935 L936 I939 D943 E944 R945 D959 V960 R963 R969 GLY GLN VAL LEU PRO ARG GLY ARG ILE VAL ALA SER VAL
LYS THR GLU ARG ALA GLU ALA VAL PRO MET VAL PRO SER GLN SER GLN SER SER HIS GLN ALA ALA SER GLN ALA GLN GLY GLN GLN SER GLN GLN GLN GLY ALA THR PRO ALA PRO ASN ALA THR PRO SER VAL PRO ILE SER GLN LEU ASN PRO PRO THR GLY PRO THR GLN PRO
PRO ASN SER SER GLY ASN THR ALA ASN ALA ASN PRO ASN THR GLY THR ASN ALA ASN THR LEU GLY GLY SER VAL PRO GLY LEU GLN GLY PHE VAL PRO VAL THR ALA ASN LEU ALA VAL ASN ALA SER GLN TRP ARG ARG CYS VAL ARG CYS ALA ALA VAL MET GLU ASP VAL TRP GLY
GLN ARG PRO GLY PHE THR PHE VAL LEU THR GLN GLN ARG ARG CYS ALA CYS GLY GLY GLY TRP GLY LEU VAL PRO ARG GLY ASP
• Molecule 4: MED15
Chain O:
8%
90%
MET ALA ALA ASN ILE PRO GLN PHE PRO ASN GLY GLN MET ALA MET LEU GLN GLN GLN GLN GLN GLN GLN GLN ALA ILE ALA ALA ASN GLN GLN TYR MET ASN VAL PHE ILE LEU ASN ASN LEU ARG GLY SER GLY THR ASN LEU PRO GLY THR TRP GLN ALA GLN ILE PRO PRO
GLN GLN LEU LEU SER GLU ARG PHE GLN LYS THR HIS ILE LEU TYR THR ASN ILE MET LEU ALA SER ASN GLY GLY ASP PRO Q88 N96 K99 K108 K118 ILE SER GLU VAL MET LYS ARG ARG GLU SER N129 G130 Q134 I138 R143 I147 Q148 Q163 L164

M165 L166 N167 R168 P177 P180 P188 G189
M249 R250 R251 R264 Q268 T272 P273 S277 S282 G283 K284 D285 Q292 V296 Q297 V298 F299 R300 E308 Q315 V316 L320

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

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

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

LEU ASP GLY THR LEU GLY GLU GLY GLN GLN GLU SER GLY GLN GLY GLN GLN GLY GLN PRO GLU VAL MET VAL ILE GLU

- Molecule 5: Unknown peptide

Chain X: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.610	Depositor
Minimum map value	-1.096	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	526.07996, 526.07996, 526.07996	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	E	0.27	0/4548	0.49	2/6191 (0.0%)
2	N	0.27	0/1464	0.52	2/1988 (0.1%)
3	P	0.27	0/6315	0.52	2/8611 (0.0%)
4	O	0.28	0/1300	0.48	2/1749 (0.1%)
All	All	0.27	0/13627	0.51	8/18539 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	254	PRO	N-CA-CB	6.93	111.61	103.30
3	P	380	PRO	N-CA-CB	6.57	111.18	103.30
3	P	869	PRO	N-CA-CB	6.48	111.08	103.30
1	E	305	PRO	N-CA-CB	6.48	111.07	103.30
4	O	188	PRO	N-CA-CB	6.04	110.55	103.30
2	N	1008	PRO	N-CA-CB	5.78	110.23	103.30
4	O	285	ASP	CB-CG-OD1	5.14	122.93	118.30
2	N	871	GLY	C-N-CA	5.04	134.29	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	E	4467	0	4409	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1439	0	1304	22	0
3	P	6178	0	6027	164	0
4	O	1290	0	1289	24	0
5	X	259	0	64	0	0
All	All	13633	0	13093	281	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 11.

All (281) 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)
1:E:228:ILE:HG21	1:E:246:LEU:HD22	1.54	0.89
1:E:409:CYS:SG	1:E:442:ARG:NH2	2.55	0.80
3:P:118:GLU:HA	3:P:548:TRP:HH2	1.51	0.76
1:E:231:GLU:HB3	1:E:239:LYS:HZ3	1.52	0.75
3:P:325:GLN:HE22	3:P:327:TRP:HB3	1.50	0.74
3:P:506:THR:HG22	3:P:507:THR:H	1.52	0.73
2:N:849:TRP:HB2	2:N:872:ASN:HD22	1.52	0.72
4:O:177:PRO:HA	4:O:308:GLU:HG2	1.71	0.72
3:P:648:ILE:HD13	3:P:945:ARG:HB2	1.70	0.72
3:P:415:PRO:HB3	3:P:433:HIS:HB2	1.72	0.72
3:P:387:PRO:HB2	3:P:416:PHE:HB3	1.71	0.72
3:P:607:LYS:NZ	3:P:635:GLN:O	2.23	0.71
3:P:624:THR:HG22	3:P:625:VAL:H	1.54	0.70
2:N:878:ILE:HG12	4:O:180:PRO:HG2	1.73	0.70
3:P:413:GLN:NE2	3:P:438:GLN:OE1	2.19	0.69
2:N:850:ARG:O	2:N:872:ASN:ND2	2.26	0.69
1:E:66:ARG:HE	3:P:206:VAL:HG21	1.59	0.68
3:P:659:GLN:NE2	3:P:764:CYS:SG	2.67	0.68
3:P:324:ILE:HG23	3:P:364:SER:HB2	1.73	0.67
2:N:958:GLU:HG2	2:N:959:GLY:H	1.59	0.67
3:P:273:ASN:O	3:P:275:ASN:ND2	2.27	0.67
4:O:315:GLN:HG2	4:O:316:VAL:H	1.60	0.67
3:P:843:ILE:HD12	3:P:927:SER:HA	1.75	0.67
3:P:273:ASN:HB2	3:P:281:SER:HB3	1.77	0.66
3:P:315:LYS:HD2	3:P:321:ARG:HE	1.61	0.65
1:E:619:GLU:HG3	1:E:620:LYS:HG3	1.78	0.65
3:P:232:GLN:HE22	3:P:241:LEU:HD22	1.63	0.64
4:O:264:ARG:O	4:O:268:GLN:NE2	2.31	0.64
3:P:118:GLU:OE2	3:P:550:LYS:NZ	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:625:VAL:HG12	3:P:766:SER:HB2	1.80	0.63
1:E:761:GLN:HG3	1:E:762:LYS:H	1.64	0.63
3:P:899:ASN:OD1	3:P:900:PRO:HD3	1.98	0.63
3:P:159:VAL:HB	3:P:178:ASP:HB3	1.81	0.62
2:N:928:LEU:HB2	2:N:936:THR:HG23	1.82	0.62
1:E:366:VAL:O	1:E:369:ASN:ND2	2.33	0.61
3:P:901:PRO:HB2	3:P:902:PRO:HD3	1.83	0.61
3:P:661:ARG:HH21	3:P:963:ARG:HH11	1.49	0.61
2:N:824:VAL:HG22	2:N:826:GLU:H	1.65	0.61
2:N:881:LEU:HD11	4:O:108:LYS:HD2	1.81	0.61
1:E:530:ASP:OD1	1:E:583:TYR:OH	2.15	0.60
3:P:90:GLN:OE1	3:P:91:GLY:N	2.36	0.59
4:O:167:ASN:HD22	4:O:168:ARG:HD3	1.67	0.59
1:E:387:PRO:HA	1:E:390:LEU:HB3	1.85	0.59
3:P:651:HIS:CG	3:P:751:LEU:HB3	2.37	0.59
1:E:707:ASN:HD21	1:E:710:ILE:HD12	1.68	0.58
4:O:164:LEU:O	4:O:168:ARG:NH2	2.35	0.58
3:P:117:TRP:CD1	3:P:592:CYS:HB3	2.38	0.58
3:P:234:ASP:OD2	3:P:236:ARG:NH2	2.36	0.58
3:P:959:ASP:OD1	3:P:960:VAL:N	2.35	0.58
1:E:696:LEU:HD11	1:E:742:VAL:HG21	1.86	0.58
3:P:180:PRO:HB3	3:P:207:ASP:H	1.67	0.58
3:P:414:GLU:OE1	3:P:415:PRO:HD3	2.04	0.57
3:P:915:ILE:HG22	3:P:918:ALA:H	1.69	0.57
3:P:179:ALA:O	3:P:181:GLY:N	2.38	0.56
1:E:447:PHE:HA	1:E:451:LEU:HD13	1.87	0.56
1:E:228:ILE:HG13	1:E:246:LEU:HB2	1.86	0.56
1:E:402:TYR:O	1:E:405:ASN:N	2.31	0.56
1:E:783:ALA:HB3	3:P:294:ILE:HD11	1.86	0.56
3:P:130:LEU:HD22	3:P:153:SER:HB3	1.88	0.56
3:P:354:THR:OG1	3:P:355:THR:N	2.39	0.56
3:P:506:THR:HG22	3:P:507:THR:HG23	1.87	0.56
3:P:257:LEU:HG	3:P:258:VAL:H	1.71	0.56
4:O:96:ASN:O	4:O:99:LYS:HG2	2.06	0.56
2:N:958:GLU:OE1	2:N:958:GLU:N	2.33	0.55
3:P:232:GLN:NE2	3:P:241:LEU:HD22	2.21	0.55
1:E:849:GLN:HE22	3:P:316:GLN:HE21	1.54	0.55
3:P:260:VAL:HA	3:P:270:PHE:HB2	1.87	0.55
3:P:442:LYS:NZ	3:P:450:SER:OG	2.24	0.55
1:E:235:GLN:OE1	1:E:235:GLN:N	2.39	0.54
3:P:418:VAL:HG12	3:P:432:PHE:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:973:GLU:HB2	2:N:975:LEU:HD22	1.87	0.54
3:P:317:LEU:HB2	3:P:319:VAL:HG22	1.90	0.54
3:P:130:LEU:HD23	3:P:151:VAL:HG23	1.89	0.54
1:E:243:ARG:NH1	1:E:247:ASP:OD1	2.40	0.54
3:P:459:ASP:OD1	3:P:459:ASP:N	2.40	0.54
3:P:328:LEU:N	3:P:329:PRO:HD3	2.22	0.54
1:E:705:ALA:HA	3:P:366:GLY:HA2	1.91	0.53
3:P:177:ILE:HG12	3:P:179:ALA:H	1.73	0.53
3:P:180:PRO:O	3:P:209:LEU:HB2	2.08	0.53
1:E:613:GLU:N	1:E:613:GLU:OE1	2.41	0.53
3:P:179:ALA:HB1	3:P:180:PRO:HD2	1.91	0.53
1:E:497:LEU:HD21	1:E:531:VAL:HG12	1.90	0.53
2:N:977:GLU:O	2:N:978:ASN:ND2	2.42	0.53
1:E:243:ARG:HD2	1:E:303:GLN:HA	1.91	0.53
3:P:262:THR:OG1	3:P:263:ASN:N	2.41	0.53
4:O:272:THR:OG1	4:O:273:PRO:HD3	2.08	0.53
4:O:134:GLN:O	4:O:138:ILE:HG13	2.08	0.53
1:E:784:ASP:OD1	1:E:784:ASP:N	2.38	0.53
3:P:922:THR:O	3:P:926:ARG:NH1	2.42	0.53
4:O:268:GLN:OE1	4:O:282:SER:OG	2.24	0.53
1:E:474:PRO:HB3	1:E:480:LYS:HE2	1.90	0.52
2:N:867:VAL:HG11	2:N:888:GLN:HB3	1.91	0.52
3:P:630:GLU:HB2	3:P:633:HIS:HB3	1.91	0.52
3:P:943:ASP:OD1	3:P:943:ASP:N	2.42	0.52
1:E:71:GLN:OE1	1:E:71:GLN:N	2.43	0.52
2:N:933:ASP:O	2:N:935:HIS:ND1	2.42	0.52
3:P:651:HIS:HB2	3:P:751:LEU:HD22	1.89	0.52
3:P:426:THR:OG1	3:P:427:ASP:N	2.35	0.52
1:E:685:ASP:HB2	1:E:731:ALA:HB2	1.90	0.51
3:P:387:PRO:HG3	3:P:418:VAL:HB	1.91	0.51
1:E:70:ASP:OD2	1:E:791:TRP:HB2	2.11	0.51
3:P:604:LYS:O	3:P:605:LYS:HD2	2.10	0.51
3:P:896:LEU:HD13	3:P:907:VAL:HG11	1.93	0.51
1:E:66:ARG:NE	3:P:206:VAL:HG21	2.25	0.51
3:P:439:LEU:HD23	3:P:455:LEU:HD11	1.93	0.51
1:E:63:PRO:HB3	1:E:66:ARG:HH11	1.76	0.50
1:E:315:GLY:HA2	1:E:879:THR:HG21	1.93	0.50
1:E:684:VAL:HA	1:E:689:LEU:HD12	1.93	0.50
3:P:907:VAL:O	3:P:908:LEU:HG	2.11	0.50
3:P:95:SER:HB3	3:P:105:LEU:HD13	1.92	0.50
3:P:489:LEU:H	3:P:489:LEU:HD23	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:536:SER:HG	3:P:548:TRP:HD1	1.57	0.50
3:P:906:GLU:N	3:P:906:GLU:OE1	2.44	0.50
3:P:249:HIS:HB2	3:P:250:PRO:HD3	1.94	0.50
3:P:269:LEU:HD12	3:P:283:GLU:HG3	1.94	0.50
1:E:705:ALA:O	1:E:711:GLN:NE2	2.45	0.50
1:E:610:GLN:HG2	1:E:611:PRO:HD3	1.93	0.50
1:E:617:GLU:HG3	1:E:618:GLN:H	1.77	0.50
1:E:85:ARG:HH12	1:E:410:ILE:HG23	1.76	0.50
3:P:263:ASN:N	3:P:263:ASN:OD1	2.43	0.50
3:P:463:ILE:O	3:P:482:PHE:HB3	2.12	0.50
4:O:315:GLN:HG2	4:O:316:VAL:N	2.27	0.50
1:E:230:ASN:HB2	3:P:72:ARG:HH21	1.77	0.49
3:P:312:MET:HG2	3:P:395:ILE:HD11	1.94	0.49
3:P:192:ILE:O	3:P:194:LYS:N	2.45	0.49
3:P:624:THR:HG22	3:P:625:VAL:N	2.25	0.49
3:P:705:ASP:OD1	3:P:706:ALA:N	2.45	0.49
3:P:231:VAL:HG22	3:P:509:ILE:HG22	1.93	0.49
1:E:218:LEU:HB2	1:E:223:PHE:CZ	2.48	0.49
3:P:512:PRO:HA	3:P:517:PHE:HB2	1.94	0.49
3:P:649:LEU:HD22	3:P:654:PHE:HB3	1.93	0.49
3:P:218:LEU:O	3:P:257:LEU:HD11	2.13	0.49
4:O:129:ASN:OD1	4:O:130:GLY:N	2.40	0.49
2:N:854:ASP:OD1	2:N:855:LEU:N	2.45	0.48
3:P:177:ILE:HG22	3:P:182:ARG:O	2.12	0.48
3:P:254:LYS:HA	3:P:254:LYS:HD3	1.67	0.48
3:P:760:HIS:CE1	3:P:900:PRO:HG2	2.48	0.48
1:E:312:THR:HG21	1:E:872:ILE:HG23	1.96	0.48
2:N:964:GLU:OE2	3:P:934:SER:OG	2.31	0.48
3:P:433:HIS:CE1	3:P:460:PRO:HD2	2.49	0.48
3:P:476:PHE:CG	3:P:477:GLY:N	2.82	0.48
3:P:316:GLN:O	3:P:316:GLN:HG2	2.13	0.48
3:P:370:ILE:HG22	3:P:372:GLN:H	1.79	0.47
1:E:390:LEU:HA	1:E:393:LEU:O	2.14	0.47
1:E:492:ASP:C	1:E:493:ARG:HD3	2.34	0.47
2:N:829:THR:O	2:N:830:LEU:HD22	2.14	0.47
1:E:361:LEU:HB3	1:E:835:MET:HE1	1.96	0.47
3:P:272:GLN:O	3:P:273:ASN:ND2	2.48	0.47
3:P:511:SER:HA	3:P:572:ALA:HB1	1.95	0.47
3:P:557:ASP:HB3	3:P:560:MET:HB2	1.96	0.47
1:E:232:THR:N	1:E:239:LYS:HE2	2.28	0.47
1:E:655:ALA:HB3	1:E:656:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:177:ILE:HG23	3:P:179:ALA:HB3	1.96	0.47
3:P:408:LEU:HD13	3:P:439:LEU:HD13	1.97	0.47
3:P:726:LEU:HG	3:P:920:ARG:HH12	1.80	0.47
3:P:852:SER:HB2	3:P:923:VAL:HG21	1.95	0.47
4:O:147:ILE:HG22	4:O:148:GLN:H	1.80	0.47
4:O:164:LEU:HD12	4:O:165:MET:HG3	1.96	0.47
1:E:492:ASP:O	1:E:493:ARG:HD3	2.15	0.47
1:E:70:ASP:HA	1:E:73:THR:HG22	1.96	0.47
3:P:327:TRP:HE3	3:P:329:PRO:HD2	1.79	0.47
3:P:466:LYS:HD3	3:P:526:LEU:O	2.15	0.47
1:E:402:TYR:N	1:E:403:PRO:HD2	2.30	0.46
1:E:415:ASN:OD1	1:E:416:GLN:N	2.37	0.46
1:E:751:LYS:HE3	1:E:751:LYS:HB2	1.74	0.46
3:P:271:PRO:HA	3:P:283:GLU:HA	1.97	0.46
3:P:475:GLN:NE2	3:P:476:PHE:O	2.48	0.46
3:P:162:ALA:HB3	3:P:174:LEU:HD21	1.96	0.46
3:P:844:GLN:O	3:P:845:THR:OG1	2.27	0.46
3:P:414:GLU:HB3	3:P:415:PRO:CD	2.45	0.46
3:P:661:ARG:HE	3:P:963:ARG:NH1	2.14	0.46
3:P:433:HIS:ND1	3:P:464:PRO:HG3	2.30	0.46
3:P:480:VAL:HG22	3:P:482:PHE:H	1.79	0.46
4:O:277:SER:O	4:O:277:SER:OG	2.31	0.46
4:O:165:MET:HA	4:O:168:ARG:HH21	1.79	0.46
1:E:468:THR:OG1	1:E:469:TYR:N	2.48	0.46
1:E:543:HIS:HE1	1:E:589:ASP:HA	1.80	0.46
2:N:875:LEU:HD11	2:N:905:ARG:HA	1.97	0.46
3:P:448:GLN:OE1	3:P:448:GLN:N	2.43	0.45
1:E:496:LYS:HE2	1:E:496:LYS:HB3	1.83	0.45
1:E:402:TYR:OH	1:E:456:SER:OG	2.12	0.45
1:E:645:SER:O	1:E:645:SER:OG	2.32	0.45
4:O:143:ARG:O	4:O:147:ILE:HG12	2.16	0.45
3:P:294:ILE:HG22	3:P:316:GLN:HE22	1.82	0.45
1:E:630:LEU:O	1:E:631:PHE:HB3	2.17	0.45
3:P:562:LEU:HB3	3:P:567:LEU:HD13	1.98	0.45
3:P:636:LEU:HD23	3:P:636:LEU:HA	1.79	0.45
3:P:716:ASP:HB3	3:P:939:ILE:HD11	1.98	0.45
3:P:578:SER:HB3	3:P:613:TRP:HH2	1.81	0.44
4:O:284:LYS:HG2	4:O:285:ASP:H	1.82	0.44
1:E:537:LYS:HE3	1:E:537:LYS:HB3	1.84	0.44
3:P:147:SER:O	3:P:147:SER:OG	2.32	0.44
3:P:299:ILE:HG21	3:P:392:PRO:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:841:ARG:NH2	3:P:845:THR:HG22	2.33	0.44
4:O:163:GLN:OE1	4:O:163:GLN:N	2.39	0.44
3:P:648:ILE:HD11	3:P:651:HIS:CE1	2.53	0.44
1:E:525:LYS:HB2	1:E:525:LYS:HE3	1.72	0.44
3:P:898:GLN:O	3:P:901:PRO:HD2	2.18	0.44
1:E:493:ARG:O	1:E:493:ARG:HG2	2.17	0.44
3:P:84:GLY:HA3	3:P:160:HIS:CE1	2.53	0.44
1:E:444:ASP:O	1:E:448:ALA:HB3	2.18	0.43
3:P:721:LEU:HA	3:P:721:LEU:HD23	1.79	0.43
3:P:214:GLY:O	3:P:262:THR:HG22	2.17	0.43
4:O:292:GLN:O	4:O:296:VAL:HG12	2.18	0.43
3:P:270:PHE:O	3:P:270:PHE:CG	2.72	0.43
3:P:418:VAL:HG12	3:P:432:PHE:CB	2.48	0.43
3:P:741:GLN:HA	3:P:905:ARG:HD2	1.99	0.43
1:E:245:LEU:HD23	1:E:245:LEU:HA	1.84	0.43
3:P:585:GLY:O	3:P:587:ASN:N	2.47	0.43
3:P:916:PHE:O	3:P:920:ARG:HB3	2.18	0.43
3:P:414:GLU:HB3	3:P:415:PRO:HD3	2.00	0.43
3:P:664:SER:HA	3:P:667:PHE:CD1	2.53	0.43
3:P:905:ARG:HG2	3:P:906:GLU:H	1.84	0.43
4:O:251:ARG:HH21	4:O:299:PHE:HB3	1.83	0.43
2:N:928:LEU:HD12	4:O:300:ARG:HD3	2.01	0.43
2:N:938:ARG:NH1	4:O:297:GLN:HE22	2.17	0.43
3:P:430:LYS:HG3	3:P:431:ALA:H	1.84	0.43
3:P:508:ASN:OD1	3:P:508:ASN:N	2.52	0.43
3:P:659:GLN:HB2	3:P:660:PRO:HD3	2.01	0.43
3:P:936:LEU:HD23	3:P:936:LEU:H	1.82	0.43
1:E:640:ASP:OD1	1:E:641:GLU:N	2.39	0.43
3:P:574:LEU:HD21	3:P:613:TRP:CD2	2.53	0.43
3:P:578:SER:HB3	3:P:613:TRP:CH2	2.54	0.43
1:E:393:LEU:HD11	1:E:395:ALA:HB3	2.01	0.43
1:E:539:HIS:HB2	1:E:543:HIS:CD2	2.54	0.43
1:E:761:GLN:C	1:E:763:ILE:H	2.22	0.43
3:P:421:ARG:O	3:P:421:ARG:NH2	2.45	0.43
3:P:724:ARG:HE	3:P:752:HIS:HE1	1.66	0.43
3:P:190:GLN:C	3:P:192:ILE:H	2.22	0.43
3:P:109:ARG:HH21	3:P:112:PRO:HD2	1.84	0.42
1:E:530:ASP:OD2	1:E:779:ARG:NH1	2.52	0.42
3:P:461:VAL:HG12	3:P:461:VAL:O	2.19	0.42
3:P:390:VAL:HG13	3:P:391:LEU:HD23	2.01	0.42
3:P:726:LEU:C	3:P:728:LEU:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:958:GLU:HG2	2:N:959:GLY:N	2.32	0.42
3:P:511:SER:OG	3:P:512:PRO:HD3	2.19	0.42
1:E:761:GLN:O	1:E:763:ILE:N	2.53	0.42
3:P:213:VAL:HG23	3:P:262:THR:HG23	2.01	0.42
3:P:478:ARG:HD3	3:P:478:ARG:HA	1.65	0.42
1:E:524:SER:OG	1:E:525:LYS:N	2.53	0.42
1:E:778:ARG:HA	1:E:778:ARG:HD3	1.87	0.42
3:P:235:TYR:HD1	3:P:235:TYR:HA	1.68	0.42
1:E:728:SER:O	1:E:731:ALA:N	2.53	0.42
2:N:956:GLU:HG3	2:N:958:GLU:OE1	2.19	0.42
1:E:586:SER:OG	1:E:587:THR:N	2.53	0.41
3:P:252:HIS:O	3:P:252:HIS:CG	2.73	0.41
3:P:385:GLU:O	3:P:386:THR:OG1	2.37	0.41
1:E:331:ASP:OD1	1:E:334:ALA:HB3	2.19	0.41
1:E:744:LYS:HB3	1:E:745:PRO:HD3	2.02	0.41
3:P:651:HIS:CE1	3:P:751:LEU:HD13	2.55	0.41
3:P:724:ARG:HE	3:P:752:HIS:CE1	2.38	0.41
3:P:642:LEU:HD23	3:P:642:LEU:H	1.86	0.41
3:P:391:LEU:HD21	3:P:465:GLY:O	2.21	0.41
1:E:729:ASN:OD1	1:E:730:GLU:N	2.53	0.41
1:E:788:LEU:HD23	1:E:788:LEU:HA	1.81	0.41
2:N:929:HIS:ND1	2:N:935:HIS:HD2	2.19	0.41
3:P:88:SER:HG	3:P:163:TRP:HE1	1.67	0.41
3:P:376:LEU:HD12	3:P:376:LEU:HA	1.91	0.41
3:P:611:THR:HA	3:P:616:GLU:HG2	2.01	0.41
3:P:235:TYR:OH	3:P:571:ALA:HB3	2.21	0.41
3:P:276:ARG:HH21	3:P:354:THR:N	2.19	0.41
3:P:512:PRO:HB2	3:P:513:LEU:HG	2.03	0.41
1:E:74:LEU:HD21	1:E:839:TYR:HD1	1.85	0.41
1:E:365:ALA:HA	1:E:369:ASN:N	2.36	0.41
1:E:739:LEU:HD23	1:E:739:LEU:HA	1.92	0.41
3:P:193:ASN:OD1	3:P:193:ASN:N	2.53	0.41
1:E:231:GLU:HB3	1:E:239:LYS:NZ	2.29	0.41
3:P:361:GLN:CD	3:P:362:GLN:H	2.24	0.41
3:P:470:THR:HG22	3:P:476:PHE:HD1	1.86	0.41
2:N:939:PHE:HB2	2:N:948:ILE:HG22	2.04	0.40
3:P:262:THR:HG1	3:P:263:ASN:H	1.69	0.40
3:P:762:LEU:HD11	3:P:897:GLY:HA3	2.03	0.40
3:P:271:PRO:HB3	3:P:283:GLU:HB3	2.03	0.40
3:P:536:SER:OG	3:P:548:TRP:HD1	2.04	0.40
3:P:843:ILE:HD12	3:P:927:SER:CA	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ARG:NH1	1:E:479:VAL:HG21	2.37	0.40
1:E:707:ASN:ND2	1:E:710:ILE:HD12	2.32	0.40
3:P:325:GLN:NE2	3:P:327:TRP:HB3	2.29	0.40
1:E:235:GLN:HG3	1:E:239:LYS:HB2	2.04	0.40
1:E:472:LEU:N	1:E:473:PRO:HD3	2.37	0.40
1:E:673:ASP:OD1	1:E:674:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	566/1099 (52%)	474 (84%)	87 (15%)	5 (1%)	17	57
2	N	192/1168 (16%)	148 (77%)	44 (23%)	0	100	100
3	P	798/1130 (71%)	618 (77%)	175 (22%)	5 (1%)	25	64
4	O	158/1625 (10%)	134 (85%)	24 (15%)	0	100	100
All	All	1714/5022 (34%)	1374 (80%)	330 (19%)	10 (1%)	29	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	254	PRO
1	E	304	VAL
1	E	305	PRO
3	P	380	PRO
3	P	180	PRO
3	P	224	VAL
3	P	868	GLN
3	P	869	PRO
1	E	236	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	491	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	481/889 (54%)	479 (100%)	2 (0%)	91 97
2	N	129/1026 (13%)	129 (100%)	0	100 100
3	P	662/947 (70%)	659 (100%)	3 (0%)	88 95
4	O	135/1327 (10%)	134 (99%)	1 (1%)	84 93
All	All	1407/4189 (34%)	1401 (100%)	6 (0%)	91 97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	243	ARG
1	E	493	ARG
3	P	270	PHE
3	P	644	PHE
3	P	841	ARG
4	O	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	369	ASN
1	E	450	GLN
1	E	485	GLN
1	E	505	ASN
1	E	543	HIS
1	E	849	GLN
2	N	872	ASN
2	N	879	ASN
2	N	955	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	190	GLN
3	P	232	GLN
3	P	274	ASN
3	P	275	ASN
3	P	325	GLN
3	P	475	GLN
3	P	587	ASN
3	P	589	HIS
3	P	659	GLN
3	P	752	HIS
3	P	861	HIS
4	O	146	GLN
4	O	167	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

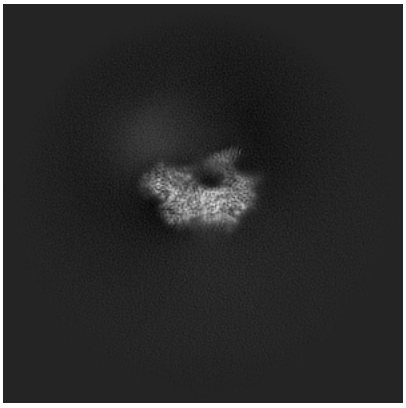
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22397. These allow visual inspection of the internal detail of the map and identification of artifacts.

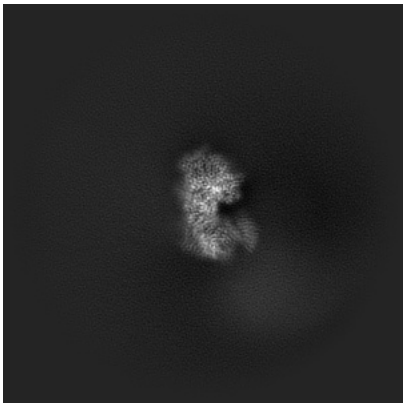
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

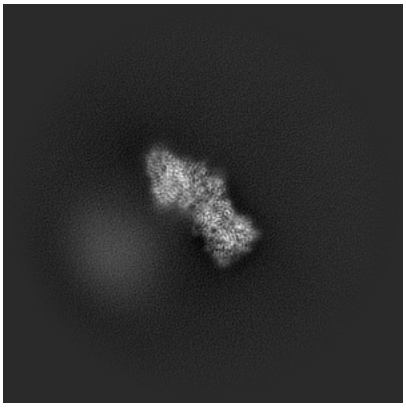
6.1.1 Primary map



X



Y

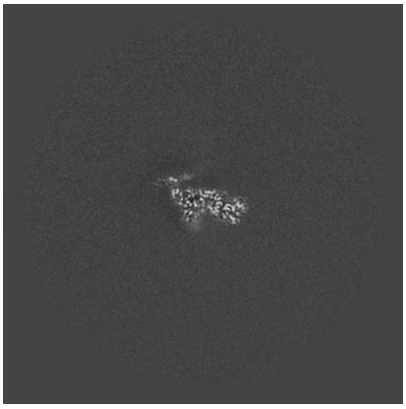


Z

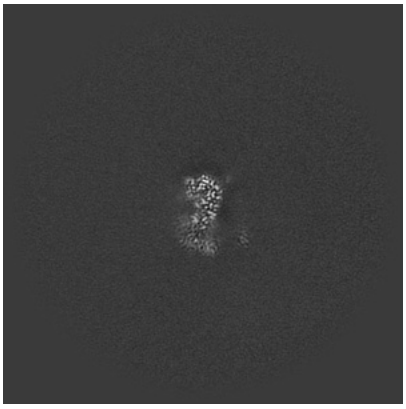
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

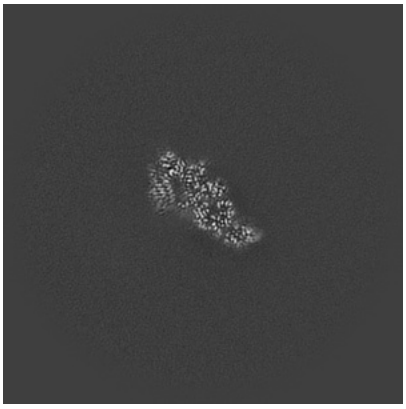
6.2.1 Primary map



X Index: 240



Y Index: 240

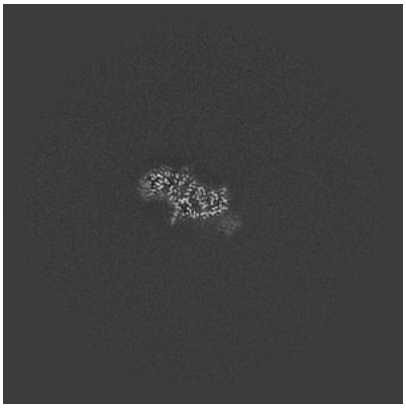


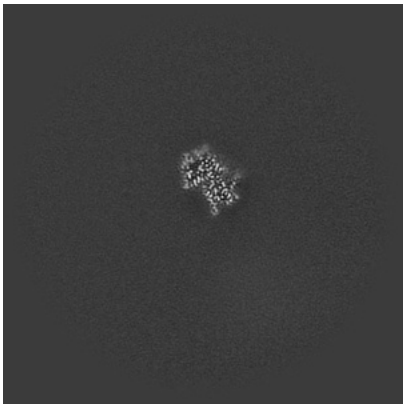
Z Index: 240

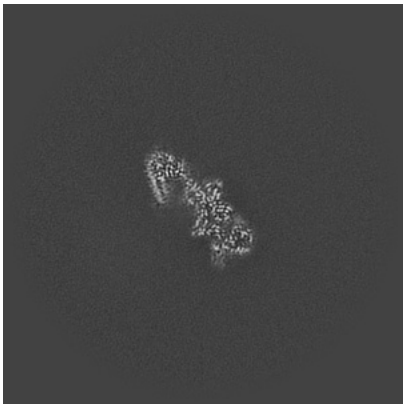
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 259

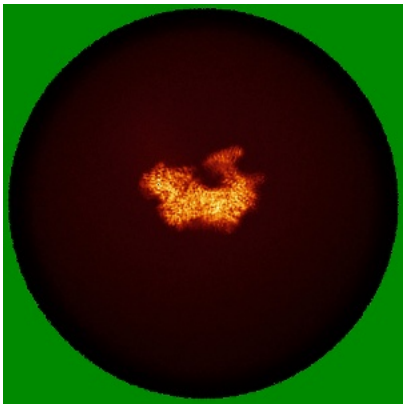

Y Index: 203

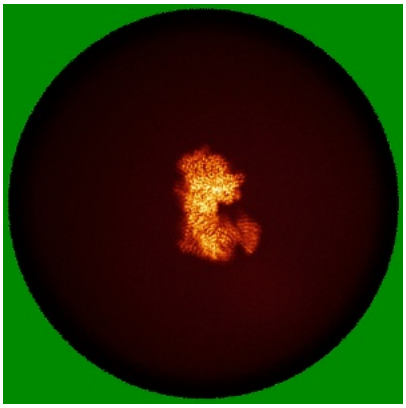

Z Index: 253

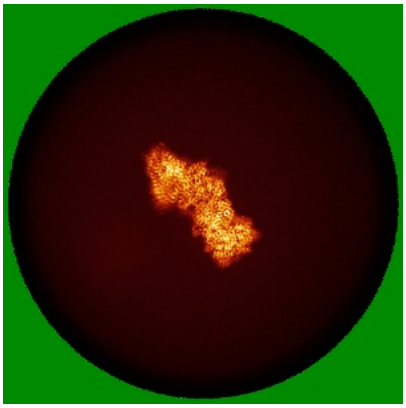
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

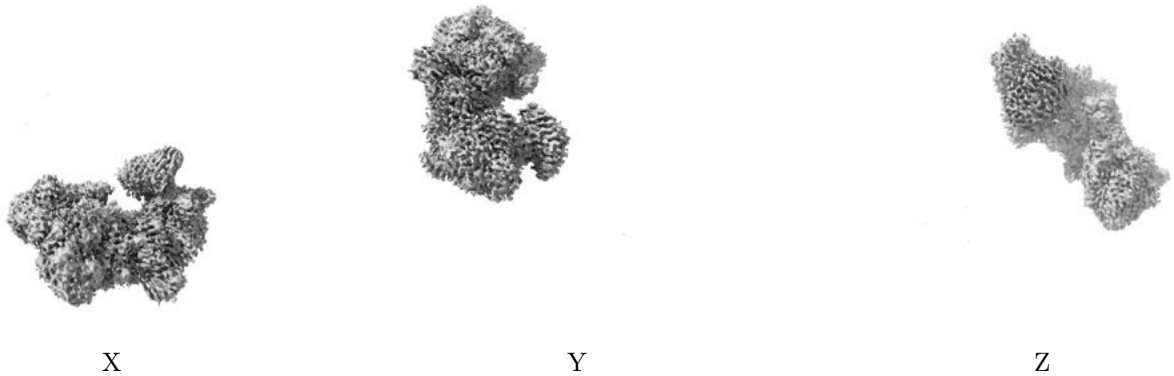

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

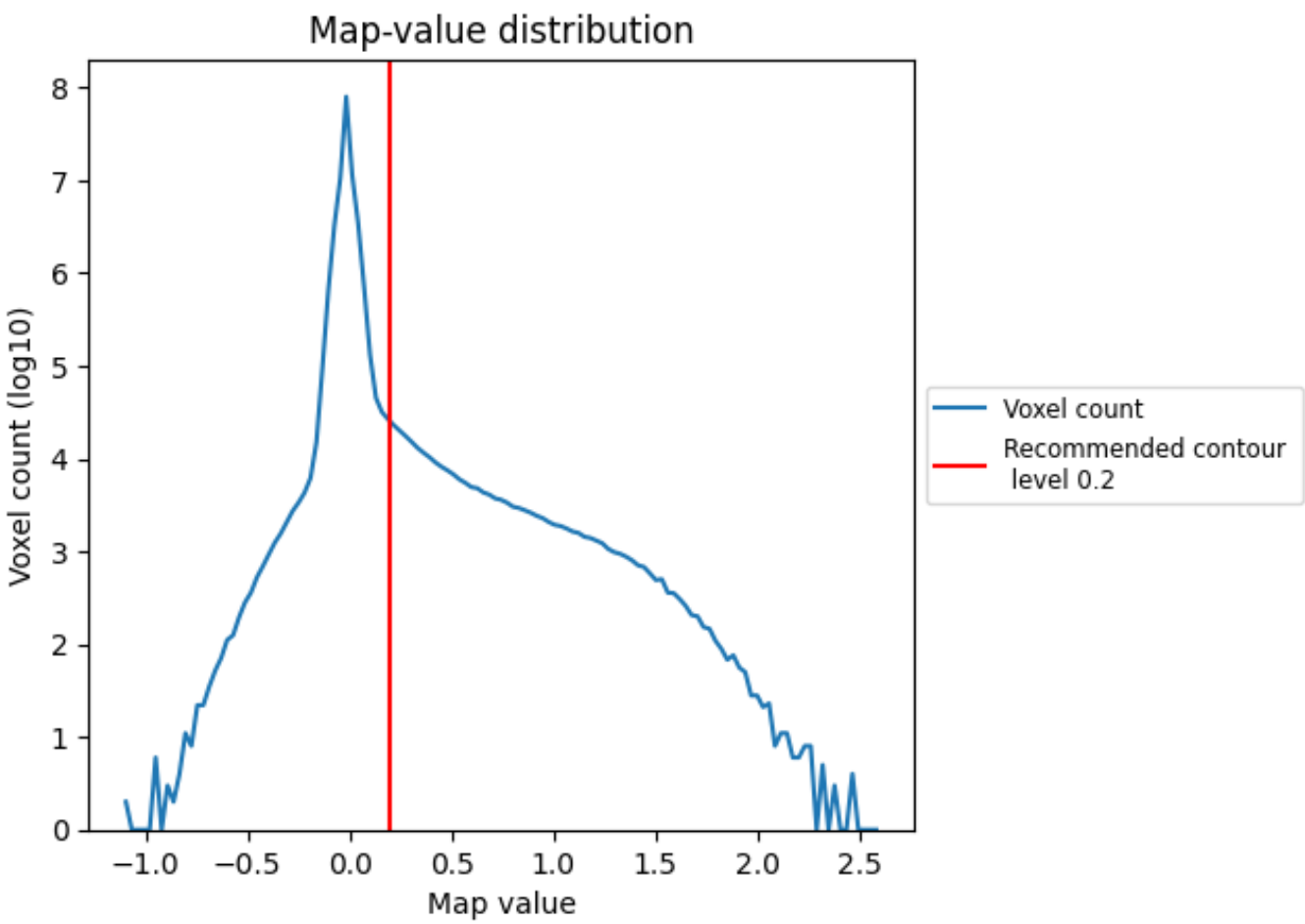
6.6 Mask visualisation (i)

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

7 Map analysis (i)

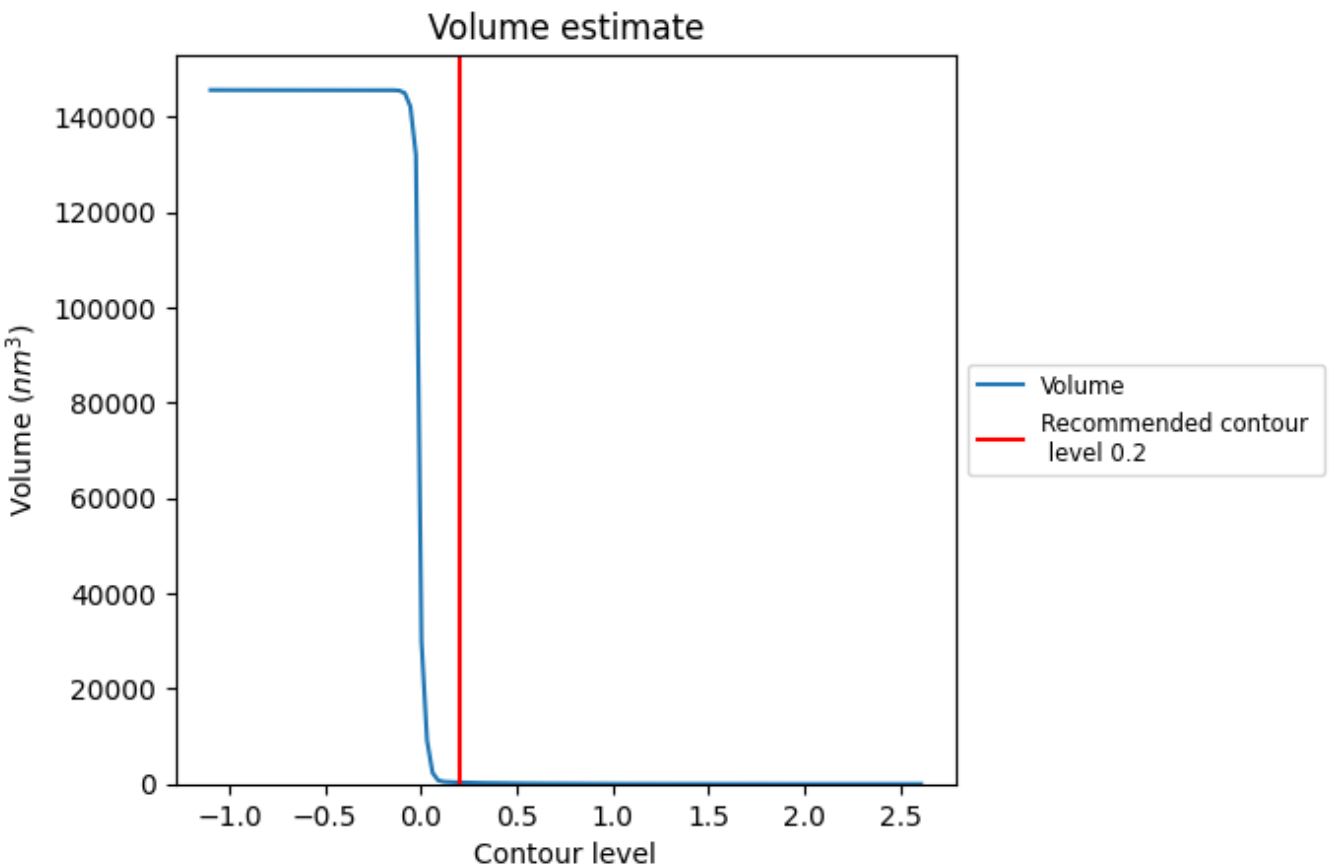
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

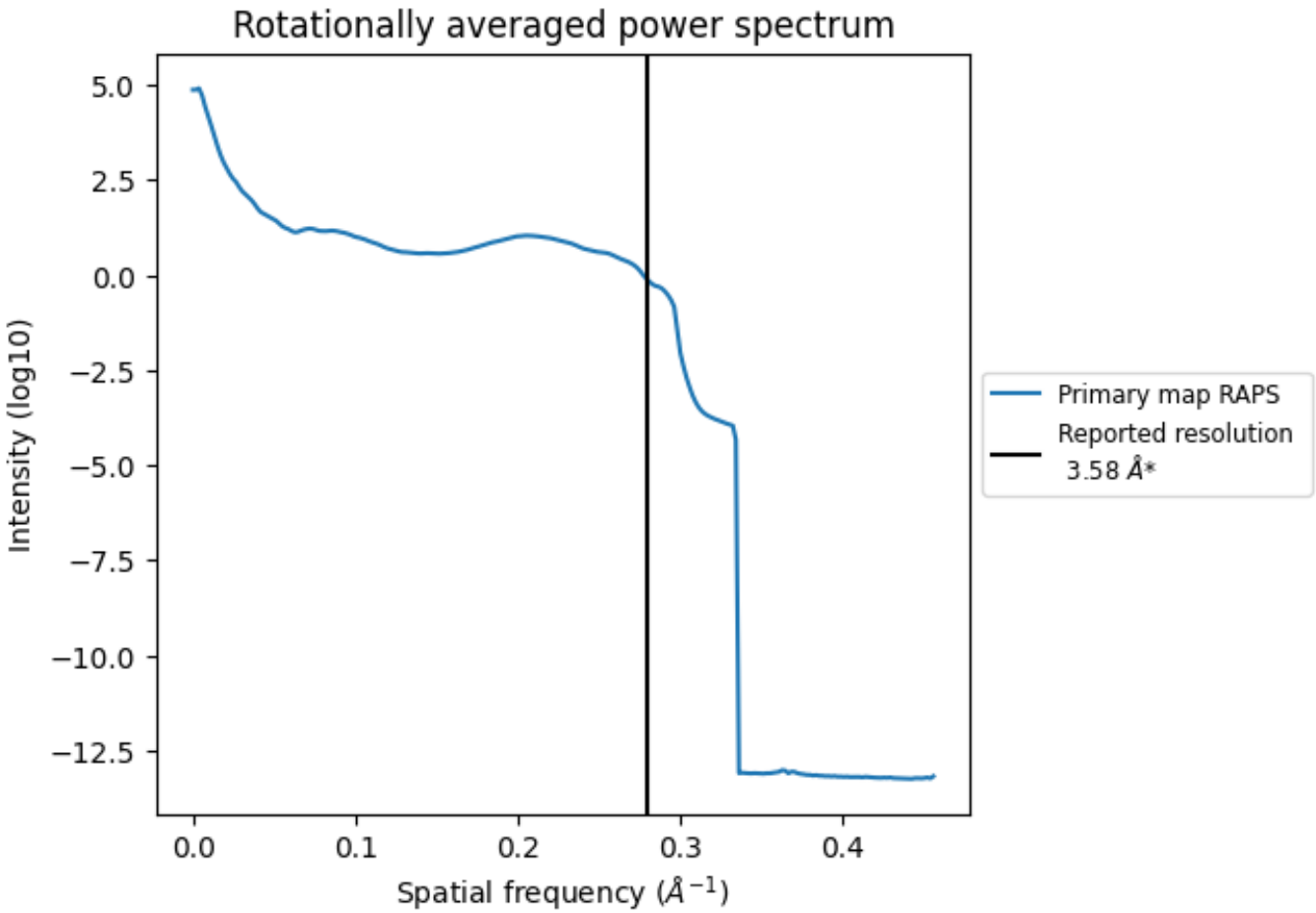
7.2 Volume estimate (i)



The volume at the recommended contour level is 317 nm^3; this corresponds to an approximate mass of 286 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

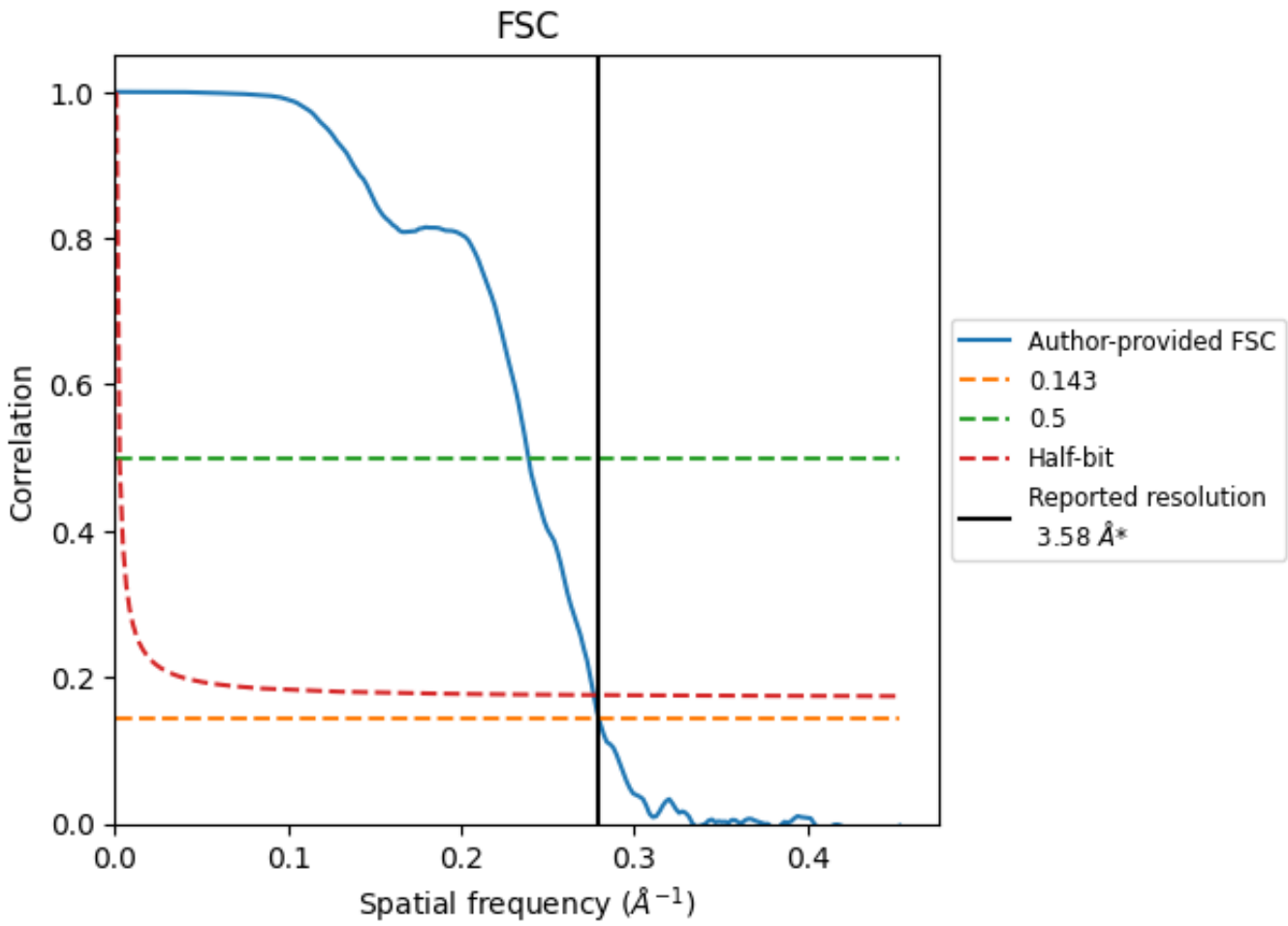


*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.279 Å^{-1}

8.2 Resolution estimates (i)

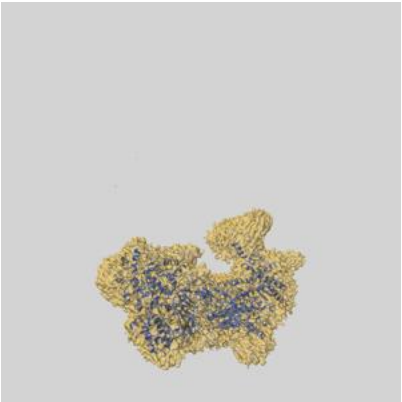
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.58	4.19	3.62
Unmasked-calculated*	-	-	-

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

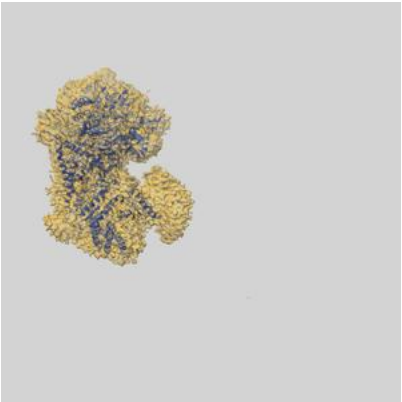
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22397 and PDB model 7JMN. Per-residue inclusion information can be found in section 3 on page 5.

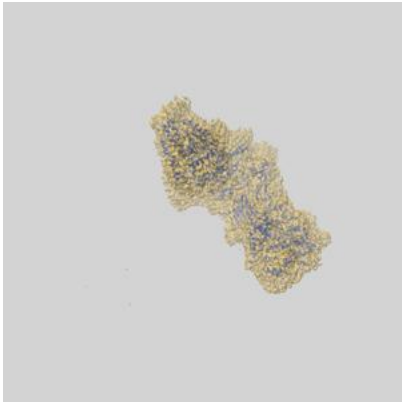
9.1 Map-model overlay (i)



X



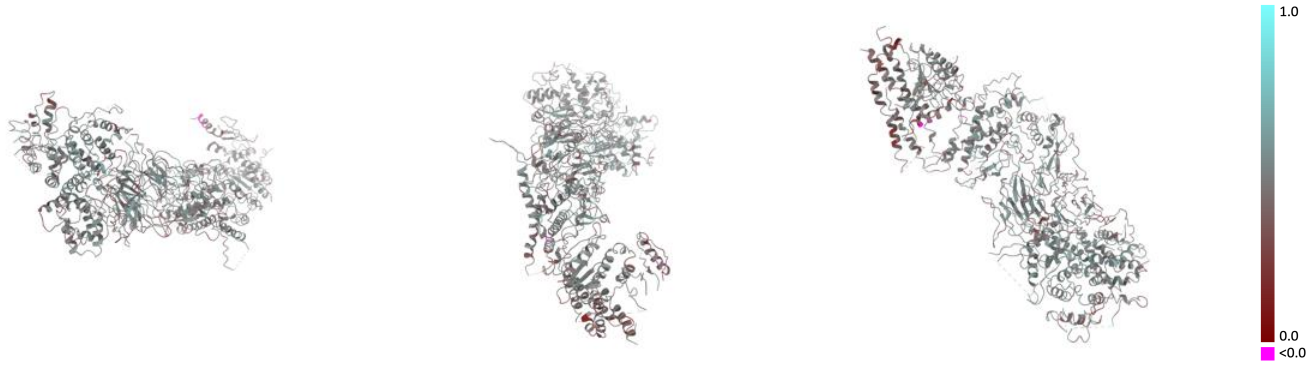
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



X Y Z

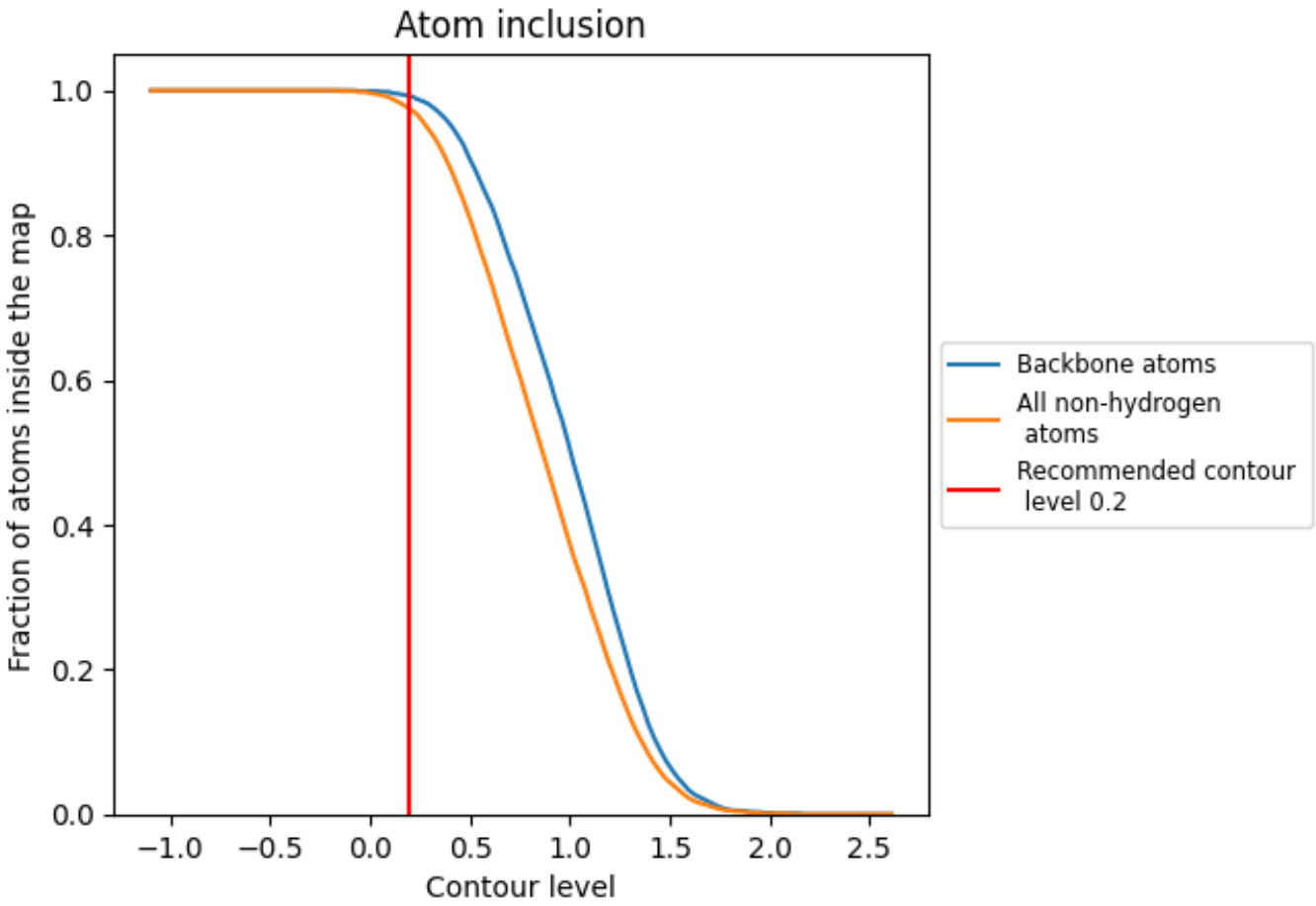
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9740	0.4650
E	0.9820	0.4830
N	0.9820	0.4530
O	0.9770	0.4230
P	0.9660	0.4640
X	0.9920	0.4970