Full wwPDB EM Validation Report

Nov 29, 2022 – 04:37 AM EST

PDB ID	:	7UY7
EMDB ID	:	EMD-26866
Title	:	Tetrahymena CST with Polymerase alpha-Primase
Authors	:	He, Y.; Song, H.; Chan, H.; Wang, Y.; Liu, B.; Susac, L.; Zhou, Z.H.; Feigon, J.
Deposited on	:	2022-05-06
Resolution	:	4.20 Å(reported)

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

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

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

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

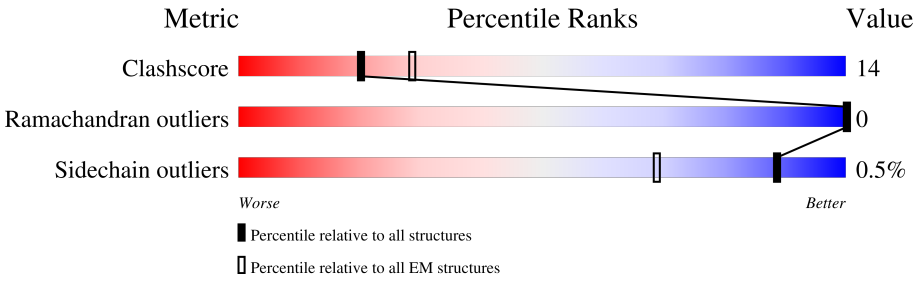
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.20 Å.

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



Metric	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	A	622	60% 28% 11%
2	B	373	53% 25% 22%
3	C	164	63% 33%
4	D	422	5% 94%
5	E	1393	38% 18% 44%
6	F	60	15% 83%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15161 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 Telomerase-associated protein of 75 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	552	Total	C	N	O	S	0	0
			4634	3014	756	847	17		

- Molecule 2 is a protein called Telomerase-associated protein of 45 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	291	Total	C	N	O	S	0	0
			2378	1542	382	446	8		

- Molecule 3 is a protein called Telomerase-associated protein of 19 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	157	Total	C	N	O	S	0	0
			1315	844	221	248	2		

- Molecule 4 is a protein called Telomerase associated protein p50.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	25	Total	C	N	O	0	0
			213	137	35	41		

- Molecule 5 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	783	Total	C	N	O	S	0	0
			6408	4137	1051	1195	25		

- Molecule 6 is a DNA chain called Telomere DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	10	Total	C	N	O	P	0	0
			212	100	38	64	10		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

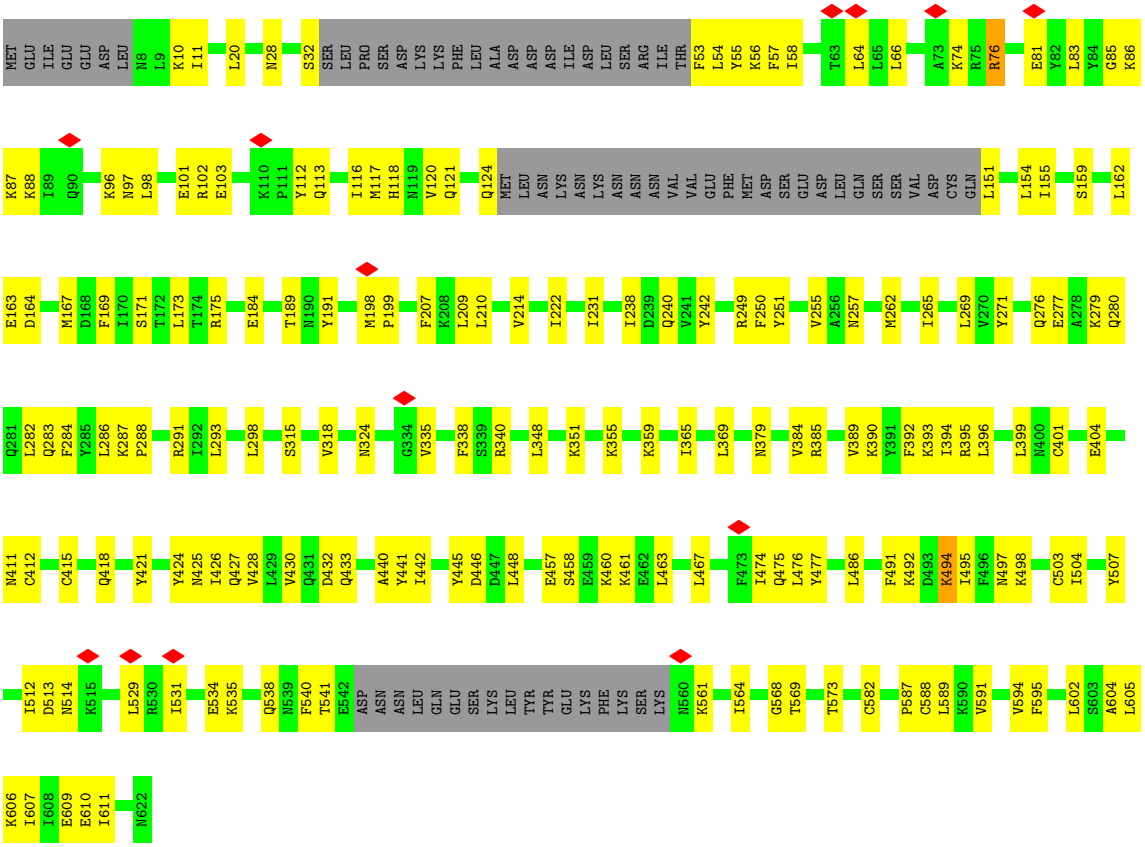
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	A	1	1	1	0

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.

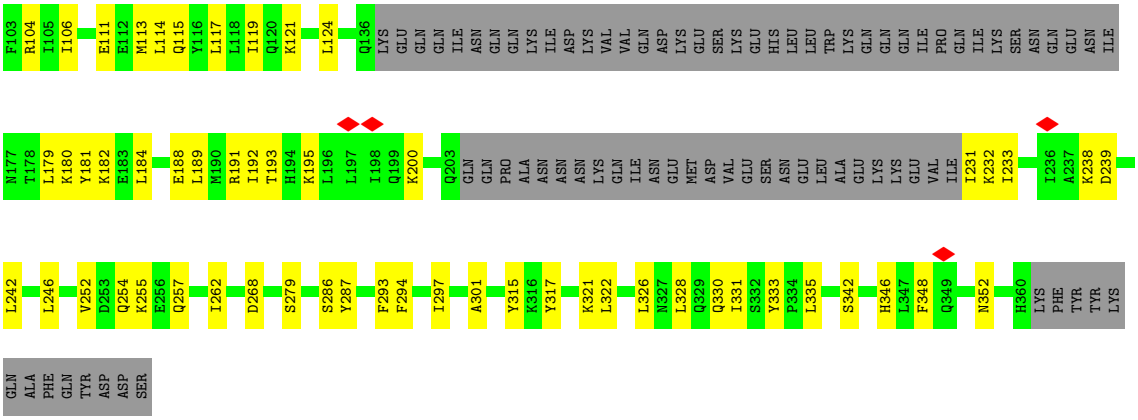
• Molecule 1: Telomerase-associated protein of 75 kDa

Chain A:



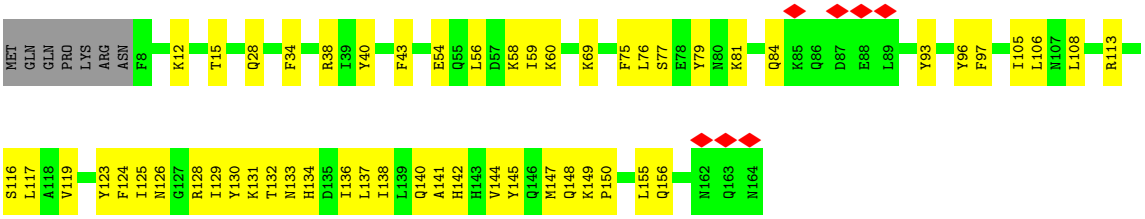
• Molecule 2: Telomerase-associated protein of 45 kDa

Chain B:



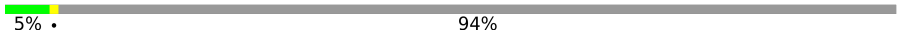
• Molecule 3: Telomerase-associated protein of 19 kDa

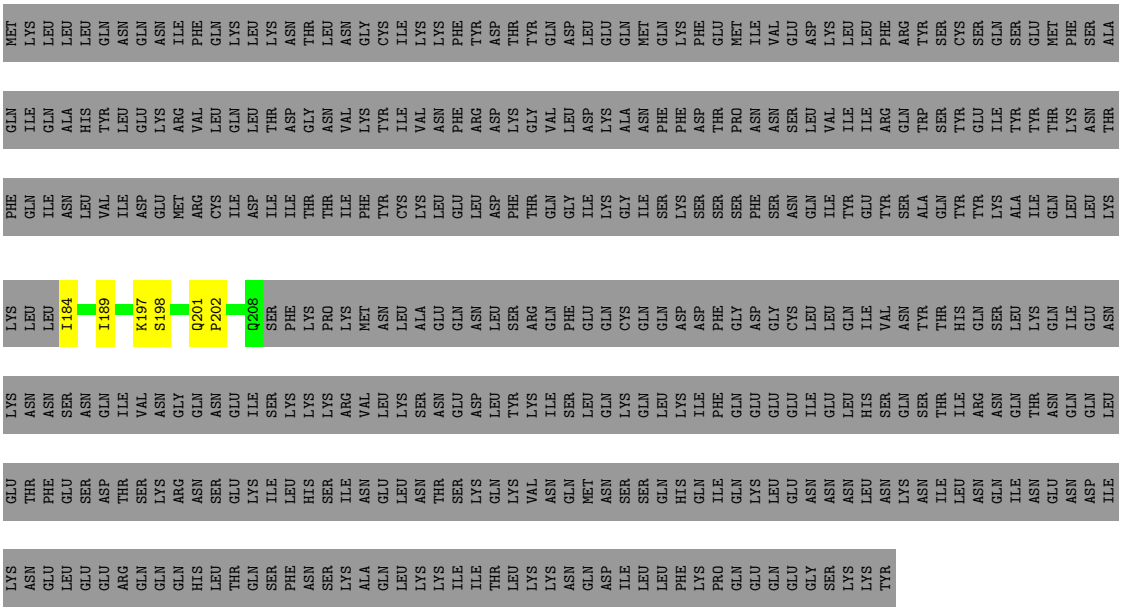
Chain C:



• Molecule 4: Telomerase associated protein p50

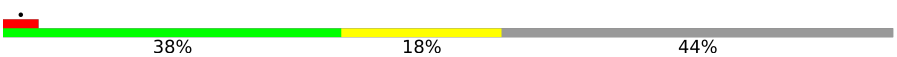
Chain D:

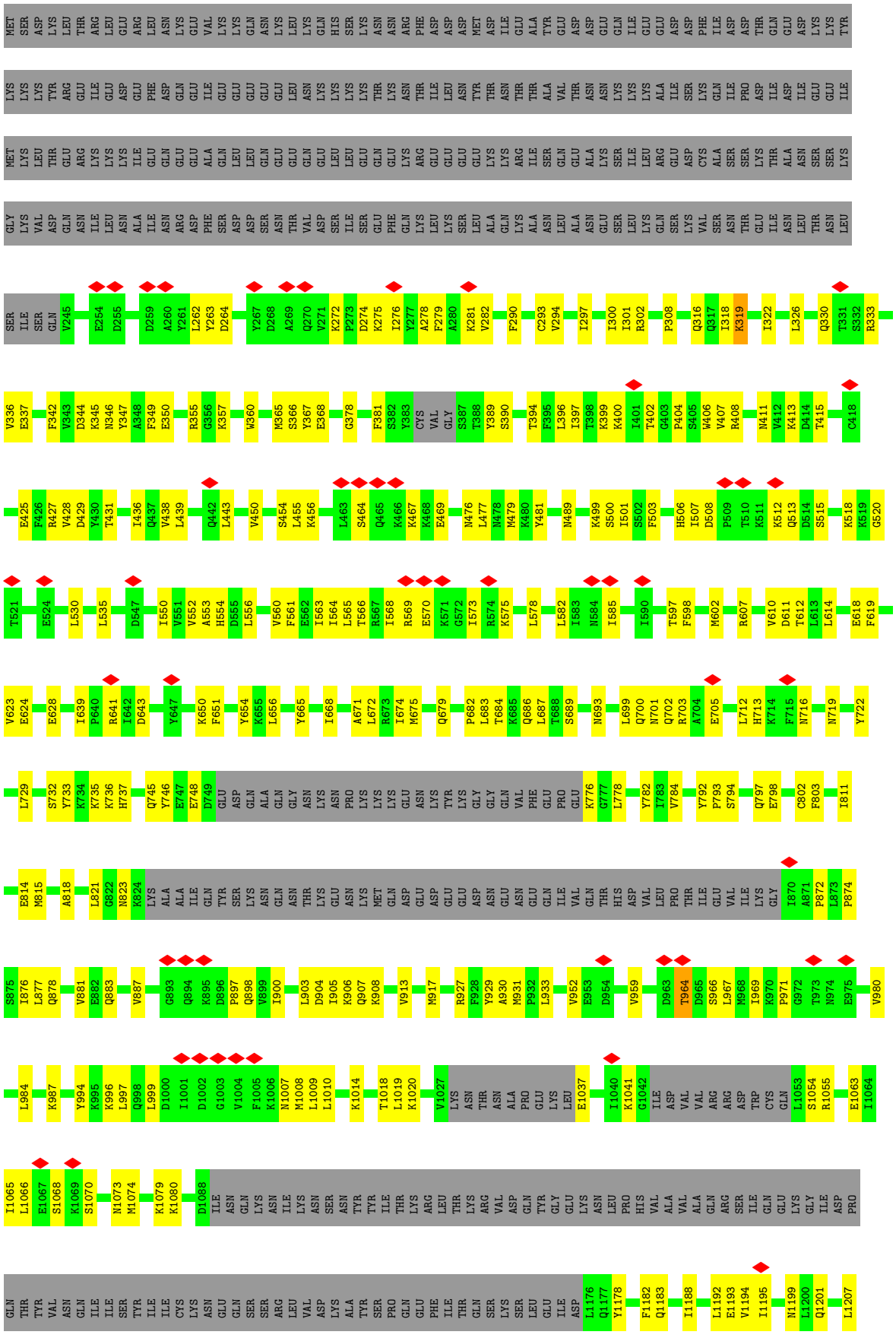


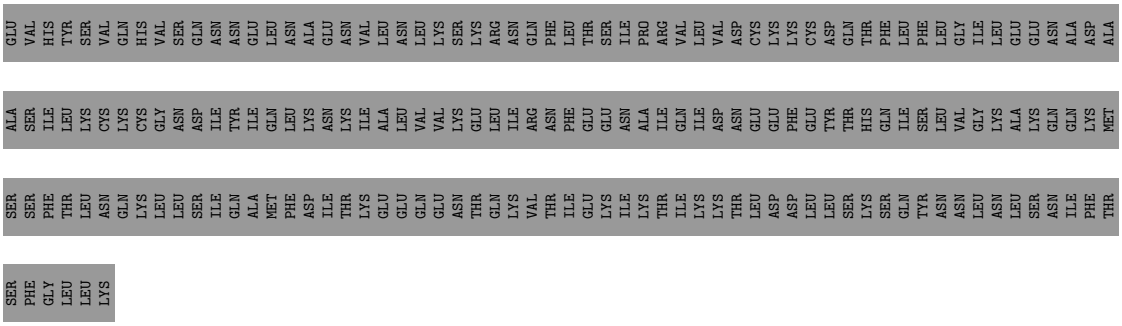


• Molecule 5: DNA polymerase

Chain E:

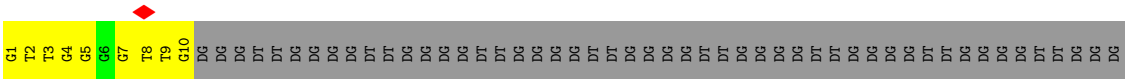



MET SER ASP LYS LEU THR ARG LEU GLU ARG LEU ASN LYS GLU VAL LYS LYS GLN ASN LYS LEU LYS GLN HIS SER LYS ASN ASN ARG PHE ASP ASP ASP GLU GLN ILE GLU GLU ASP ASP PHE ILE ASP ASP THR GLN GLU ASP LYS LYS TYR
LYS LYS LYS TYR ARG GLU ILE GLU ASP GLU PHE ASP GLN GLU ILE GLU GLU GLU ASP THR LYS ASN THR ILE ILE LEU ASN TYR THR ASN ASN LYS LYS LYS ALA ILE SER LYS GLN LYS GLU ILE PRO ASP ILE ASP ILE GLU GLU ILE
MET LYS LEU THR GLU ARG LYS LYS ILE GLU GLN GLU GLU ALA GLN LEU LEU GLN GLU GLU GLU GLU GLN LEU LEU GLU GLN LEU GLU GLU LYS ARG GLU GLU GLU LYS LYS ARG ILE SER GLN GLU GLU ALA LYS SER ILE LEU LEU ARG GLU ASP CYS ALA SER SER THR LYS THR ALA ASN SER SER LYS
GLY LYS VAL ASP GLN ASN ILE LEU ASN ALA ILE ASN ARG ASP PHE SER ASP ASP SER ASN THR VAL ASP SER ILE SER GLU PHE GLN LYS LEU LYS SER LEU ALA GLN LYS ALA ASN LEU ALA ALA ASN GLU SER LEU LYS GLN SER LYS VAL SER ASN THR GLU ILE ASN LEU THR ASN LEU
SER ILE SER GLN V245 E264 D255 D259 A260 Y261 L262 Y263 D264 Y267 D268 A269 Q270 V271 K272 P273 D274 K275 I276 Y277 A278 F279 A280 K281 V282 F290 C293 V294 I297 I300 I301 R302 P308 Q316 Q317 I318 K319 I322 L326 Q330 T331 S332 R333
V336 E337 F342 V343 D344 K345 N346 Y347 A348 F349 E350 R355 G356 K357 W360 M365 S366 Y367 E368 G378 F381 S382 Y383 CYS VAL GLY S387 T388 Y389 S390 T394 F395 L396 I397 T398 K399 K400 I401 T402 G403 P404 S405 W406 V407 R408 N411 V412 K413 D414 T415 C418
E425 F426 R427 V428 D429 Y430 T431 I436 Q437 V438 L439 Q442 L443 V450 S454 L455 K456 L463 S464 Q465 K466 K467 K468 E469 N476 L477 M478 M479 K480 Y481 N489 K499 S500 I501 S502 P503 H506 I507 D508 P509 T510 K511 K512 Q513 D514 S515 K518 K519 G520
T521 E524 L530 L535 D547 I550 V551 V552 A553 H554 D555 L556 V560 F561 E562 I563 I564 L565 T566 R567 I568 R569 E570 K571 G572 I573 R574 K575 L578 L582 I583 N584 I585 I590 T597 F598 M602 R607 V610 D611 T612 L613 L614 E618 F619
V623 E624 E628 I639 P640 R641 I642 D643 Y647 K650 F651 Y654 K655 L656 Y665 I668 A671 L672 R673 I674 M675 Q679 P682 L683 T684 K685 Q686 L687 T688 S689 N693 L699 Q700 N701 Q702 R703 A704 E705 L712 H713 K714 F715 N716 N719 Y722
L729 S732 Y733 K734 K735 K736 H737 Q745 Y746 E747 E748 D749 GLU ASP GLN ALA GLN GLY ASN LYS ASN PRO LYS LYS LYS GLU ASN LYS TYR LYS GLY GLY GLN VAL PHE GLU PRO GLU K776 G777 L778 Y782 I783 V784 Y792 P793 S794 Q797 E798 C802 F803 I811
E814 M815 A818 L821 G822 N823 K824 LYS ALA ALA ILE GLN TYR SER LYS ASN GLN ASN THR LYS GLU ASN LYS MET GLN ASP GLU ASP GLU GLU ASP ASN GLU ASN GLU GLN ILE VAL GLN THR HIS ASP VAL LEU PRO THR ILE GLU VAL ILE LYS GLY I870 A871 P872 L873 P874
S875 I876 L877 Q878 V881 E882 Q883 V887 G893 Q894 K895 D896 P897 Q898 V899 I900 L903 D904 I905 K906 Q907 K908 V913 M917 R927 F928 Y929 A930 M931 P932 L933 V952 E953 D954 V959 D963 T964 D965 S966 L967 N968 I969 K970 P971 Q972 T973 N974 E975 V980
L984 K987 Y994 K995 K996 L997 Q998 L999 D1000 I1001 D1002 G1003 V1004 F1005 K1006 N1007 M1008 L1009 L1010 K1014 T1018 L1019 K1020 V1027 LYS ASN THR ASN ALA PRO GLU LYS LEU E1037 I1040 K1041 G1042 ILE ASP VAL VAL ARG ARG ASP TRP CYS GLN L1053 S1054 R1055 E1063 I1064
I1065 L1066 E1067 S1068 K1069 S1070 N1073 M1074 K1079 K1080 D1088 ILE ASN GLN LYS ASN ILE LYS ASN SER ASN TYR TYR ILE THR LYS ARG LEU THR LYS ARG VAL ASP GLN TYR GLY GLU LYS ASN LEU PRO HIS VAL ALA VAL ALA GLN ARG SER ILE GLN GLU LYS GLY ILE ASP PRO
GLN THR TYR VAL ASN GLN ILE ILE SER TYR ILE ILE CYS LYS ASN GLU GLN SER SER ARG LEU VAL ASP LYS ALA TYR SER PRO GLN GLU PHE ILE THR GLN SER LYS SER LEU GLU ILE ASP L1176 Q1177 Y1178 F1182 Q1183 I1188 L1192 E1193 V1194 I1195 N1199 L1200 Q1201 L1207



• Molecule 6: Telomere DNA

Chain F: 15% 83%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142912	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/4726	0.47	0/6358
2	B	0.25	0/2417	0.45	0/3251
3	C	0.25	0/1341	0.46	0/1805
4	D	0.25	0/217	0.42	0/291
5	E	0.25	0/6526	0.45	0/8791
6	F	0.48	0/237	0.96	0/366
All	All	0.26	0/15464	0.47	0/20862

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	A	4634	0	4681	146	0
2	B	2378	0	2434	76	0
3	C	1315	0	1295	40	0
4	D	213	0	209	6	0
5	E	6408	0	6550	166	0
6	F	212	0	115	8	0
7	A	1	0	0	0	0
All	All	15161	0	15284	417	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 14.

All (417) 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)
2:B:179:LEU:HD22	2:B:333:TYR:HB3	1.16	1.08
5:E:966:SER:O	5:E:967:LEU:HD22	1.59	1.01
1:A:497:ASN:ND2	2:B:65:MET:HG3	1.77	0.98
2:B:179:LEU:CD2	2:B:333:TYR:HB3	2.03	0.87
1:A:494:LYS:HB2	1:A:494:LYS:NZ	1.96	0.81
1:A:494:LYS:HG3	1:A:495:ILE:HD12	1.63	0.80
2:B:7:LEU:HG	2:B:119:ILE:HD13	1.64	0.78
5:E:553:ALA:HB1	5:E:560:VAL:HG21	1.66	0.76
1:A:495:ILE:HD12	1:A:495:ILE:H	1.50	0.75
2:B:179:LEU:HD22	2:B:333:TYR:CB	2.09	0.74
1:A:494:LYS:HB2	1:A:494:LYS:HZ2	1.53	0.73
1:A:497:ASN:ND2	2:B:65:MET:CG	2.52	0.73
3:C:129:ILE:HG22	3:C:137:LEU:HD12	1.72	0.72
5:E:456:LYS:HB2	5:E:476:ASN:HB3	1.71	0.72
2:B:342:SER:O	2:B:346:HIS:ND1	2.22	0.71
5:E:994:TYR:HB3	5:E:997:LEU:HB3	1.72	0.71
5:E:262:LEU:HD11	5:E:278:ALA:HB1	1.70	0.71
1:A:392:PHE:HB2	1:A:426:ILE:HG12	1.72	0.70
2:B:279:SER:HB3	2:B:286:SER:H	1.57	0.69
3:C:108:LEU:HD21	3:C:113:ARG:HD2	1.75	0.69
1:A:534:GLU:O	1:A:538:GLN:NE2	2.26	0.69
5:E:301:ILE:HA	5:E:366:SER:HA	1.74	0.69
5:E:575:LYS:HD3	5:E:578:LEU:HD11	1.74	0.69
2:B:89:ASN:HA	2:B:94:GLN:HG2	1.75	0.69
1:A:395:ARG:HD3	1:A:475:GLN:HE21	1.57	0.69
3:C:132:THR:HG23	3:C:134:HIS:H	1.58	0.68
5:E:575:LYS:HB3	5:E:578:LEU:HD12	1.74	0.67
5:E:952:VAL:HG11	5:E:959:VAL:HG12	1.76	0.67
5:E:302:ARG:N	5:E:365:MET:O	2.28	0.67
5:E:563:ILE:HA	5:E:566:THR:HG22	1.75	0.67
4:D:197:LYS:O	4:D:201:GLN:NE2	2.28	0.65
1:A:242:TYR:O	1:A:324:ASN:ND2	2.24	0.65
1:A:401:CYS:HB3	5:E:467:LYS:HZ3	1.61	0.65
1:A:102:ARG:NH2	1:A:103:GLU:OE2	2.30	0.65
5:E:966:SER:C	5:E:967:LEU:HD22	2.17	0.65
3:C:93:TYR:HA	3:C:108:LEU:HB3	1.78	0.65
1:A:495:ILE:HD12	1:A:495:ILE:N	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1070:SER:HB3	5:E:1073:ASN:HB2	1.78	0.64
2:B:231:ILE:N	2:B:287:TYR:O	2.31	0.64
3:C:128:ARG:H	3:C:140:GLN:HB2	1.62	0.64
1:A:389:VAL:HG12	1:A:428:VAL:HG22	1.80	0.63
3:C:130:TYR:HE2	3:C:140:GLN:HE21	1.48	0.62
1:A:315:SER:HB3	1:A:318:VAL:HG23	1.81	0.61
1:A:457:GLU:HA	1:A:460:LYS:HD2	1.81	0.61
5:E:1008:MET:HA	5:E:1018:THR:HA	1.82	0.61
1:A:238:ILE:HG22	1:A:240:GLN:H	1.64	0.61
5:E:802:CYS:SG	5:E:803:PHE:N	2.73	0.61
1:A:293:LEU:HB2	1:A:338:PHE:HE1	1.65	0.61
2:B:233:ILE:HD11	2:B:262:ILE:HG21	1.82	0.60
1:A:58:ILE:HB	1:A:112:TYR:HA	1.82	0.60
5:E:964:THR:HG23	5:E:964:THR:O	2.01	0.60
4:D:184:ILE:HG13	4:D:189:ILE:HD13	1.84	0.60
5:E:397:ILE:HD11	5:E:713:HIS:HA	1.84	0.60
5:E:355:ARG:HH22	5:E:803:PHE:HB2	1.66	0.59
5:E:794:SER:HB3	5:E:997:LEU:HA	1.85	0.59
1:A:393:LYS:HB3	1:A:475:GLN:HE22	1.66	0.59
5:E:686:GLN:HG2	5:E:906:LYS:HA	1.83	0.59
1:A:64:LEU:HD12	1:A:74:LYS:HB3	1.85	0.59
1:A:262:MET:HB3	1:A:379:ASN:HD22	1.68	0.59
1:A:395:ARG:NH1	6:F:9:DT:O4	2.35	0.59
1:A:474:ILE:HG13	1:A:476:LEU:H	1.66	0.59
5:E:294:VAL:HB	5:E:425:GLU:HG2	1.84	0.58
1:A:396:LEU:HB2	1:A:467:LEU:HD21	1.84	0.58
3:C:60:LYS:HA	3:C:134:HIS:HE1	1.68	0.58
3:C:149:LYS:NZ	3:C:150:PRO:O	2.37	0.58
2:B:317:TYR:O	2:B:321:LYS:HG2	2.04	0.57
5:E:913:VAL:O	5:E:917:MET:HG2	2.03	0.57
1:A:445:TYR:CZ	6:F:4:DG:H2"	2.40	0.57
1:A:394:ILE:HD12	1:A:476:LEU:HD22	1.86	0.57
1:A:573:THR:OG1	1:A:582:CYS:SG	2.62	0.57
2:B:85:LEU:HA	2:B:98:ILE:HG22	1.85	0.57
2:B:232:LYS:HA	2:B:286:SER:HA	1.86	0.57
5:E:503:PHE:HB3	5:E:535:LEU:HD11	1.87	0.57
5:E:575:LYS:HB3	5:E:578:LEU:CD1	2.34	0.57
5:E:797:GLN:HB2	5:E:877:LEU:HD11	1.87	0.57
5:E:1054:SER:HB3	5:E:1183:GLN:HB3	1.87	0.56
1:A:98:LEU:O	1:A:102:ARG:HB2	2.05	0.56
1:A:390:LYS:NZ	1:A:441:TYR:OH	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:PHE:O	1:A:495:ILE:CD1	2.53	0.56
3:C:125:ILE:HD11	3:C:141:ALA:HB1	1.88	0.56
5:E:330:GLN:O	5:E:333:ARG:NH1	2.36	0.56
2:B:104:ARG:HG2	2:B:106:ILE:HG23	1.86	0.55
1:A:11:ILE:HG13	1:A:280:GLN:HE22	1.71	0.55
1:A:541:THR:HA	2:B:238:LYS:HE3	1.89	0.55
1:A:430:VAL:O	1:A:440:ALA:N	2.40	0.55
1:A:424:TYR:HB2	1:A:446:ASP:HA	1.89	0.55
5:E:365:MET:HG2	5:E:366:SER:H	1.72	0.55
1:A:76:ARG:NH1	1:A:97:ASN:O	2.29	0.54
5:E:1199:ASN:HD21	5:E:1201:GLN:HE21	1.55	0.54
1:A:568:GLY:HA2	1:A:588:CYS:H	1.72	0.54
2:B:184:LEU:O	2:B:188:GLU:HG2	2.08	0.54
5:E:272:LYS:HB3	5:E:275:LYS:HB2	1.89	0.54
5:E:566:THR:HA	5:E:569:ARG:HH12	1.72	0.54
2:B:45:VAL:HG23	2:B:46:PRO:HD3	1.90	0.54
3:C:81:LYS:O	3:C:84:GLN:HG2	2.08	0.54
5:E:610:VAL:HG22	5:E:699:LEU:HD13	1.90	0.54
5:E:798:GLU:HA	5:E:996:LYS:HE3	1.89	0.54
5:E:987:LYS:HA	5:E:999:LEU:HD23	1.90	0.54
2:B:348:PHE:O	2:B:352:ASN:N	2.42	0.53
1:A:189:THR:HG1	1:A:191:TYR:HD2	1.56	0.53
1:A:284:PHE:O	1:A:340:ARG:NH1	2.42	0.53
1:A:611:ILE:HD13	2:B:121:LYS:HE2	1.90	0.53
2:B:246:LEU:HD13	2:B:252:VAL:HB	1.90	0.53
5:E:506:HIS:ND1	5:E:508:ASP:O	2.41	0.53
1:A:57:PHE:HB3	1:A:81:GLU:H	1.72	0.53
1:A:498:LYS:O	2:B:102:ARG:NH2	2.36	0.53
5:E:297:ILE:HA	5:E:428:VAL:O	2.08	0.53
1:A:411:ASN:OD1	1:A:418:GLN:NE2	2.39	0.53
5:E:455:LEU:HD11	5:E:564:ILE:HD11	1.91	0.53
1:A:365:ILE:HD11	1:A:587:PRO:HG2	1.90	0.53
3:C:131:LYS:HA	3:C:137:LEU:HA	1.90	0.53
5:E:512:LYS:HG3	5:E:513:GLN:HG2	1.89	0.53
1:A:504:ILE:HD12	1:A:591:VAL:HG12	1.89	0.53
2:B:68:PHE:N	5:E:746:TYR:OH	2.42	0.53
5:E:302:ARG:HG3	5:E:367:TYR:HE1	1.73	0.53
1:A:399:LEU:HB2	1:A:421:TYR:HD1	1.74	0.52
1:A:604:ALA:HB2	2:B:114:LEU:HD21	1.91	0.52
5:E:611:ASP:HB3	5:E:614:LEU:HG	1.90	0.52
1:A:495:ILE:H	1:A:495:ILE:CD1	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:411:ASN:O	5:E:413:LYS:NZ	2.41	0.52
5:E:929:TYR:OH	5:E:931:MET:SD	2.64	0.52
1:A:169:PHE:CZ	1:A:173:LEU:HD11	2.44	0.52
2:B:47:HIS:ND1	2:B:64:ASP:OD1	2.41	0.52
1:A:458:SER:O	1:A:461:LYS:HG2	2.09	0.52
5:E:671:ALA:HA	5:E:674:ILE:HD12	1.92	0.52
1:A:486:LEU:HD11	5:E:746:TYR:HA	1.91	0.52
2:B:294:PHE:HA	2:B:297:ILE:HD12	1.92	0.52
1:A:495:ILE:O	2:B:102:ARG:NH2	2.42	0.52
1:A:491:PHE:O	1:A:495:ILE:HD13	2.10	0.52
3:C:147:MET:SD	3:C:148:GLN:N	2.83	0.52
5:E:515:SER:HA	5:E:518:LYS:HD3	1.92	0.52
1:A:269:LEU:HD21	1:A:335:VAL:HG21	1.91	0.51
5:E:489:ASN:ND2	5:E:898:GLN:HG2	2.25	0.51
3:C:124:PHE:HE2	3:C:147:MET:HB2	1.75	0.51
3:C:105:ILE:HD13	3:C:138:ILE:HG12	1.93	0.51
6:F:2:DT:H2"	6:F:3:DT:H5'	1.92	0.51
5:E:782:TYR:O	5:E:971:PRO:HD2	2.11	0.51
1:A:66:LEU:HB2	1:A:74:LYS:HE3	1.93	0.51
5:E:408:ARG:HB2	5:E:439:LEU:HD21	1.92	0.51
2:B:331:ILE:HG21	2:B:335:LEU:HD21	1.92	0.51
3:C:124:PHE:N	3:C:145:TYR:O	2.34	0.51
1:A:76:ARG:HD3	1:A:76:ARG:H	1.76	0.50
3:C:93:TYR:O	3:C:108:LEU:N	2.42	0.50
5:E:406:TRP:O	5:E:439:LEU:N	2.42	0.50
1:A:251:TYR:HB2	1:A:269:LEU:HB2	1.93	0.50
3:C:15:THR:HG21	3:C:156:GLN:HG2	1.93	0.50
5:E:396:LEU:O	5:E:400:LYS:N	2.45	0.50
1:A:445:TYR:HB2	1:A:448:LEU:HD13	1.94	0.50
3:C:126:ASN:O	3:C:142:HIS:N	2.41	0.50
5:E:308:PRO:HA	5:E:381:PHE:HA	1.94	0.50
1:A:494:LYS:NZ	1:A:494:LYS:CB	2.73	0.50
2:B:182:LYS:HD3	2:B:333:TYR:CZ	2.46	0.50
2:B:39:GLN:HB3	2:B:47:HIS:HD2	1.77	0.50
5:E:479:MET:N	5:E:501:ILE:O	2.41	0.50
5:E:582:LEU:HD12	5:E:585:ILE:HD11	1.92	0.50
1:A:385:ARG:HH21	2:B:82:ILE:HG23	1.76	0.50
5:E:512:LYS:HE3	5:E:530:LEU:HA	1.94	0.50
5:E:872:PRO:O	5:E:876:ILE:HG13	2.11	0.50
1:A:611:ILE:HD11	2:B:124:LEU:HD13	1.92	0.49
1:A:602:LEU:HD13	1:A:605:LEU:HD21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:407:VAL:HG12	5:E:438:VAL:HG22	1.94	0.49
1:A:282:LEU:HD21	1:A:286:LEU:HD13	1.93	0.49
5:E:897:PRO:HA	5:E:900:ILE:HB	1.94	0.49
1:A:514:ASN:HD22	1:A:569:THR:HG21	1.76	0.49
5:E:612:THR:HB	5:E:674:ILE:HG21	1.93	0.49
1:A:85:GLY:O	1:A:87:LYS:NZ	2.39	0.49
2:B:192:ILE:HA	2:B:195:LYS:HD3	1.95	0.49
5:E:1014:LYS:O	5:E:1041:LYS:NZ	2.34	0.49
1:A:76:ARG:NH1	1:A:98:LEU:HA	2.28	0.49
1:A:83:LEU:HD12	1:A:86:LYS:HA	1.95	0.49
2:B:326:LEU:HB3	2:B:328:LEU:HD23	1.94	0.49
5:E:455:LEU:HD21	5:E:564:ILE:HG13	1.94	0.49
5:E:1068:SER:HB2	5:E:1073:ASN:HB3	1.95	0.49
2:B:48:LYS:HG3	2:B:66:TYR:CZ	2.47	0.49
3:C:28:GLN:HB3	3:C:133:ASN:HA	1.95	0.49
3:C:128:ARG:NE	3:C:140:GLN:OE1	2.41	0.49
5:E:389:TYR:OH	5:E:722:TYR:O	2.28	0.49
5:E:930:ALA:HB1	5:E:933:LEU:HD23	1.94	0.49
2:B:53:GLN:HB2	2:B:58:GLU:HG3	1.95	0.48
5:E:281:LYS:HE3	5:E:290:PHE:HB3	1.93	0.48
5:E:406:TRP:NE1	5:E:443:LEU:HB2	2.28	0.48
2:B:7:LEU:HB3	2:B:23:CYS:HB3	1.95	0.48
5:E:618:GLU:OE2	5:E:703:ARG:NH2	2.46	0.48
5:E:776:LYS:HA	5:E:1010:LEU:HD23	1.95	0.48
5:E:818:ALA:HB1	5:E:823:ASN:HB3	1.95	0.48
5:E:390:SER:O	5:E:394:THR:OG1	2.20	0.48
5:E:467:LYS:NZ	5:E:469:GLU:OE2	2.46	0.48
2:B:200:LYS:HE2	2:B:231:ILE:HD11	1.95	0.48
5:E:566:THR:HA	5:E:569:ARG:NH1	2.28	0.48
3:C:54:GLU:O	3:C:58:LYS:HG2	2.13	0.48
5:E:347:TYR:CZ	5:E:349:PHE:HB2	2.48	0.48
1:A:198:MET:N	1:A:199:PRO:HD3	2.28	0.48
3:C:60:LYS:HA	3:C:134:HIS:CE1	2.48	0.48
2:B:192:ILE:HD12	2:B:195:LYS:HB2	1.96	0.48
2:B:328:LEU:HD12	2:B:330:GLN:HE22	1.78	0.48
5:E:732:SER:O	5:E:735:LYS:HG2	2.13	0.48
1:A:83:LEU:HA	1:A:88:LYS:HA	1.96	0.47
1:A:271:TYR:HE2	1:A:279:LYS:HE2	1.79	0.47
2:B:189:LEU:O	2:B:193:THR:HG23	2.14	0.47
3:C:116:SER:O	3:C:123:TYR:OH	2.21	0.47
1:A:249:ARG:HB2	1:A:271:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HA	1:A:351:LYS:HZ2	1.80	0.47
2:B:315:TYR:HE2	2:B:342:SER:HA	1.80	0.47
1:A:379:ASN:OD1	1:A:507:TYR:HB3	2.13	0.47
1:A:393:LYS:HB2	1:A:425:ASN:HB3	1.96	0.47
1:A:448:LEU:HD22	1:A:591:VAL:HG23	1.96	0.47
5:E:675:MET:O	5:E:679:GLN:N	2.47	0.47
1:A:98:LEU:O	1:A:102:ARG:CB	2.63	0.47
1:A:293:LEU:HB2	1:A:338:PHE:CE1	2.48	0.47
5:E:345:LYS:HB2	5:E:360:TRP:CD1	2.49	0.47
5:E:507:ILE:HB	5:E:651:PHE:HE2	1.78	0.47
1:A:262:MET:HB3	1:A:379:ASN:ND2	2.29	0.47
1:A:393:LYS:N	1:A:425:ASN:O	2.40	0.47
1:A:442:ILE:HD13	1:A:589:LEU:HB2	1.96	0.47
2:B:47:HIS:HB3	2:B:62:PHE:HE1	1.80	0.47
3:C:77:SER:O	3:C:81:LYS:HG2	2.15	0.47
5:E:1192:LEU:HD23	5:E:1195:ILE:HD12	1.97	0.47
5:E:618:GLU:HG2	5:E:701:ASN:HD21	1.78	0.46
5:E:643:ASP:N	5:E:643:ASP:OD1	2.45	0.46
5:E:904:ASP:O	5:E:907:GLN:HG3	2.15	0.46
3:C:76:LEU:HD22	3:C:96:TYR:HB2	1.96	0.46
5:E:406:TRP:CG	5:E:443:LEU:HD12	2.50	0.46
1:A:412:CYS:HB3	1:A:415:CYS:O	2.14	0.46
2:B:114:LEU:HD13	2:B:117:LEU:HD12	1.96	0.46
5:E:476:ASN:OD1	5:E:477:LEU:N	2.48	0.46
5:E:1188:ILE:HD11	5:E:1207:LEU:HD11	1.97	0.46
1:A:207:PHE:HA	1:A:210:LEU:HD13	1.98	0.46
2:B:63:LEU:HD13	2:B:66:TYR:HB3	1.98	0.46
5:E:1063:GLU:HA	5:E:1066:LEU:HD12	1.98	0.46
1:A:54:LEU:HD12	1:A:120:VAL:HG11	1.97	0.46
1:A:175:ARG:CZ	1:A:175:ARG:HB3	2.46	0.46
3:C:34:PHE:HB3	3:C:130:TYR:HD2	1.80	0.46
5:E:778:LEU:HD13	5:E:1009:LEU:HB2	1.97	0.46
1:A:512:ILE:HD12	1:A:564:ILE:HG12	1.98	0.46
2:B:11:LYS:NZ	2:B:12:GLU:OE2	2.40	0.46
5:E:556:LEU:H	5:E:611:ASP:CG	2.18	0.46
5:E:565:LEU:HD13	5:E:568:ILE:HD12	1.97	0.46
5:E:282:VAL:HG22	5:E:293:CYS:SG	2.56	0.46
5:E:628:GLU:HA	5:E:639:ILE:HD13	1.98	0.46
5:E:650:LYS:HD2	5:E:656:LEU:HB3	1.98	0.46
5:E:345:LYS:H	5:E:360:TRP:HD1	1.63	0.46
5:E:429:ASP:OD2	5:E:431:THR:OG1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:LEU:HD11	2:B:76:PHE:HA	1.98	0.45
5:E:326:LEU:HD13	5:E:336:VAL:HG12	1.98	0.45
5:E:618:GLU:HG2	5:E:701:ASN:ND2	2.31	0.45
1:A:164:ASP:HB2	4:D:202:PRO:HG3	1.97	0.45
1:A:222:ILE:HG13	1:A:288:PRO:HA	1.97	0.45
2:B:10:LEU:HA	2:B:13:LEU:HD13	1.99	0.45
3:C:75:PHE:HB3	3:C:79:TYR:CZ	2.51	0.45
5:E:565:LEU:HA	5:E:568:ILE:HD12	1.98	0.45
6:F:7:DG:H2"	6:F:8:DT:C6	2.51	0.45
1:A:291:ARG:HB3	1:A:338:PHE:HB2	1.99	0.45
1:A:395:ARG:NH2	1:A:404:GLU:OE1	2.49	0.45
2:B:106:ILE:HB	2:B:111:GLU:HG3	1.99	0.45
2:B:239:ASP:OD1	2:B:242:LEU:N	2.33	0.45
5:E:814:GLU:HG2	5:E:815:MET:HE3	1.98	0.45
1:A:384:VAL:HG12	1:A:432:ASP:HA	1.99	0.45
5:E:883:GLN:O	5:E:887:VAL:HG23	2.15	0.45
5:E:1055:ARG:HG3	5:E:1183:GLN:HG2	1.98	0.45
1:A:58:ILE:HD12	1:A:113:GLN:H	1.80	0.45
1:A:395:ARG:NH1	1:A:474:ILE:O	2.40	0.45
1:A:10:LYS:HZ1	4:D:198:SER:HB3	1.81	0.45
2:B:252:VAL:HG12	2:B:252:VAL:O	2.16	0.45
2:B:293:PHE:CE2	2:B:297:ILE:HD11	2.52	0.45
1:A:11:ILE:HG13	1:A:280:GLN:NE2	2.31	0.45
5:E:264:ASP:OD1	5:E:279:PHE:HB2	2.17	0.45
3:C:43:PHE:CE2	3:C:119:VAL:HA	2.52	0.45
1:A:287:LYS:HG2	1:A:288:PRO:HD2	1.98	0.45
3:C:60:LYS:HG2	3:C:133:ASN:HD21	1.82	0.45
1:A:355:LYS:O	1:A:359:LYS:HG3	2.17	0.44
5:E:350:GLU:O	5:E:811:ILE:N	2.47	0.44
1:A:531:ILE:O	1:A:535:LYS:HG2	2.17	0.44
5:E:745:GLN:HA	5:E:748:GLU:HG2	1.99	0.44
3:C:117:LEU:HD12	3:C:144:VAL:HG21	1.99	0.44
5:E:344:ASP:HB3	5:E:357:LYS:HE3	1.98	0.44
5:E:684:THR:HG21	5:E:699:LEU:HD23	1.99	0.44
5:E:1007:ASN:HB2	5:E:1019:LEU:HD12	2.00	0.44
1:A:56:LYS:HB2	1:A:117:MET:HG3	1.99	0.44
2:B:188:GLU:OE1	2:B:191:ARG:NH1	2.50	0.44
2:B:293:PHE:CZ	2:B:297:ILE:HD11	2.52	0.44
5:E:365:MET:HG2	5:E:366:SER:N	2.33	0.44
5:E:500:SER:HB3	5:E:665:TYR:CE1	2.52	0.44
5:E:693:ASN:ND2	5:E:705:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:454:SER:HB3	5:E:668:ILE:HG13	2.00	0.44
6:F:9:DT:H2"	6:F:10:DG:C8	2.53	0.44
5:E:570:GLU:OE1	5:E:570:GLU:N	2.47	0.44
5:E:1079:LYS:HE3	5:E:1080:LYS:NZ	2.33	0.44
5:E:1020:LYS:HG2	5:E:1037:GLU:HB2	2.00	0.44
5:E:980:VAL:O	5:E:984:LEU:HG	2.18	0.44
1:A:53:PHE:HD1	1:A:118:HIS:HA	1.83	0.44
1:A:255:VAL:N	1:A:265:ILE:O	2.39	0.44
1:A:384:VAL:HA	1:A:433:GLN:H	1.83	0.44
3:C:130:TYR:HE2	3:C:140:GLN:NE2	2.13	0.43
1:A:432:ASP:OD1	1:A:432:ASP:N	2.51	0.43
1:A:529:LEU:HD22	1:A:561:LYS:HE3	2.00	0.43
5:E:520:GLY:HA3	5:E:654:TYR:CZ	2.53	0.43
5:E:554:HIS:ND1	5:E:612:THR:OG1	2.44	0.43
5:E:887:VAL:HG13	5:E:903:LEU:HD22	2.01	0.43
1:A:175:ARG:HH22	1:A:293:LEU:HD22	1.84	0.43
5:E:556:LEU:HD11	5:E:561:PHE:CD2	2.54	0.43
5:E:623:VAL:HG13	5:E:624:GLU:HG2	2.00	0.43
1:A:121:GLN:HB2	1:A:154:LEU:HD21	1.99	0.43
1:A:540:PHE:HA	2:B:255:LYS:NZ	2.33	0.43
2:B:42:GLN:HE21	5:E:736:LYS:HD3	1.83	0.43
5:E:346:ASN:ND2	5:E:719:ASN:O	2.32	0.43
1:A:209:LEU:HD11	2:B:181:TYR:HA	2.01	0.43
5:E:712:LEU:HD11	5:E:927:ARG:HH22	1.83	0.43
1:A:504:ILE:HG22	1:A:594:VAL:HG12	2.01	0.43
5:E:668:ILE:O	5:E:672:LEU:HG	2.18	0.43
5:E:702:GLN:O	5:E:705:GLU:HG3	2.19	0.43
1:A:53:PHE:CD1	1:A:118:HIS:HA	2.54	0.43
1:A:163:GLU:C	4:D:202:PRO:HB3	2.39	0.43
1:A:55:TYR:OH	1:A:173:LEU:HD13	2.19	0.43
5:E:399:LYS:NZ	5:E:436:ILE:O	2.34	0.43
1:A:118:HIS:HB3	1:A:159:SER:HA	2.00	0.43
2:B:67:LYS:O	2:B:70:GLN:HG2	2.19	0.43
1:A:10:LYS:NZ	4:D:198:SER:HB3	2.33	0.43
1:A:184:GLU:HG3	1:A:257:ASN:OD1	2.19	0.43
1:A:396:LEU:HD12	1:A:421:TYR:O	2.18	0.43
1:A:497:ASN:HD21	2:B:65:MET:HG3	1.71	0.43
2:B:3:ASP:HB3	2:B:4:ASN:H	1.65	0.43
3:C:40:TYR:HB2	3:C:124:PHE:CE1	2.53	0.43
5:E:300:ILE:HD12	5:E:367:TYR:HD2	1.84	0.43
5:E:464:SER:OG	5:E:469:GLU:OE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:515:SER:O	5:E:518:LYS:NZ	2.49	0.43
5:E:619:PHE:HE2	5:E:908:LYS:HZ2	1.66	0.43
5:E:263:TYR:HB3	5:E:404:PRO:HB3	2.01	0.42
5:E:318:ILE:HG21	5:E:342:PHE:CZ	2.54	0.42
5:E:318:ILE:HG21	5:E:342:PHE:HZ	1.84	0.42
1:A:20:LEU:HG	1:A:53:PHE:CG	2.54	0.42
1:A:369:LEU:HD11	1:A:587:PRO:HD3	2.01	0.42
5:E:597:THR:HG21	5:E:700:GLN:HE22	1.84	0.42
5:E:878:GLN:HA	5:E:881:VAL:HG12	2.01	0.42
1:A:390:LYS:HB3	1:A:427:GLN:HG2	2.01	0.42
1:A:458:SER:O	1:A:461:LYS:N	2.51	0.42
2:B:113:MET:HE3	3:C:155:LEU:HA	2.01	0.42
5:E:337:GLU:OE1	5:E:337:GLU:N	2.51	0.42
5:E:415:THR:HG22	5:E:425:GLU:OE1	2.18	0.42
1:A:124:GLN:HB3	1:A:151:LEU:N	2.34	0.42
5:E:552:VAL:HG11	5:E:675:MET:CE	2.50	0.42
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.91	0.42
5:E:274:ASP:HB3	5:E:368:GLU:HB3	2.00	0.42
5:E:276:ILE:HB	5:E:297:ILE:HB	2.01	0.42
5:E:276:ILE:N	5:E:297:ILE:O	2.48	0.42
3:C:132:THR:HB	3:C:138:ILE:HD11	2.02	0.42
1:A:28:ASN:O	1:A:32:SER:N	2.47	0.42
1:A:385:ARG:NH2	2:B:23:CYS:SG	2.93	0.42
1:A:396:LEU:HB2	1:A:467:LEU:CD2	2.49	0.42
5:E:556:LEU:HA	5:E:560:VAL:HB	2.02	0.42
1:A:606:LYS:O	1:A:609:GLU:HG3	2.20	0.42
5:E:1188:ILE:O	5:E:1192:LEU:HG	2.19	0.42
1:A:231:ILE:HA	1:A:250:PHE:CZ	2.55	0.42
1:A:477:TYR:O	1:A:492:LYS:NZ	2.52	0.42
1:A:610:GLU:OE2	2:B:121:LYS:HE3	2.20	0.42
3:C:149:LYS:HD2	3:C:150:PRO:HD2	2.01	0.42
5:E:274:ASP:HA	5:E:300:ILE:HG12	2.00	0.42
1:A:271:TYR:CE2	1:A:279:LYS:HE2	2.55	0.42
5:E:322:ILE:O	5:E:326:LEU:HG	2.19	0.41
5:E:568:ILE:HG23	5:E:573:ILE:HB	2.01	0.41
5:E:598:PHE:O	5:E:602:MET:HG3	2.19	0.41
5:E:792:TYR:HB2	5:E:793:PRO:HD3	2.02	0.41
1:A:81:GLU:HB3	1:A:88:LYS:HD2	2.02	0.41
3:C:12:LYS:O	3:C:38:ARG:N	2.44	0.41
5:E:481:TYR:CE2	5:E:499:LYS:HD2	2.54	0.41
5:E:683:LEU:O	5:E:687:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:378:GLY:HA3	5:E:381:PHE:CE1	2.56	0.41
5:E:1192:LEU:HA	5:E:1195:ILE:HD12	2.03	0.41
1:A:513:ASP:OD1	1:A:513:ASP:N	2.52	0.41
5:E:316:GLN:O	5:E:319:LYS:HG3	2.21	0.41
5:E:682:PRO:HB2	5:E:905:ILE:HD13	2.03	0.41
1:A:277:GLU:OE1	1:A:277:GLU:N	2.40	0.41
1:A:460:LYS:O	1:A:463:LEU:HG	2.20	0.41
2:B:113:MET:O	2:B:117:LEU:HG	2.21	0.41
2:B:180:LYS:O	2:B:184:LEU:HD12	2.20	0.41
3:C:56:LEU:HA	3:C:59:ILE:HG22	2.02	0.41
5:E:300:ILE:HG13	5:E:367:TYR:HB2	2.02	0.41
5:E:729:LEU:HD23	5:E:733:TYR:CD2	2.55	0.41
5:E:874:PRO:HA	5:E:877:LEU:HG	2.02	0.41
1:A:167:MET:O	1:A:171:SER:N	2.37	0.41
2:B:268:ASP:OD2	2:B:333:TYR:OH	2.38	0.41
2:B:293:PHE:O	2:B:297:ILE:HG13	2.19	0.41
3:C:97:PHE:HB2	3:C:106:LEU:HD12	2.02	0.41
5:E:344:ASP:HB3	5:E:357:LYS:HB3	2.03	0.41
5:E:1178:TYR:HA	5:E:1182:PHE:CD2	2.56	0.41
6:F:4:DG:H2'	6:F:5:DG:O4'	2.21	0.41
2:B:34:PHE:HB3	2:B:39:GLN:HE21	1.86	0.41
1:A:96:LYS:NZ	1:A:155:ILE:O	2.53	0.41
1:A:494:LYS:O	1:A:498:LYS:CB	2.69	0.41
2:B:111:GLU:O	2:B:115:GLN:HG2	2.20	0.41
2:B:191:ARG:O	2:B:195:LYS:HG3	2.20	0.41
3:C:43:PHE:HE2	3:C:119:VAL:HA	1.86	0.41
6:F:4:DG:H2'	6:F:5:DG:C8	2.55	0.41
1:A:276:GLN:OE1	1:A:276:GLN:N	2.54	0.41
2:B:34:PHE:HB3	2:B:39:GLN:NE2	2.36	0.41
3:C:69:LYS:HG2	3:C:136:ILE:HD11	2.03	0.41
5:E:784:VAL:HG23	5:E:971:PRO:HG3	2.03	0.41
1:A:116:ILE:HD11	1:A:162:LEU:HD23	2.03	0.41
1:A:392:PHE:HA	1:A:426:ILE:HA	2.02	0.40
5:E:450:VAL:HG22	5:E:550:ILE:HB	2.02	0.40
5:E:737:HIS:ND1	5:E:821:LEU:HD13	2.36	0.40
5:E:952:VAL:HG13	5:E:969:ILE:HD13	2.03	0.40
1:A:64:LEU:HA	1:A:76:ARG:HA	2.04	0.40
1:A:607:ILE:O	1:A:611:ILE:HG22	2.21	0.40
6:F:1:DG:H2"	6:F:2:DT:H71	2.03	0.40
2:B:5:PHE:CG	2:B:21:LYS:HB3	2.55	0.40
2:B:10:LEU:HA	2:B:10:LEU:HD23	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:LEU:HD23	2:B:17:PRO:O	2.21	0.40
1:A:76:ARG:HH22	1:A:101:GLU:HB2	1.87	0.40
1:A:214:VAL:HA	1:A:298:LEU:HA	2.03	0.40
1:A:279:LYS:O	1:A:283:GLN:HG2	2.21	0.40
1:A:503:CYS:HB3	1:A:595:PHE:HB2	2.03	0.40
5:E:402:THR:O	5:E:689:SER:HA	2.21	0.40
5:E:1065:ILE:HG23	5:E:1074:MET:HG2	2.04	0.40
5:E:1193:GLU:HG2	5:E:1194:VAL:HG13	2.02	0.40
2:B:254:GLN:OE1	2:B:257:GLN:N	2.52	0.40
2:B:301:ALA:HA	2:B:322:LEU:HD21	2.04	0.40
5:E:479:MET:HB2	5:E:501:ILE:HB	2.02	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	A	544/622 (88%)	523 (96%)	21 (4%)	0	100	100
2	B	285/373 (76%)	274 (96%)	11 (4%)	0	100	100
3	C	155/164 (94%)	147 (95%)	8 (5%)	0	100	100
4	D	23/422 (6%)	22 (96%)	1 (4%)	0	100	100
5	E	769/1393 (55%)	742 (96%)	27 (4%)	0	100	100
All	All	1776/2974 (60%)	1708 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	529/598 (88%)	527 (100%)	2 (0%)	91 94
2	B	268/347 (77%)	268 (100%)	0	100 100
3	C	146/153 (95%)	146 (100%)	0	100 100
4	D	25/406 (6%)	25 (100%)	0	100 100
5	E	725/1297 (56%)	719 (99%)	6 (1%)	81 89
All	All	1693/2801 (60%)	1685 (100%)	8 (0%)	89 93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	494	LYS
5	E	319	LYS
5	E	427	ARG
5	E	607	ARG
5	E	641	ARG
5	E	716	ASN
5	E	964	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	497	ASN
1	A	538	GLN
2	B	203	GLN
5	E	1007	ASN
5	E	1199	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

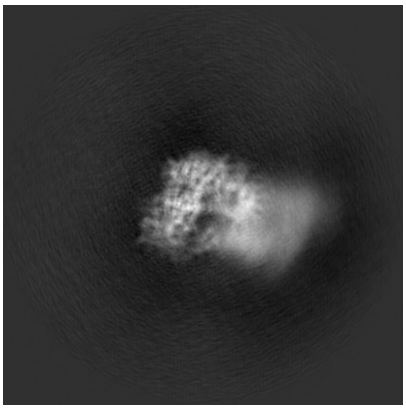
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26866. These allow visual inspection of the internal detail of the map and identification of artifacts.

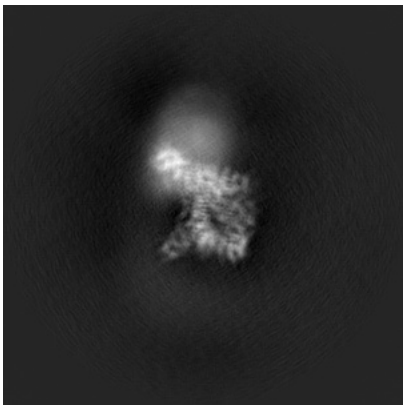
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

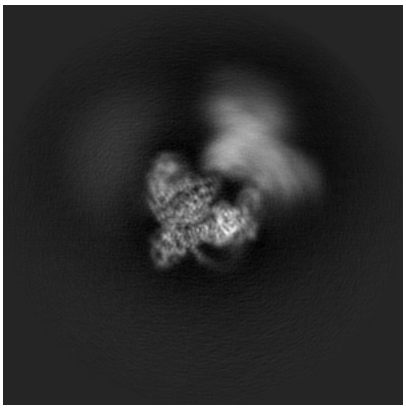
6.1.1 Primary map



X

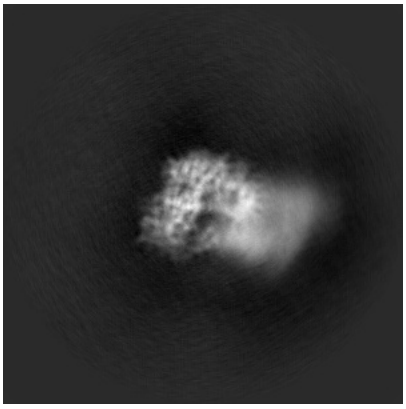


Y

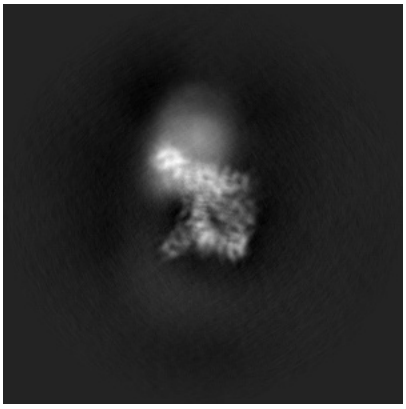


Z

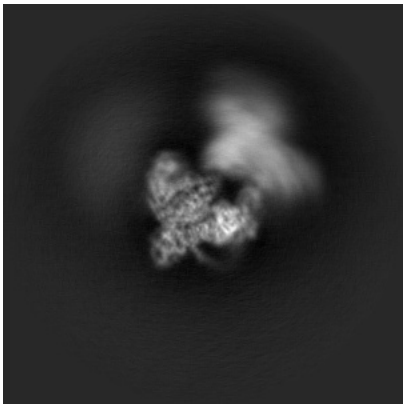
6.1.2 Raw map



X



Y

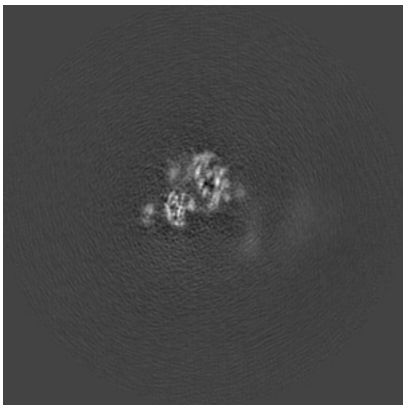


Z

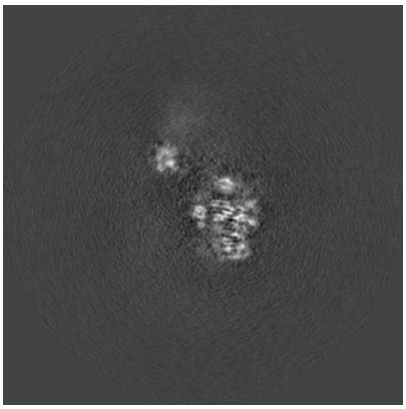
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

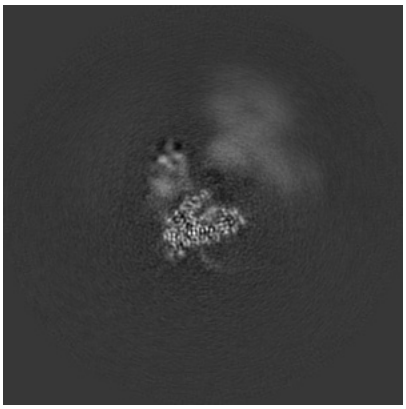
6.2.1 Primary map



X Index: 200

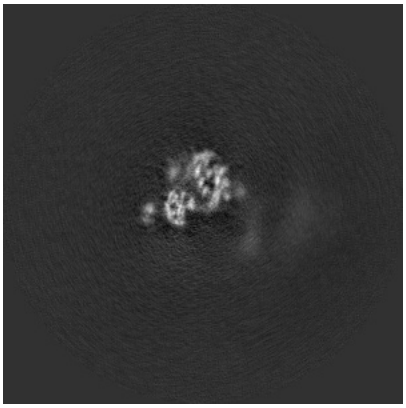


Y Index: 200

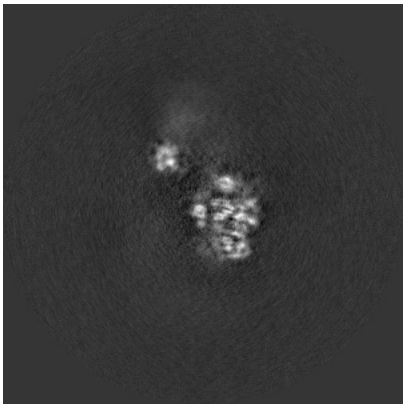


Z Index: 200

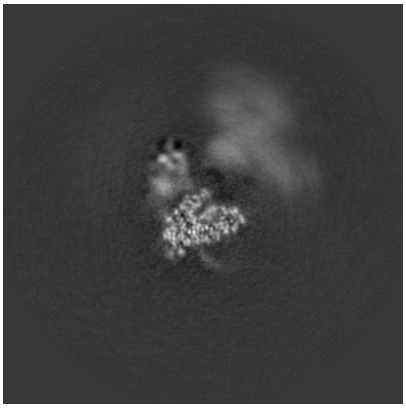
6.2.2 Raw map



X Index: 200



Y Index: 200

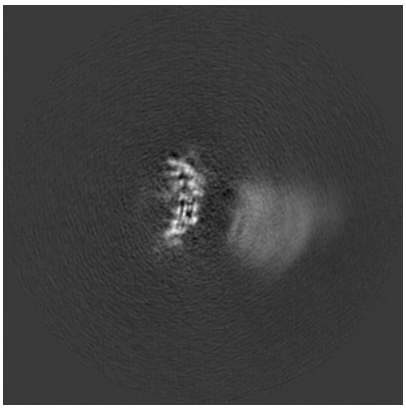


Z Index: 200

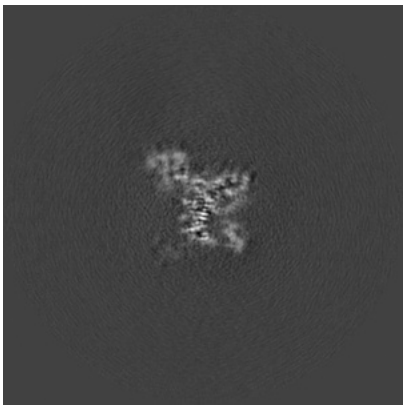
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

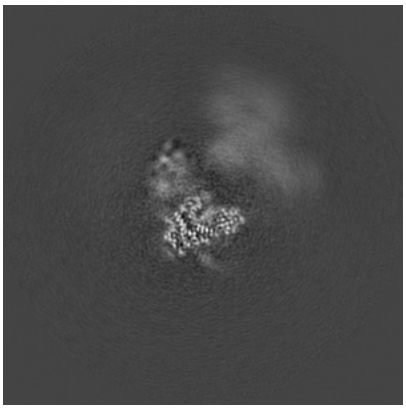
6.3.1 Primary map



X Index: 227

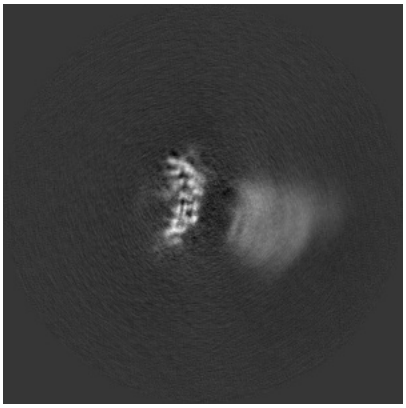


Y Index: 171

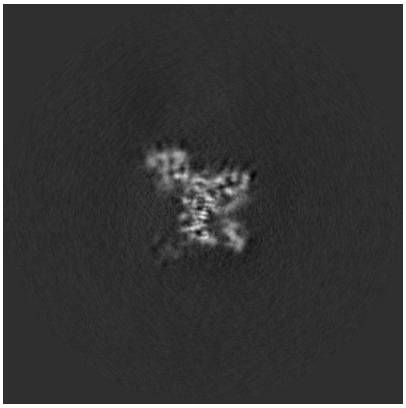


Z Index: 198

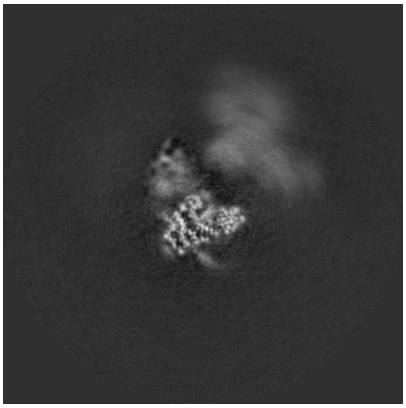
6.3.2 Raw map



X Index: 227



Y Index: 171



Z Index: 197

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

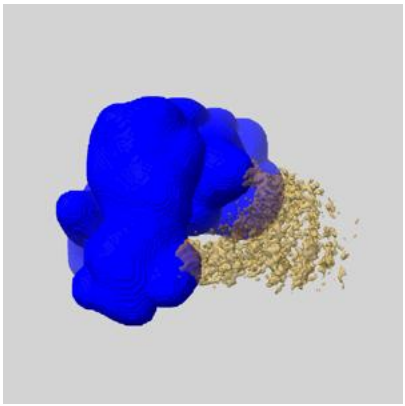
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

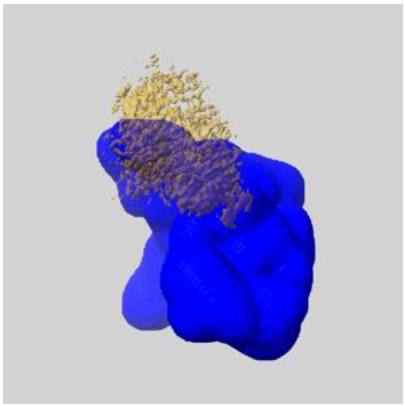
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

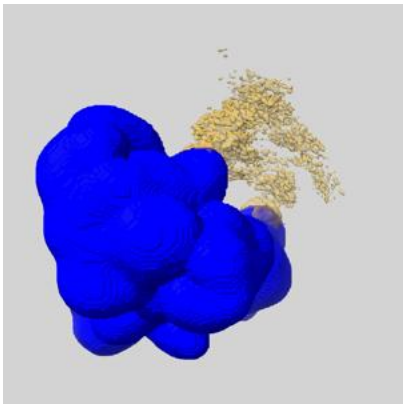
6.5.1 emd_26866_msk_1.map (i)



X



Y

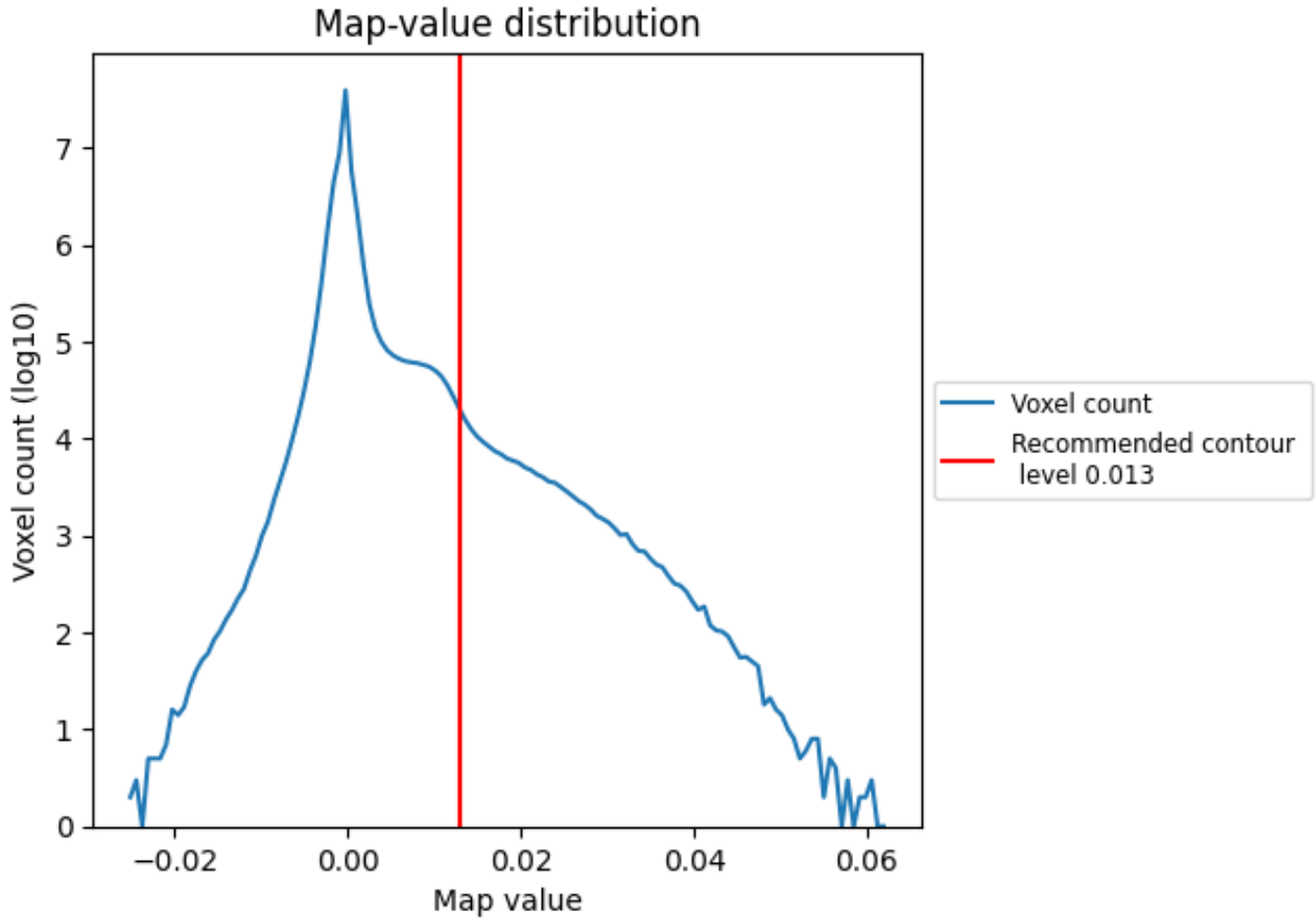


Z

7 Map analysis

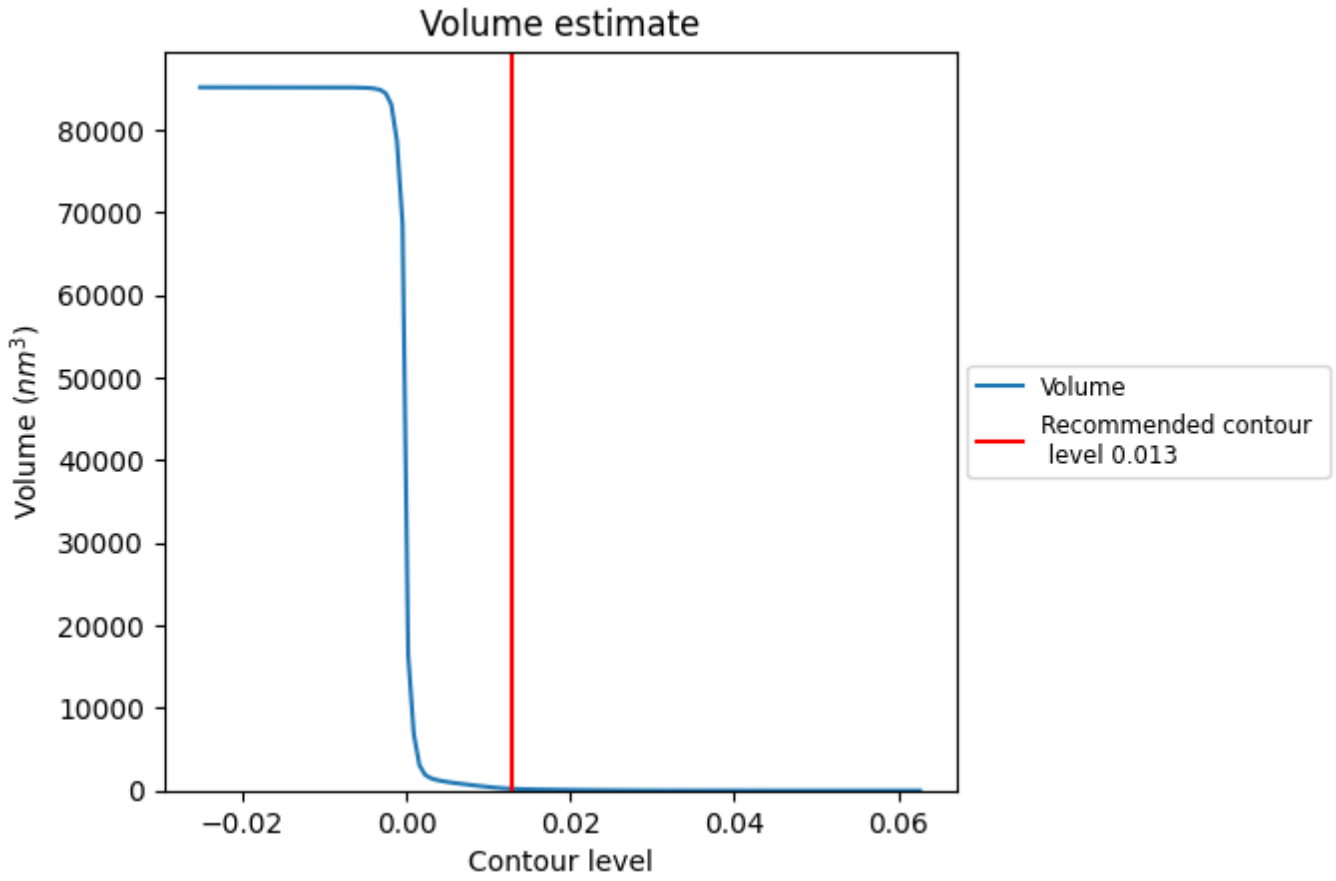
This section contains the results of statistical analysis of the map.

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.

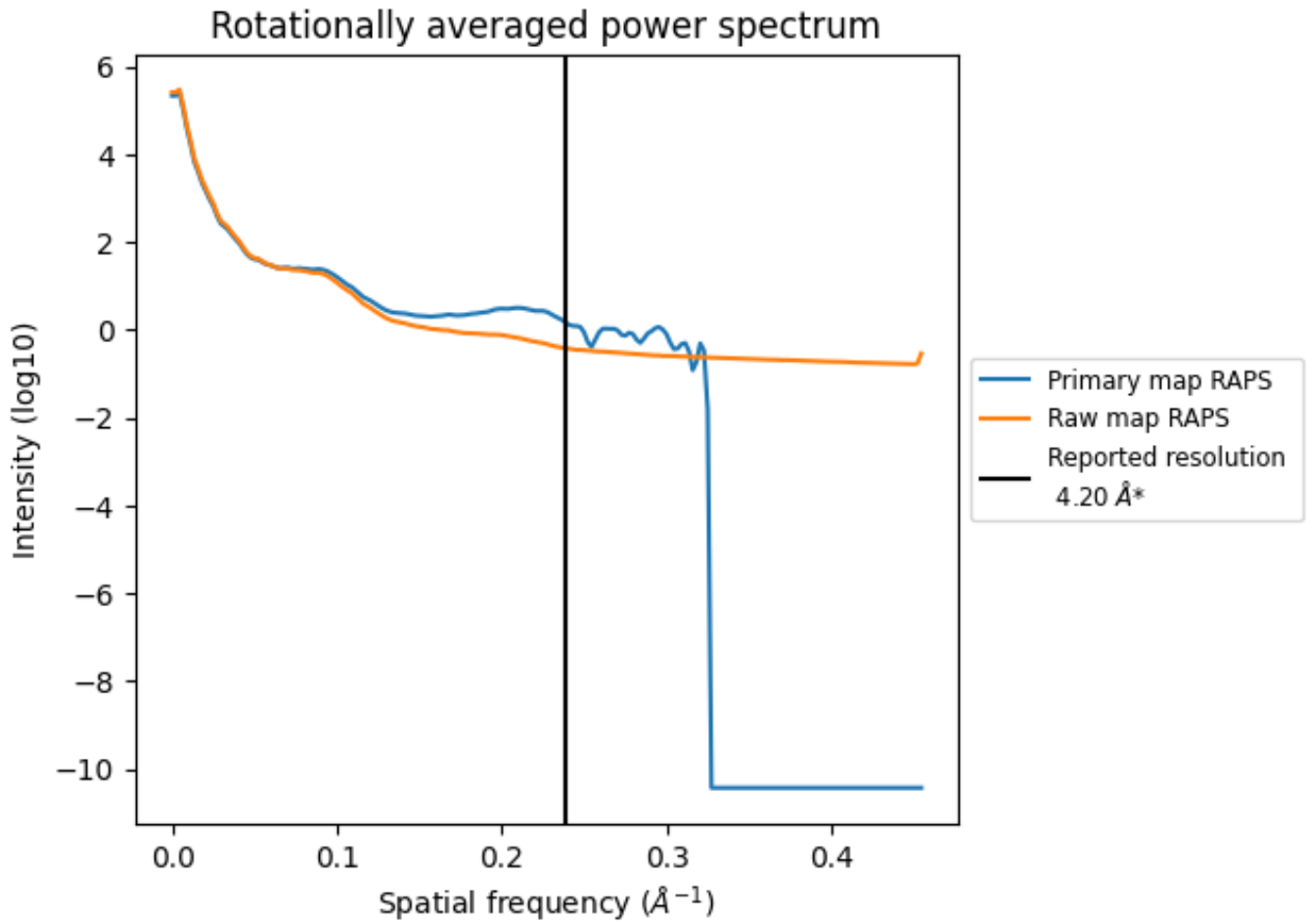
7.2 Volume estimate



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 192 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)

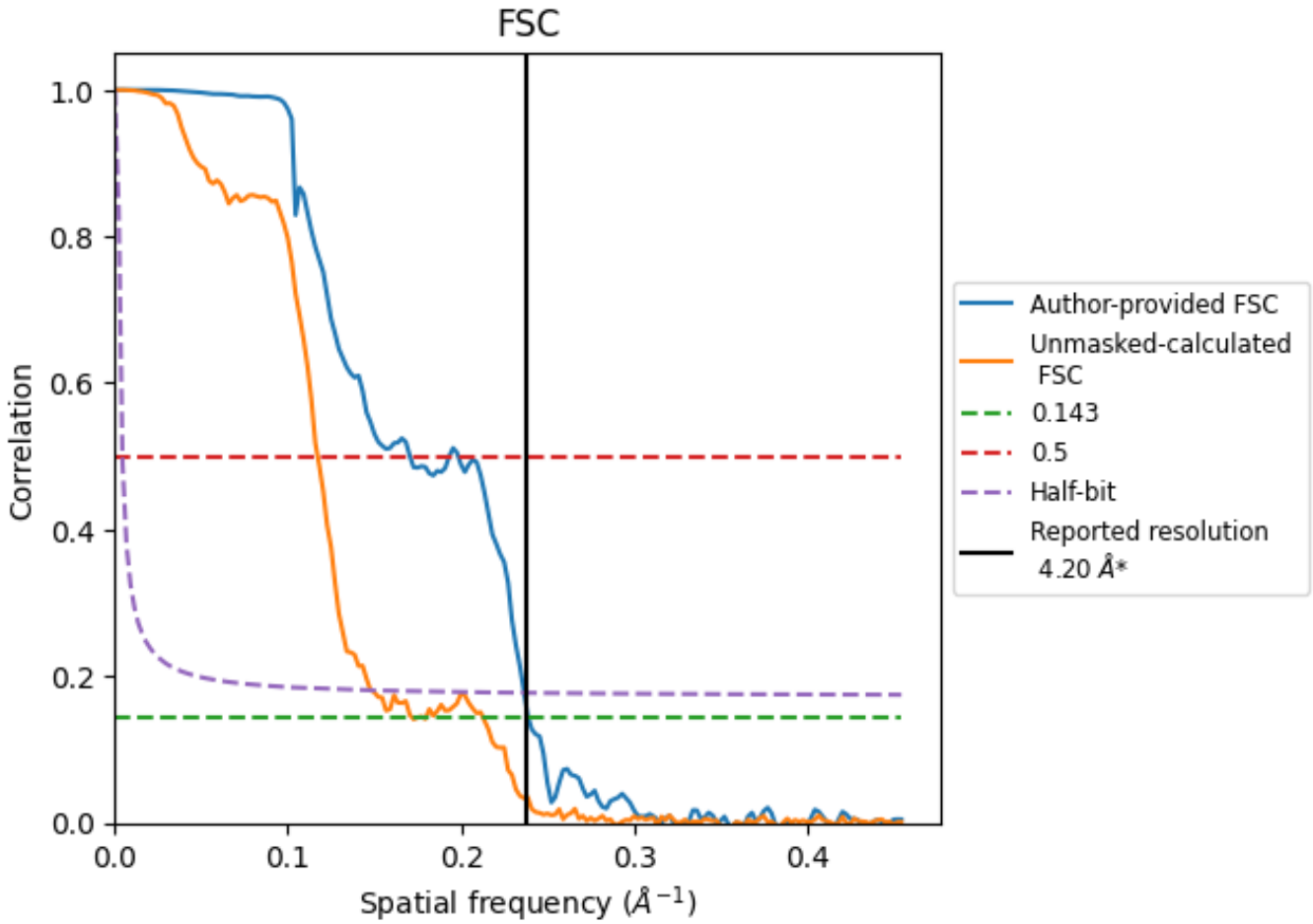


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

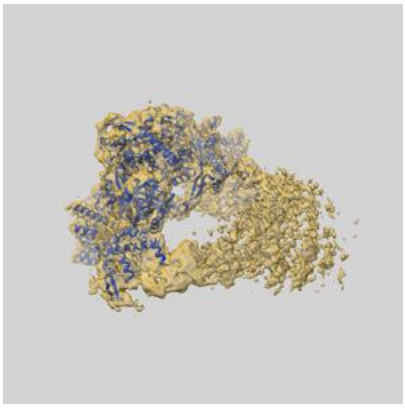
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	5.87	4.23
Unmasked-calculated*	5.81	8.53	6.75

*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 5.81 differs from the reported value 4.2 by more than 10 %

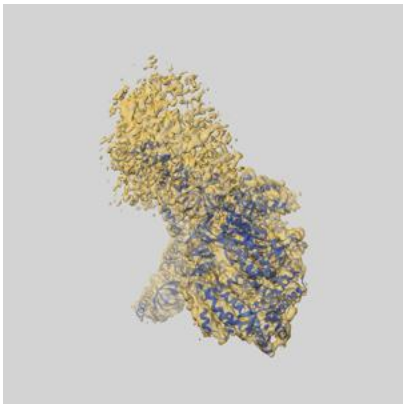
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26866 and PDB model 7UY7. Per-residue inclusion information can be found in section 3 on page 5.

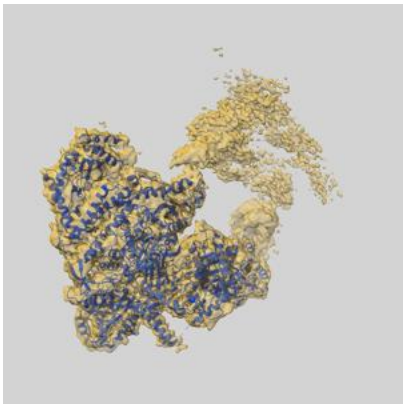
9.1 Map-model overlay



X



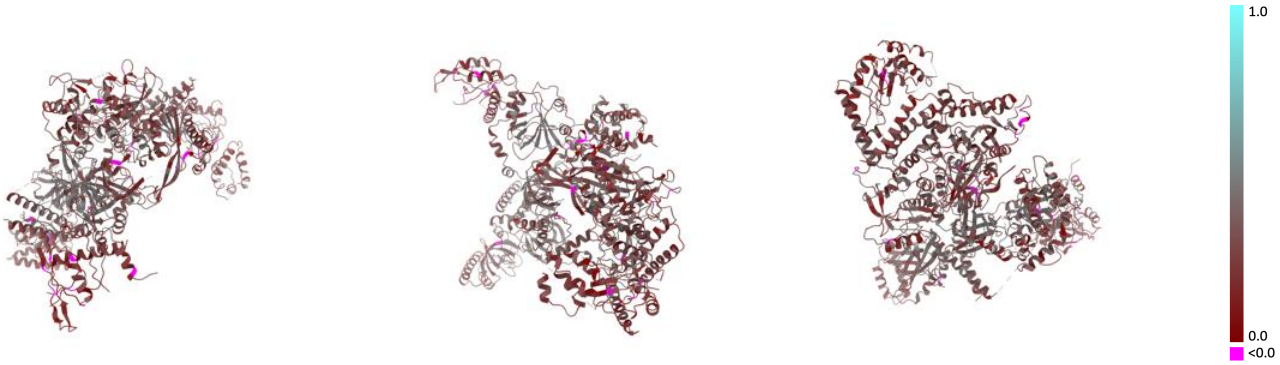
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

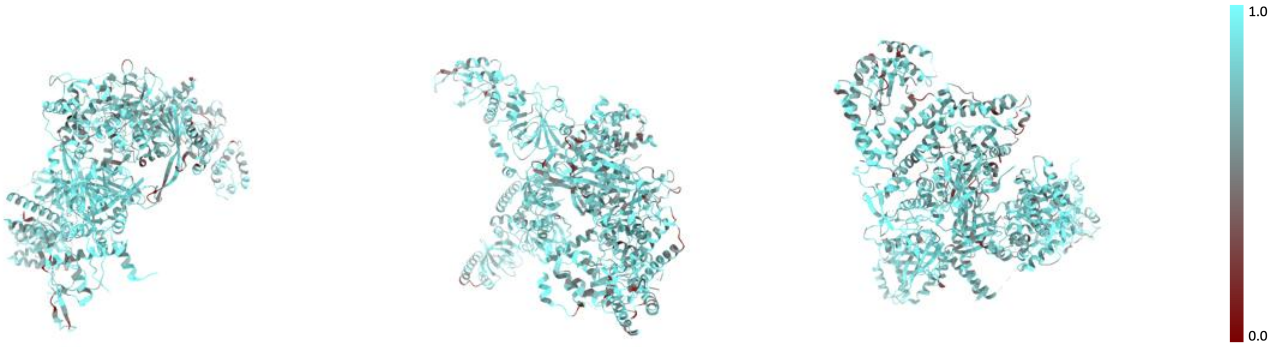
9.2 Q-score mapped to coordinate model (i)



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.

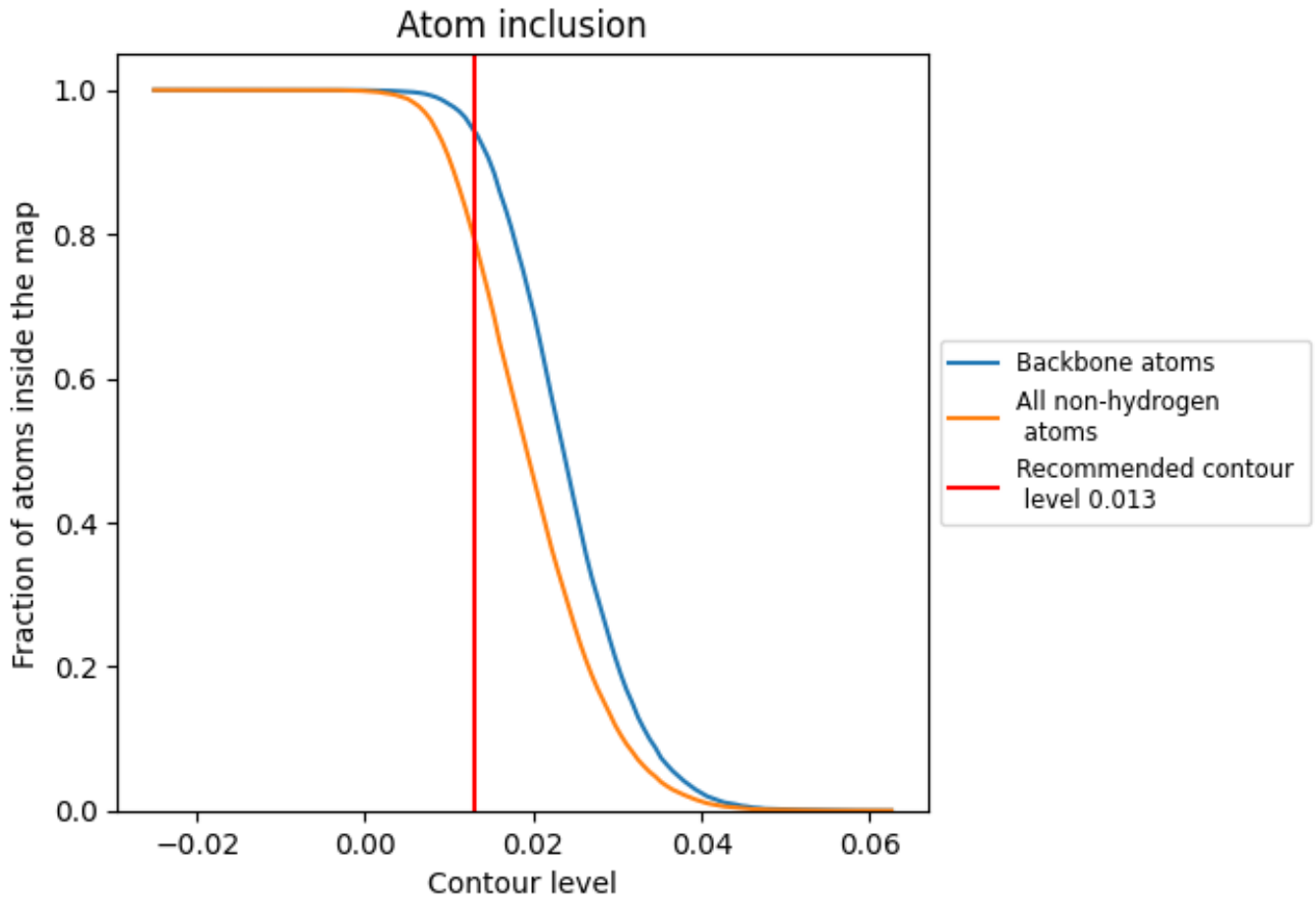
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7934	0.2930
A	0.8309	0.3180
B	0.8369	0.3280
C	0.7631	0.2740
D	0.8756	0.2560
E	0.7544	0.2710
F	0.7689	0.1700