Full wwPDB EM Validation Report ⓘ

Nov 27, 2023 – 10:13 PM JST

PDB ID	:	7XYG
EMDB ID	:	EMD-33521
Title	:	Cryo-EM structure of Fft3-nucleosome complex with Fft3 bound to SHL+3 position of the nucleosome
Authors	:	Nan, Z.; Tao, J.; Yangao, H.
Deposited on	:	2022-06-01
Resolution	:	5.40 Å(reported)

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

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

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

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

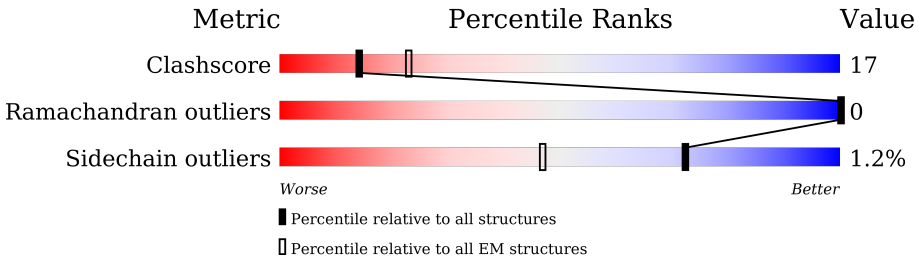
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.40 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	135	7% 42% 30% · 27%
1	E	135	11% 44% 28% 27%
2	B	103	6% 38% 41% 21%
2	F	103	12% 42% 42% 17%
3	C	123	12% 53% 33% · 14%
3	G	123	11% 63% 22% 15%
4	D	123	7% 54% 23% 23%
4	H	123	· 50% 24% · 24%

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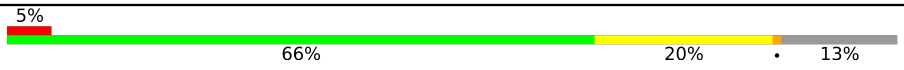
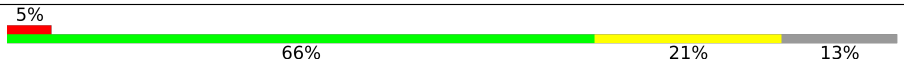
Mol	Chain	Length	Quality of chain
5	J	167	
6	I	167	
7	K	922	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17273 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total 807	C 508	N 156	O 140	S 3	0	0
1	E	98	Total 807	C 508	N 156	O 140	S 3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total 646	C 407	N 126	O 112	S 1	0	0
2	F	86	Total 694	C 436	N 140	O 117	S 1	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	106	Total 812	C 512	N 158	O 141	S 1	0	0
3	G	105	Total 803	C 506	N 156	O 140	S 1	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total 753	C 474	N 137	O 140	S 2	0	0
4	H	93	Total 732	C 462	N 131	O 137	S 2	0	0

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	146	Total	C	N	O	P	0	0
			3009	1424	565	874	146		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	146	Total	C	N	O	P	0	0
			2977	1414	539	878	146		

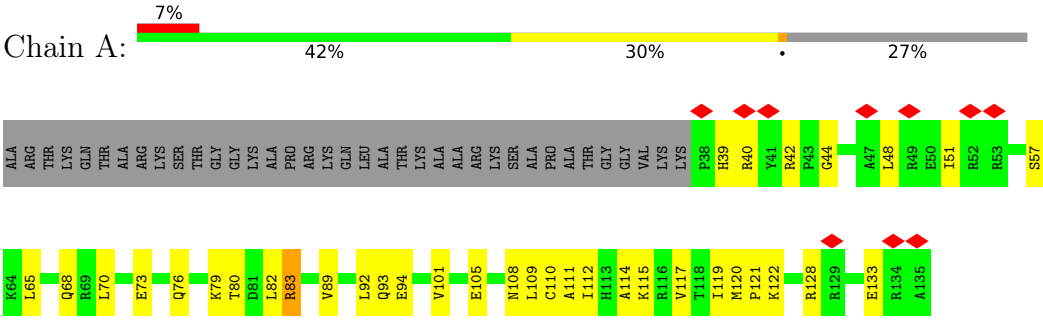
- Molecule 7 is a protein called ATP-dependent helicase fft3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	650	Total	C	N	O	S	0	0
			5233	3348	894	962	29		

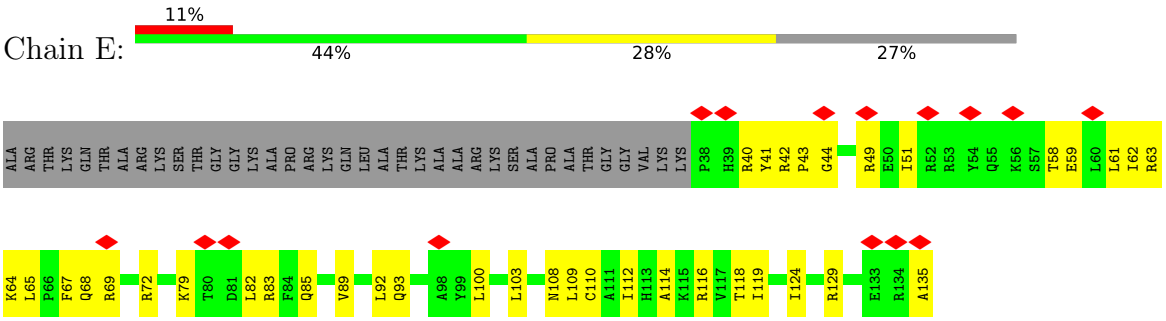
3 Residue-property plots (i)

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.

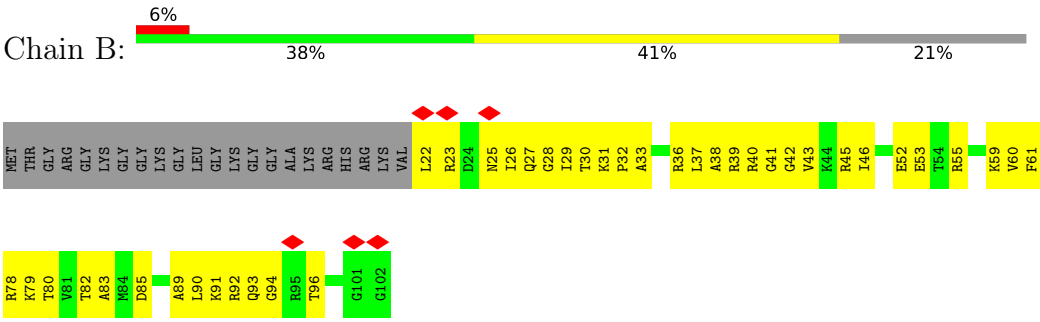
• Molecule 1: Histone H3



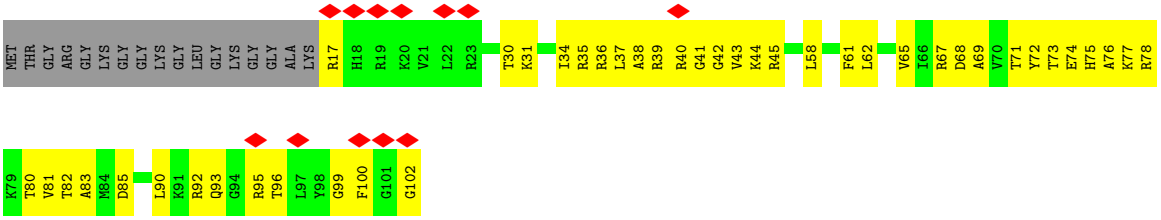
• Molecule 1: Histone H3



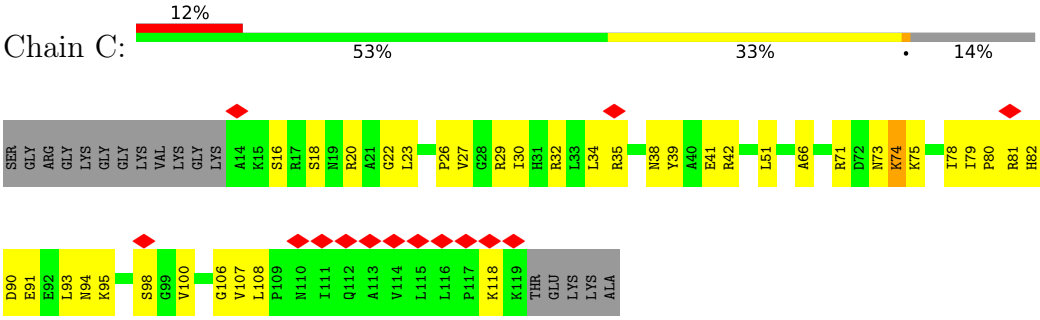
• Molecule 2: Histone H4



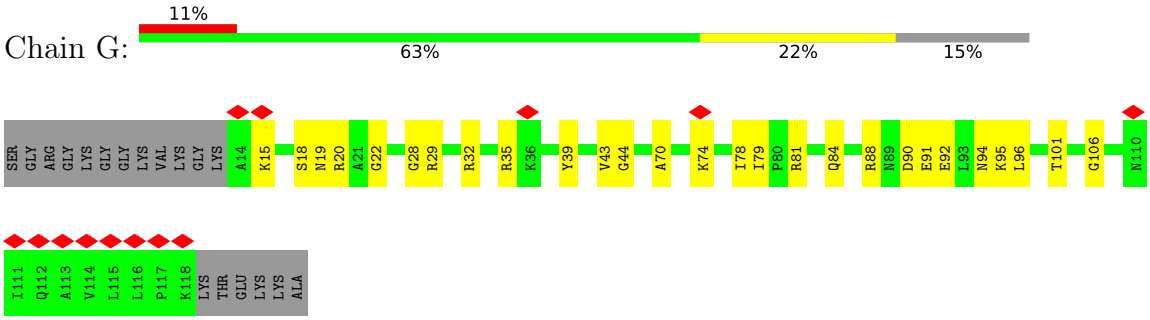
• Molecule 2: Histone H4



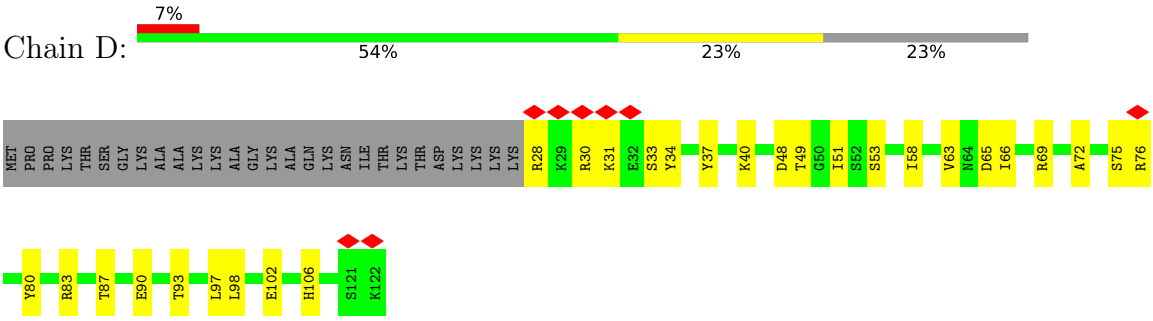
• Molecule 3: Histone H2A



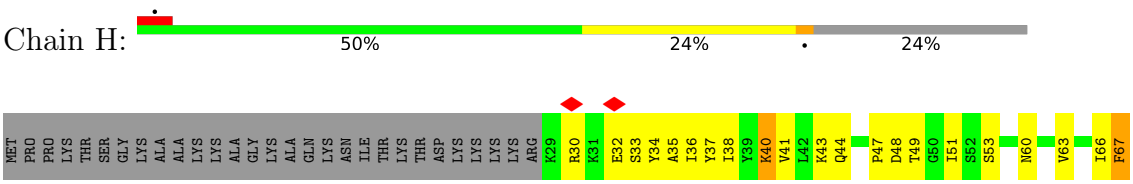
• Molecule 3: Histone H2A

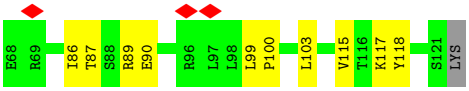


• Molecule 4: Histone H2B



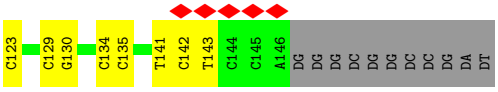
• Molecule 4: Histone H2B





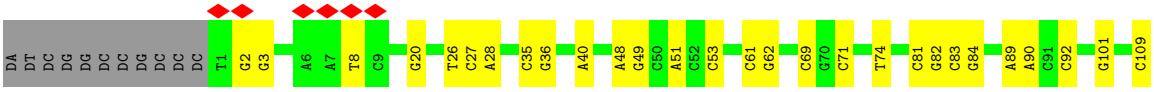
• Molecule 5: DNA (167-MER)

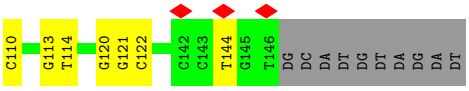
Chain J:



• Molecule 6: DNA (167-MER)

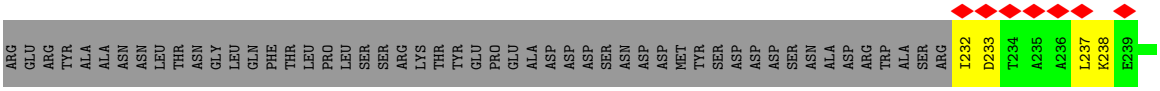
Chain I:

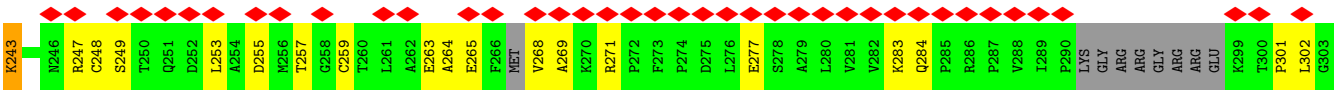


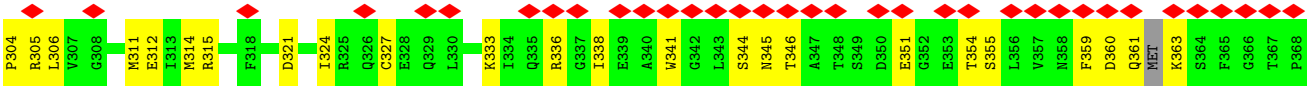


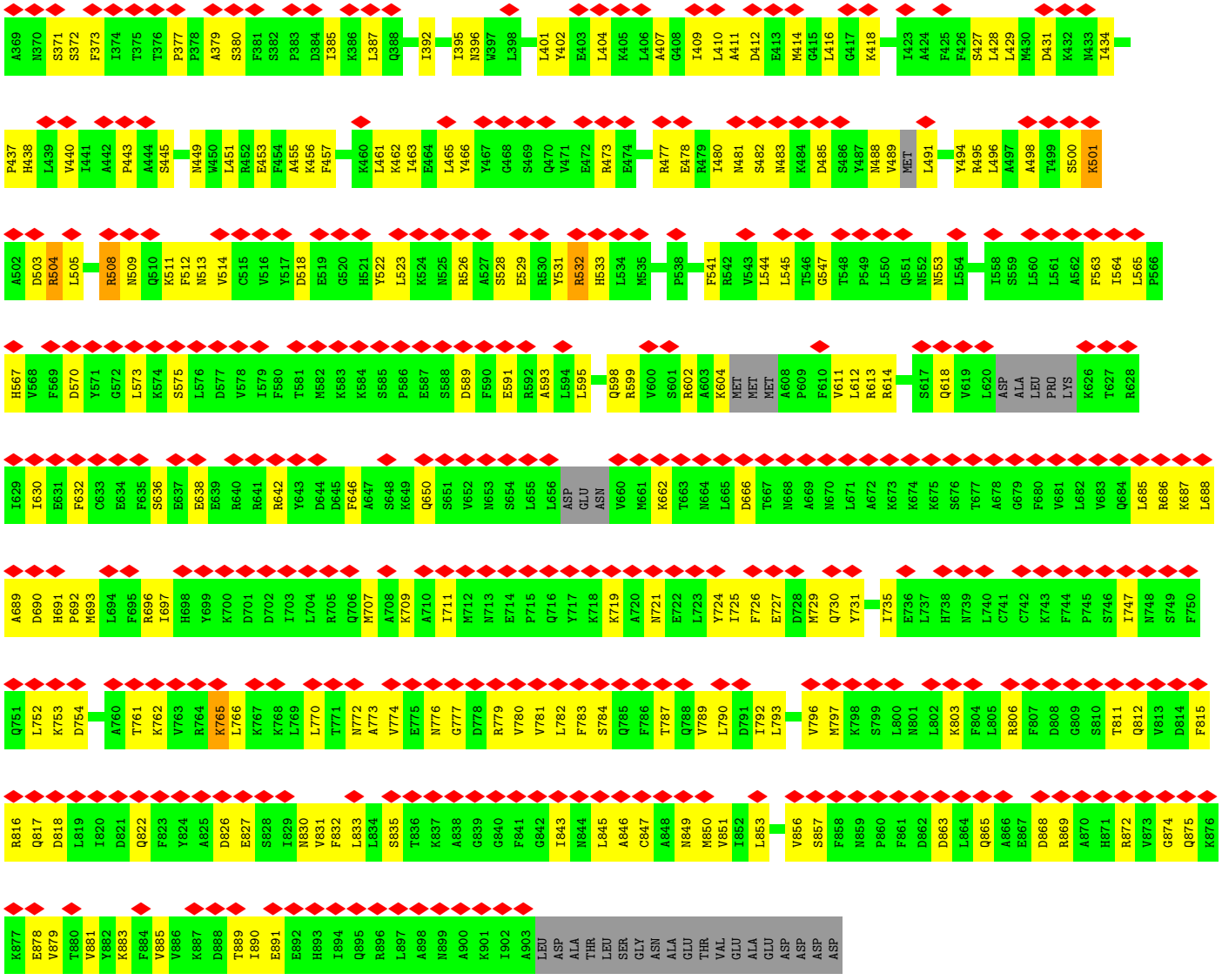
• Molecule 7: ATP-dependent helicase fft3

Chain K:








A369 N370 S371 S372 F373 I374 T375 T376 P377 P378 A379 S380 F381 S382 P383 D384 I385 K386 L387 Q388 I392 I395 N396 W397 L398 L401 Y402 E403 L404 K405 L406 A407 G408 I409 L410 A411 D412 E413 M414 G415 L416 G417 K418 I423 A424 F425 F426 S427 L428 L429 M430 D431 K432 N433 I434
P437 H438 L439 V440 I441 A442 P443 A444 S445 N449 W450 L451 R452 E453 F454 A455 K456 F457 K460 L461 K462 I463 E464 L465 Y466 Y467 G468 S469 Q470 V471 E472 R473 E474 R477 E478 R479 I480 N481 S482 N483 K484 D485 S486 Y487 N488 V489 MET L491 Y494 R495 L496 A497 A498 T499 S500 K501
A502 D503 R504 L505 R508 N509 Q510 K511 F512 N513 V514 C515 V516 Y517 D518 E519 G520 H521 Y522 L523 K524 N525 R526 A527 S528 E529 R530 Y531 R532 H533 L534 M535 P538 F541 R542 V543 L544 L545 T546 G547 T548 P549 L550 Q551 N552 N553 L554 I558 S559 L560 L561 A562 F563 I564 L565 P566
H567 V568 F569 D570 Y571 G572 L573 K574 S575 L576 D577 V578 I579 F580 T581 M582 K583 K584 S585 P586 E587 S588 D589 F590 E591 R592 A593 L594 L595 Q598 R599 V600 S601 R602 A603 K604 MET MET MET A608 P609 F610 V611 L612 R613 R614 S617 Q618 V619 L620 ASP ALA LEU PRO LYS K626 T627 R628
I629 I630 E631 F632 C633 E634 F635 S636 E637 E638 E639 R640 R641 R642 Y643 D644 D645 F646 A647 S648 K649 Q650 S651 V652 N653 S654 L655 L656 ASP GLU ASN V660 M661 K662 T663 N664 L665 D666 T667 N668 A669 N670 L671 A672 K673 K674 K675 S676 T677 A678 G679 F680 V681 L682 V683 Q684 L685 R686 K687 L688
A689 D690 H691 P692 M693 L694 F695 R696 I697 H698 Y699 K700 D701 D702 I703 L704 R705 Q706 M707 A708 K709 A710 I711 M712 N713 E714 P715 Q716 Y717 K718 K719 A720 N721 E722 L723 Y724 I725 F726 E727 D728 M729 Q730 Y731 I735 E736 L737 H738 N739 L740 C741 C742 K743 F744 P745 S746 I747 N748 S749 F750
Q751 L752 K753 D754 A760 T761 K762 V763 R764 K765 L766 K767 K768 L769 L770 T771 N772 A773 V774 E775 N776 G777 D778 R779 V780 V781 L782 F783 S784 Q785 F786 T787 Q788 V789 L790 D791 I792 L793 V796 M797 K798 S799 L800 N801 L802 K803 F804 L805 R806 F807 D808 G809 S810 T811 Q812 V813 D814 F815
R816 Q817 D818 L819 I820 D821 Q822 F823 Y824 A825 D826 E827 S828 I829 N830 V831 F832 L833 L834 S835 T836 K837 A838 G839 G840 F841 G842 I843 N844 L845 A846 C847 A848 N849 M850 V851 I852 L853 V856 S857 F858 N859 P860 F861 D862 D863 L864 Q865 A866 E867 D868 R869 A870 H871 R872 V873 G874 Q875 K876
K877 E878 V879 T880 V881 Y882 K883 F884 V885 V886 K887 D888 T889 I890 E891 E892 H893 I894 Q895 R896 L897 A898 N899 A900 K901 I902 A903 LEU ASP ALA THR LEU SER GLY ASN ALA GLU THR VAL GLU ALA GLU ASP ASP ASP ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19730	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0173	Depositor
Map size (Å)	232.95999, 232.95999, 232.95999	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.35	0/819	0.50	0/1097
1	E	0.35	0/819	0.51	0/1097
2	B	0.38	0/653	0.56	0/873
2	F	0.36	0/702	0.54	0/937
3	C	0.33	0/822	0.56	0/1108
3	G	0.33	0/813	0.54	0/1097
4	D	0.34	0/764	0.50	0/1024
4	H	0.36	0/743	0.53	0/999
5	J	0.96	0/3379	1.06	2/5217 (0.0%)
6	I	0.98	0/3335	1.05	0/5141
7	K	0.31	0/5325	0.54	0/7171
All	All	0.65	0/18174	0.79	2/25761 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	41	DG	O4'-C1'-N9	5.43	111.80	108.00
5	J	32	DG	O4'-C1'-N9	5.15	111.60	108.00

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	807	0	844	34	0
1	E	807	0	844	32	0
2	B	646	0	687	37	0
2	F	694	0	742	38	0
3	C	812	0	866	30	0
3	G	803	0	853	21	0
4	D	753	0	785	24	0
4	H	732	0	759	25	0
5	J	3009	0	1638	36	0
6	I	2977	0	1640	35	0
7	K	5233	0	5308	235	0
All	All	17273	0	14966	461	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 17.

All (461) 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)
7:K:501:LYS:HA	7:K:504:ARG:CD	1.33	1.58
7:K:501:LYS:HA	7:K:504:ARG:CG	1.54	1.35
7:K:501:LYS:CA	7:K:504:ARG:CD	2.24	1.14
7:K:284:GLN:HB2	7:K:302:LEU:HD22	1.21	1.13
7:K:263:GLU:CD	7:K:305:ARG:HH22	1.52	1.11
7:K:501:LYS:CA	7:K:504:ARG:CG	2.33	1.04
7:K:501:LYS:HA	7:K:504:ARG:NE	1.72	1.03
7:K:501:LYS:HA	7:K:504:ARG:HD3	1.40	1.01
7:K:284:GLN:HB2	7:K:302:LEU:CD2	1.91	1.00
7:K:505:LEU:HD22	7:K:508:ARG:HH11	1.28	0.98
7:K:501:LYS:HE2	7:K:505:LEU:HD11	1.46	0.95
7:K:263:GLU:CG	7:K:305:ARG:HH22	1.81	0.94
7:K:263:GLU:CD	7:K:305:ARG:NH2	2.22	0.92
7:K:501:LYS:HE2	7:K:505:LEU:CD1	1.99	0.91
4:H:37:TYR:HA	4:H:40:LYS:HD2	1.50	0.91
7:K:501:LYS:HB2	7:K:504:ARG:NE	1.85	0.91
7:K:263:GLU:CG	7:K:305:ARG:NH2	2.38	0.85
7:K:501:LYS:C	7:K:504:ARG:HG2	1.98	0.82
7:K:501:LYS:O	7:K:504:ARG:CG	2.26	0.82
7:K:501:LYS:CA	7:K:504:ARG:HG2	2.09	0.81
7:K:501:LYS:CA	7:K:504:ARG:NE	2.40	0.81
7:K:501:LYS:CA	7:K:504:ARG:HD3	2.00	0.81
7:K:598:GLN:O	7:K:602:ARG:HB2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:505:LEU:HB3	7:K:508:ARG:NH1	1.97	0.80
7:K:263:GLU:HG2	7:K:305:ARG:NH2	1.98	0.78
7:K:501:LYS:CB	7:K:504:ARG:NE	2.47	0.78
7:K:529:GLU:O	7:K:532:ARG:HG2	1.85	0.77
7:K:501:LYS:N	7:K:504:ARG:HD3	2.01	0.76
7:K:636:SER:H	7:K:761:THR:HG22	1.51	0.76
7:K:501:LYS:HE2	7:K:505:LEU:CG	2.16	0.75
7:K:505:LEU:HD22	7:K:508:ARG:NH1	1.99	0.74
7:K:501:LYS:O	7:K:504:ARG:HG3	1.86	0.74
7:K:505:LEU:CD2	7:K:508:ARG:HH11	2.00	0.74
7:K:501:LYS:O	7:K:504:ARG:HG2	1.86	0.73
7:K:263:GLU:HG2	7:K:305:ARG:HH22	1.54	0.73
7:K:305:ARG:HG3	7:K:306:LEU:N	2.04	0.71
7:K:779:ARG:HH21	7:K:847:CYS:HB3	1.55	0.71
7:K:501:LYS:HA	7:K:504:ARG:HG3	1.68	0.70
7:K:508:ARG:HD2	7:K:509:ASN:N	2.07	0.70
7:K:501:LYS:HB2	7:K:504:ARG:HE	1.58	0.69
3:C:32:ARG:HA	3:C:35:ARG:HD2	1.75	0.68
7:K:311:MET:HB3	7:K:315:ARG:HH21	1.59	0.68
7:K:501:LYS:HB2	7:K:504:ARG:CZ	2.23	0.68
2:B:29:ILE:O	2:B:55:ARG:NH2	2.27	0.67
7:K:501:LYS:C	7:K:504:ARG:CG	2.57	0.67
7:K:243:LYS:O	7:K:247:ARG:HB3	1.94	0.67
7:K:341:TRP:HD1	7:K:371:SER:HB3	1.59	0.67
1:E:63:ARG:HH21	6:I:92:DC:H5'	1.60	0.66
1:E:42:ARG:HG2	5:J:143:DT:H3'	1.77	0.65
7:K:338:ILE:HG21	7:K:345:ASN:HB2	1.78	0.64
7:K:477:ARG:O	7:K:481:ASN:HB2	1.98	0.64
7:K:826:ASP:O	7:K:830:ASN:ND2	2.31	0.64
1:E:108:ASN:ND2	2:F:42:GLY:O	2.32	0.63
7:K:773:ALA:O	7:K:830:ASN:ND2	2.32	0.63
7:K:772:ASN:ND2	7:K:850:MET:SD	2.72	0.63
3:C:80:PRO:HA	3:C:83:LEU:HD13	1.82	0.62
7:K:781:VAL:HG21	7:K:869:ARG:HD3	1.80	0.62
4:D:37:TYR:HA	4:D:40:LYS:HD2	1.80	0.62
7:K:523:LEU:HD12	7:K:544:LEU:HD13	1.82	0.62
3:C:26:PRO:HB2	3:C:29:ARG:HB3	1.83	0.61
7:K:691:HIS:HB3	7:K:792:ILE:HD13	1.81	0.61
7:K:411:ALA:O	7:K:613:ARG:NH2	2.34	0.61
7:K:501:LYS:HE2	7:K:505:LEU:HG	1.81	0.61
7:K:532:ARG:NE	7:K:533:HIS:CE1	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:780:VAL:HG12	7:K:850:MET:HB3	1.82	0.61
7:K:324:ILE:HG21	7:K:602:ARG:HG3	1.81	0.61
7:K:284:GLN:CB	7:K:302:LEU:HD22	2.14	0.60
7:K:872:ARG:HG3	7:K:874:GLY:H	1.67	0.60
1:E:62:ILE:HB	1:E:93:GLN:HE21	1.66	0.60
5:J:96:DT:H2"	5:J:97:DG:H2'	1.82	0.60
7:K:630:ILE:HD12	7:K:883:LYS:HE3	1.83	0.60
2:F:58:LEU:O	2:F:61:PHE:HB3	2.01	0.60
7:K:851:VAL:HG13	7:K:881:VAL:HG23	1.84	0.60
3:C:39:TYR:HB3	4:D:75:SER:HB3	1.83	0.60
2:F:74:GLU:O	4:H:89:ARG:NH2	2.35	0.60
7:K:402:TYR:OH	7:K:513:ASN:ND2	2.35	0.59
1:E:44:GLY:HA3	2:F:44:LYS:HE3	1.84	0.59
5:J:64:DG:N2	6:I:83:DC:C2	2.70	0.59
7:K:514:VAL:HA	7:K:541:PHE:O	2.01	0.59
7:K:259:CYS:HB3	7:K:306:LEU:HD21	1.84	0.59
7:K:437:PRO:HG2	7:K:512:PHE:HA	1.85	0.59
1:A:63:ARG:HH21	5:J:91:DA:H5'	1.68	0.59
6:I:109:DC:H4'	6:I:110:DC:H5'	1.83	0.58
3:G:15:LYS:O	3:G:20:ARG:NH2	2.37	0.58
2:F:78:ARG:HH22	2:F:81:VAL:HA	1.69	0.58
2:B:36:ARG:NH1	6:I:61:DC:OP2	2.36	0.58
2:B:38:ALA:HB1	2:B:43:VAL:HB	1.85	0.58
7:K:532:ARG:NE	7:K:533:HIS:HE1	2.02	0.58
7:K:259:CYS:HB2	7:K:263:GLU:HB2	1.85	0.58
1:A:40:ARG:NH2	5:J:82:DG:O3'	2.37	0.57
7:K:414:MET:HG2	7:K:547:GLY:HA3	1.86	0.57
7:K:846:ALA:HB1	7:K:875:GLN:HG3	1.86	0.57
7:K:301:PRO:HB2	7:K:304:PRO:HD2	1.86	0.57
7:K:501:LYS:CB	7:K:504:ARG:HE	2.15	0.57
2:B:78:ARG:NH1	2:B:80:THR:O	2.38	0.57
7:K:333:LYS:HG3	7:K:336:ARG:HH21	1.69	0.57
7:K:248:CYS:O	7:K:271:ARG:NH1	2.37	0.57
7:K:302:LEU:HA	7:K:305:ARG:HG2	1.85	0.57
7:K:255:ASP:HB3	7:K:593:ALA:HB2	1.86	0.57
1:A:79:LYS:HB3	1:A:82:LEU:HD11	1.85	0.57
1:A:121:PRO:HB3	2:B:53:GLU:HG2	1.86	0.57
7:K:232:ILE:HG21	7:K:315:ARG:HB2	1.86	0.56
2:F:45:ARG:HE	6:I:81:DC:H4'	1.70	0.56
2:F:68:ASP:O	2:F:71:THR:HB	2.04	0.56
1:E:89:VAL:HA	1:E:92:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:28:ARG:NH2	6:I:26:DT:O2	2.36	0.56
7:K:265:GLU:HA	7:K:268:VAL:HB	1.88	0.56
7:K:532:ARG:HE	7:K:533:HIS:CE1	2.22	0.56
7:K:632:PHE:O	7:K:765:LYS:NZ	2.38	0.56
1:E:40:ARG:NH1	6:I:84:DG:O4'	2.38	0.56
7:K:707:MET:HA	7:K:747:ILE:HG21	1.88	0.56
7:K:429:LEU:HB3	7:K:434:ILE:HB	1.88	0.56
3:G:78:ILE:HB	4:H:51:ILE:HG13	1.87	0.56
2:B:22:LEU:HD23	2:B:23:ARG:HB2	1.88	0.56
2:B:23:ARG:HH11	2:B:28:GLY:HA2	1.71	0.56
7:K:283:LYS:HE3	7:K:301:PRO:HB3	1.88	0.56
7:K:377:PRO:HB3	7:K:387:LEU:HD12	1.88	0.56
1:E:40:ARG:NH1	6:I:83:DC:O3'	2.38	0.55
7:K:686:ARG:NH2	7:K:856:VAL:O	2.39	0.55
7:K:849:ASN:HB2	7:K:879:VAL:HG13	1.88	0.55
1:E:109:LEU:HA	1:E:112:ILE:HD12	1.89	0.55
7:K:411:ALA:N	7:K:612:LEU:O	2.39	0.55
7:K:501:LYS:CE	7:K:505:LEU:HG	2.37	0.55
7:K:567:HIS:HA	7:K:570:ASP:HB3	1.88	0.55
7:K:243:LYS:HB2	7:K:247:ARG:HH21	1.72	0.55
7:K:263:GLU:HG2	7:K:302:LEU:HD21	1.88	0.55
1:A:59:GLU:O	2:B:40:ARG:NH1	2.39	0.55
7:K:752:LEU:HG	7:K:754:ASP:H	1.72	0.55
2:B:60:VAL:O	2:B:64:ASN:ND2	2.40	0.54
4:H:41:VAL:HA	4:H:44:GLN:HB2	1.89	0.54
4:H:48:ASP:OD1	4:H:48:ASP:N	2.36	0.54
7:K:414:MET:SD	7:K:418:LYS:NZ	2.70	0.54
1:E:40:ARG:HD2	6:I:83:DC:H4'	1.90	0.54
1:E:42:ARG:NH1	5:J:68:DG:OP1	2.41	0.54
7:K:477:ARG:NH1	7:K:503:ASP:OD1	2.40	0.54
1:A:108:ASN:ND2	2:B:42:GLY:O	2.40	0.54
2:B:92:ARG:HE	4:D:97:LEU:HD12	1.71	0.54
7:K:889:THR:HG23	7:K:891:GLU:H	1.72	0.54
7:K:485:ASP:N	7:K:485:ASP:OD1	2.40	0.54
7:K:495:ARG:HA	7:K:498:ALA:HB3	1.89	0.54
7:K:501:LYS:CA	7:K:504:ARG:HG3	2.32	0.54
1:E:42:ARG:H	5:J:143:DT:H5"	1.71	0.54
3:G:88:ARG:HD3	3:G:94:ASN:HD21	1.73	0.53
7:K:249:SER:O	7:K:253:LEU:N	2.39	0.53
7:K:685:LEU:HD23	7:K:688:LEU:HD12	1.90	0.53
6:I:121:DG:H1'	6:I:122:DC:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:508:ARG:HD2	7:K:508:ARG:C	2.28	0.53
2:B:85:ASP:N	2:B:85:ASP:OD1	2.39	0.53
5:J:74:DG:N2	6:I:74:DT:O2	2.41	0.53
2:F:82:THR:OG1	2:F:85:ASP:N	2.40	0.53
7:K:392:ILE:O	7:K:396:ASN:ND2	2.35	0.53
4:H:100:PRO:HD2	4:H:103:LEU:HD12	1.90	0.53
7:K:265:GLU:O	7:K:269:ALA:N	2.41	0.53
7:K:766:LEU:HD21	7:K:782:LEU:HD13	1.90	0.53
1:A:44:GLY:O	1:A:48:LEU:N	2.41	0.53
5:J:40:DA:H2"	5:J:41:DG:H2'	1.90	0.53
7:K:410:LEU:HD13	7:K:612:LEU:HD23	1.91	0.53
7:K:505:LEU:HB3	7:K:508:ARG:HH11	1.73	0.53
3:C:84:GLN:NE2	3:C:106:GLY:O	2.42	0.53
7:K:784:SER:H	7:K:835:SER:HA	1.74	0.53
3:C:90:ASP:OD2	3:C:93:LEU:N	2.41	0.53
4:D:33:SER:OG	4:D:34:TYR:N	2.42	0.53
7:K:553:ASN:ND2	7:K:591:GLU:OE2	2.41	0.53
7:K:696:ARG:NH2	7:K:731:TYR:O	2.42	0.53
2:F:35:ARG:O	2:F:39:ARG:NH1	2.43	0.52
3:G:29:ARG:HH22	4:H:32:GLU:HB3	1.74	0.52
7:K:849:ASN:ND2	7:K:878:GLU:O	2.42	0.52
1:A:62:ILE:O	1:A:93:GLN:NE2	2.40	0.52
7:K:465:LEU:HD12	7:K:491:LEU:HB3	1.91	0.52
7:K:770:LEU:HD21	7:K:797:MET:HE1	1.92	0.52
4:H:117:LYS:N	7:K:666:ASP:OD1	2.42	0.52
7:K:257:THR:HB	7:K:306:LEU:HD22	1.92	0.52
7:K:360:ASP:OD1	7:K:360:ASP:N	2.41	0.52
7:K:797:MET:HE2	7:K:831:VAL:HG21	1.91	0.52
1:A:39:HIS:HE1	6:I:144:DT:H4'	1.74	0.52
2:B:27:GLN:HA	2:B:55:ARG:HH21	1.74	0.52
2:B:78:ARG:HD2	5:J:101:DG:H5"	1.91	0.52
7:K:642:ARG:HE	7:K:697:ILE:HG21	1.75	0.52
6:I:89:DA:H4'	6:I:90:DA:H5'	1.92	0.52
7:K:449:ASN:O	7:K:453:GLU:HB2	2.09	0.52
6:I:35:DC:H2"	6:I:36:DG:H5'	1.92	0.52
7:K:344:SER:HB3	7:K:361:GLN:HE21	1.74	0.52
3:C:27:VAL:HA	3:C:30:ILE:HB	1.91	0.51
7:K:379:ALA:N	7:K:431:ASP:OD2	2.43	0.51
1:A:68:GLN:HE22	1:A:89:VAL:HG11	1.75	0.51
7:K:783:PHE:HB2	7:K:853:LEU:HA	1.91	0.51
2:F:100:PHE:H	2:F:102:GLY:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:284:GLN:H	7:K:302:LEU:HB2	1.75	0.51
7:K:500:SER:C	7:K:504:ARG:HD3	2.31	0.51
3:C:16:SER:O	3:C:20:ARG:N	2.42	0.51
3:C:78:ILE:H	4:D:51:ILE:HA	1.75	0.51
5:J:46:DC:O5'	7:K:495:ARG:NH1	2.44	0.51
7:K:480:ILE:O	7:K:483:ASN:ND2	2.44	0.51
1:E:83:ARG:HB2	2:F:80:THR:HA	1.92	0.51
4:D:30:ARG:HB2	5:J:122:DG:H4'	1.92	0.51
7:K:243:LYS:O	7:K:247:ARG:CB	2.57	0.51
7:K:264:ALA:O	7:K:268:VAL:N	2.43	0.51
7:K:843:ILE:HD13	7:K:872:ARG:HH22	1.76	0.51
7:K:856:VAL:HG11	7:K:885:VAL:HG22	1.93	0.51
7:K:346:THR:N	7:K:355:SER:O	2.41	0.51
1:A:57:SER:O	2:B:40:ARG:NH2	2.44	0.51
5:J:56:DG:N2	6:I:92:DC:O2	2.44	0.51
7:K:766:LEU:HD11	7:K:782:LEU:HD22	1.92	0.51
7:K:789:VAL:HA	7:K:792:ILE:HD12	1.93	0.51
1:E:129:ARG:NH1	1:E:135:ALA:O	2.44	0.50
7:K:523:LEU:HD22	7:K:531:TYR:HD1	1.75	0.50
1:A:61:LEU:HD11	2:B:36:ARG:HE	1.75	0.50
2:F:36:ARG:NH1	5:J:60:DA:OP2	2.44	0.50
2:F:96:THR:HG23	3:C:100:VAL:HA	1.92	0.50
7:K:355:SER:OG	7:K:618:GLN:OE1	2.27	0.50
7:K:727:GLU:HA	7:K:730:GLN:HE21	1.76	0.50
7:K:885:VAL:HG13	7:K:891:GLU:HG2	1.92	0.50
5:J:23:DG:H2"	5:J:24:DT:H2'	1.92	0.50
7:K:434:ILE:HG22	7:K:438:HIS:HE1	1.76	0.50
5:J:134:DC:H2"	5:J:135:DC:H2'	1.94	0.50
7:K:453:GLU:HG2	7:K:457:PHE:HB2	1.92	0.50
2:B:27:GLN:NE2	2:B:52:GLU:OE1	2.44	0.50
4:H:90:GLU:N	4:H:90:GLU:OE1	2.44	0.50
7:K:354:THR:HB	7:K:612:LEU:HA	1.93	0.50
4:D:83:ARG:NH1	6:I:40:DA:OP2	2.44	0.50
7:K:811:THR:HA	7:K:816:ARG:HD3	1.94	0.50
1:A:44:GLY:N	5:J:82:DG:OP1	2.44	0.49
7:K:529:GLU:HA	7:K:532:ARG:HB3	1.94	0.49
7:K:770:LEU:O	7:K:774:VAL:N	2.43	0.49
4:H:36:ILE:O	4:H:40:LYS:HG3	2.12	0.49
3:G:96:LEU:HD11	4:H:99:LEU:HG	1.93	0.49
7:K:410:LEU:HA	7:K:612:LEU:HB3	1.94	0.49
3:C:18:SER:O	3:C:23:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:LEU:O	2:F:41:GLY:N	2.41	0.49
7:K:505:LEU:CG	7:K:508:ARG:HH11	2.24	0.49
3:C:91:GLU:O	3:C:95:LYS:N	2.35	0.49
4:H:53:SER:N	5:J:19:DA:OP1	2.46	0.49
2:B:37:LEU:O	2:B:41:GLY:N	2.42	0.48
2:F:73:THR:O	2:F:77:LYS:N	2.45	0.48
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.48	0.48
7:K:461:LEU:HB3	7:K:463:ILE:HD11	1.95	0.48
7:K:687:LYS:HA	7:K:690:ASP:HB2	1.94	0.48
7:K:889:THR:OG1	7:K:890:ILE:N	2.45	0.48
3:C:73:ASN:O	3:C:75:LYS:NZ	2.36	0.48
1:E:85:GLN:OE1	2:F:83:ALA:N	2.46	0.48
4:D:53:SER:N	6:I:20:DG:OP1	2.42	0.48
6:I:113:DG:H2'	6:I:114:DT:H71	1.96	0.48
7:K:354:THR:O	7:K:613:ARG:N	2.47	0.48
7:K:443:PRO:HD3	7:K:494:TYR:HE1	1.79	0.48
4:H:30:ARG:NH2	5:J:28:DT:OP1	2.42	0.48
7:K:395:ILE:HD12	7:K:428:LEU:HD22	1.95	0.48
5:J:23:DG:H1'	5:J:24:DT:H5'	1.95	0.48
5:J:28:DT:O2	6:I:120:DG:N2	2.47	0.48
1:E:79:LYS:HB3	1:E:82:LEU:HD11	1.95	0.48
2:B:89:ALA:O	2:B:93:GLN:N	2.41	0.48
3:G:18:SER:OG	3:G:19:ASN:N	2.46	0.48
7:K:462:LYS:N	7:K:488:ASN:OD1	2.46	0.48
7:K:253:LEU:O	7:K:257:THR:OG1	2.28	0.48
1:E:61:LEU:HD21	2:F:36:ARG:HB2	1.96	0.47
1:E:116:ARG:NH1	1:E:118:THR:O	2.47	0.47
7:K:341:TRP:HE1	7:K:372:SER:HB3	1.79	0.47
1:A:109:LEU:HA	1:A:112:ILE:HD12	1.96	0.47
1:E:59:GLU:O	2:F:40:ARG:NH1	2.45	0.47
7:K:238:LYS:NZ	7:K:277:GLU:OE2	2.47	0.47
1:E:100:LEU:HA	1:E:103:LEU:HD12	1.96	0.47
4:D:72:ALA:O	4:D:76:ARG:NE	2.43	0.47
7:K:638:GLU:O	7:K:642:ARG:NH1	2.47	0.47
7:K:646:PHE:HB3	7:K:688:LEU:HD11	1.96	0.47
7:K:284:GLN:HB3	7:K:302:LEU:HD13	1.96	0.47
7:K:857:SER:OG	7:K:863:ASP:OD2	2.33	0.47
1:E:83:ARG:HH21	6:I:101:DG:H5'	1.79	0.47
3:C:78:ILE:HG23	3:C:82:HIS:HD1	1.80	0.47
3:C:107:VAL:HG22	3:C:108:LEU:HD23	1.95	0.47
7:K:761:THR:OG1	7:K:762:LYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:787:THR:HA	7:K:790:LEU:HB2	1.96	0.47
4:H:33:SER:OG	4:H:34:TYR:N	2.47	0.47
7:K:283:LYS:HA	7:K:302:LEU:HB2	1.96	0.47
7:K:312:GLU:O	7:K:575:SER:OG	2.33	0.47
7:K:373:PHE:HA	7:K:396:ASN:HB3	1.96	0.47
7:K:451:LEU:HB3	7:K:815:PHE:H	1.79	0.47
7:K:255:ASP:OD1	7:K:589:ASP:N	2.46	0.47
7:K:494:TYR:OH	7:K:518:ASP:N	2.48	0.47
5:J:81:DC:H1'	5:J:82:DG:H5'	1.97	0.47
7:K:721:ASN:HA	7:K:724:TYR:HB2	1.97	0.47
1:A:83:ARG:HE	6:I:51:DA:H4'	1.80	0.46
1:E:68:GLN:HE21	1:E:72:ARG:HE	1.63	0.46
5:J:96:DT:H1'	5:J:97:DG:H5'	1.96	0.46
6:I:48:DA:H1'	6:I:49:DG:H5'	1.96	0.46
7:K:509:ASN:O	7:K:511:LYS:NZ	2.45	0.46
7:K:522:TYR:O	7:K:528:SER:OG	2.33	0.46
7:K:711:ILE:HG21	7:K:725:ILE:HG21	1.97	0.46
7:K:806:ARG:HG3	7:K:833:LEU:HD12	1.96	0.46
7:K:321:ASP:HA	7:K:324:ILE:HD12	1.97	0.46
7:K:407:ALA:HB3	7:K:564:ILE:HA	1.97	0.46
1:A:42:ARG:NH1	6:I:69:DC:OP1	2.47	0.46
2:F:31:LYS:HA	2:F:34:ILE:HD12	1.97	0.46
3:C:71:ARG:NH1	4:D:49:THR:OG1	2.46	0.46
3:G:91:GLU:O	3:G:95:LYS:N	2.44	0.46
2:B:92:ARG:HH11	4:D:98:LEU:HD23	1.81	0.46
3:G:18:SER:O	3:G:22:GLY:N	2.49	0.46
7:K:410:LEU:HG	7:K:418:LYS:HD2	1.97	0.46
7:K:412:ASP:HB3	7:K:416:LEU:HD13	1.97	0.46
7:K:529:GLU:HB3	7:K:532:ARG:HE	1.81	0.46
1:E:58:THR:HG21	3:C:81:ARG:HB2	1.98	0.46
3:G:35:ARG:NH2	6:I:113:DG:OP2	2.33	0.46
4:D:90:GLU:N	4:D:90:GLU:OE1	2.48	0.46
6:I:2:DG:H1'	6:I:3:DG:H5'	1.96	0.46
7:K:233:ASP:OD1	7:K:233:ASP:N	2.38	0.46
2:B:30:THR:OG1	6:I:62:DG:OP2	2.34	0.46
3:G:84:GLN:NE2	3:G:106:GLY:O	2.49	0.46
7:K:826:ASP:OD1	7:K:826:ASP:N	2.48	0.46
2:B:30:THR:HG23	2:B:33:ALA:H	1.80	0.46
7:K:359:PHE:O	7:K:363:LYS:N	2.49	0.46
1:A:65:LEU:N	5:J:91:DA:OP2	2.48	0.46
2:F:72:TYR:O	2:F:76:ALA:N	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:PHE:N	2:F:102:GLY:OXT	2.46	0.46
7:K:429:LEU:HD22	7:K:434:ILE:HD13	1.98	0.46
7:K:642:ARG:HH11	7:K:692:PRO:HB2	1.80	0.46
3:G:19:ASN:N	3:G:19:ASN:OD1	2.46	0.45
3:C:34:LEU:HD11	3:C:51:LEU:HD21	1.99	0.45
1:A:60:LEU:HD11	1:A:94:GLU:HG2	1.98	0.45
4:D:28:ARG:NH1	6:I:27:DC:O4'	2.49	0.45
4:H:63:VAL:HA	4:H:66:ILE:HG22	1.98	0.45
2:F:67:ARG:O	2:F:71:THR:OG1	2.27	0.45
7:K:354:THR:N	7:K:611:VAL:O	2.49	0.45
2:F:73:THR:HA	2:F:76:ALA:HB3	1.98	0.45
2:B:82:THR:OG1	2:B:83:ALA:N	2.50	0.45
1:E:43:PRO:O	3:C:118:LYS:NZ	2.45	0.45
2:F:92:ARG:HA	2:F:92:ARG:HD2	1.74	0.45
3:G:29:ARG:HA	3:G:32:ARG:HB3	1.99	0.45
3:G:44:GLY:H	4:H:86:ILE:HG13	1.82	0.45
7:K:409:ILE:HB	7:K:611:VAL:HA	1.98	0.45
1:A:111:ALA:HA	1:A:114:ALA:HB3	1.98	0.45
2:F:38:ALA:O	2:F:42:GLY:N	2.50	0.45
4:D:63:VAL:HA	4:D:66:ILE:HD12	1.98	0.45
1:A:115:LYS:HE2	1:A:115:LYS:HB2	1.86	0.44
2:F:75:HIS:HA	4:H:89:ARG:HH21	1.82	0.44
3:C:88:ARG:HA	3:C:88:ARG:HD3	1.81	0.44
2:B:96:THR:O	3:G:101:THR:N	2.50	0.44
4:H:35:ALA:HA	4:H:38:ILE:HD12	1.99	0.44
4:H:115:VAL:N	7:K:666:ASP:OD2	2.50	0.44
1:E:110:CYS:O	1:E:114:ALA:N	2.48	0.44
7:K:595:LEU:HD23	7:K:599:ARG:HH12	1.82	0.44
7:K:638:GLU:HG2	7:K:642:ARG:HH22	1.82	0.44
7:K:531:TYR:HE1	7:K:563:PHE:HB2	1.82	0.44
1:A:119:ILE:HD11	2:B:46:ILE:HG22	1.99	0.44
3:C:81:ARG:HD2	3:C:84:GLN:HB3	1.99	0.44
7:K:505:LEU:CB	7:K:508:ARG:HH11	2.31	0.44
7:K:774:VAL:HG13	7:K:827:GLU:HG3	1.98	0.44
4:H:34:TYR:N	4:H:60:ASN:OD1	2.49	0.44
3:C:94:ASN:O	3:C:98:SER:OG	2.28	0.44
1:E:64:LYS:HB2	1:E:64:LYS:HE2	1.77	0.44
5:J:141:DT:H2"	5:J:142:DC:C5	2.53	0.44
7:K:689:ALA:HB2	7:K:889:THR:HG21	2.00	0.44
1:A:51:ILE:HG12	2:B:42:GLY:HA2	2.00	0.43
3:G:43:VAL:N	6:I:113:DG:OP1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:602:ARG:HD2	7:K:602:ARG:HA	1.80	0.43
7:K:725:ILE:O	7:K:729:MET:HB2	2.18	0.43
1:A:63:ARG:HA	1:A:63:ARG:HD2	1.75	0.43
1:A:110:CYS:O	1:A:114:ALA:N	2.51	0.43
1:E:65:LEU:HG	1:E:69:ARG:HH11	1.83	0.43
2:B:45:ARG:NH1	5:J:80:DA:O3'	2.51	0.43
2:F:90:LEU:HD23	2:F:93:GLN:HE22	1.84	0.43
7:K:505:LEU:CD2	7:K:508:ARG:HE	2.30	0.43
7:K:790:LEU:HD23	7:K:790:LEU:HA	1.90	0.43
7:K:401:LEU:HA	7:K:404:LEU:HD12	2.01	0.43
1:E:119:ILE:HD13	2:F:43:VAL:HG11	2.00	0.43
3:G:70:ALA:O	3:G:74:LYS:N	2.51	0.43
7:K:473:ARG:NH2	7:K:503:ASP:OD2	2.36	0.43
3:G:79:ILE:HG13	3:G:81:ARG:HB3	2.00	0.43
4:H:87:THR:OG1	4:H:90:GLU:OE1	2.31	0.43
6:I:27:DC:H2"	6:I:28:DA:N7	2.33	0.43
7:K:418:LYS:HB3	7:K:545:LEU:HD22	1.99	0.43
1:E:41:TYR:HA	5:J:143:DT:H4'	2.00	0.43
7:K:735:ILE:HD13	7:K:735:ILE:HA	1.92	0.43
2:B:90:LEU:O	2:B:94:GLY:N	2.52	0.43
2:F:93:GLN:HG2	2:F:95:ARG:H	1.83	0.43
3:G:28:GLY:HA3	5:J:29:DG:H5"	2.01	0.43
4:D:48:ASP:OD1	4:D:48:ASP:N	2.41	0.43
7:K:327:CYS:HB3	7:K:565:LEU:HD11	2.00	0.43
6:I:61:DC:H2"	6:I:62:DG:H8	1.84	0.43
2:F:69:ALA:O	2:F:72:TYR:HB2	2.19	0.43
7:K:380:SER:OG	7:K:427:SER:O	2.37	0.43
7:K:776:ASN:OD1	7:K:777:GLY:N	2.52	0.43
5:J:104:DC:H2'	5:J:105:DT:C6	2.54	0.42
7:K:445:SER:HA	7:K:812:GLN:HG2	2.01	0.42
3:G:90:ASP:OD1	3:G:92:GLU:N	2.52	0.42
4:D:28:ARG:HH11	6:I:27:DC:H5'	1.83	0.42
7:K:456:LYS:HB2	7:K:817:GLN:HE22	1.84	0.42
7:K:797:MET:HB2	7:K:803:LYS:HB2	2.00	0.42
1:A:117:VAL:N	6:I:71:DC:OP1	2.52	0.42
2:B:36:ARG:HA	2:B:39:ARG:HG2	2.00	0.42
7:K:351:GLU:HA	7:K:604:LYS:HE3	2.01	0.42
7:K:466:TYR:OH	7:K:477:ARG:NH1	2.50	0.42
2:F:58:LEU:O	2:F:62:LEU:N	2.41	0.42
3:C:66:ALA:HB1	3:C:78:ILE:HG21	2.00	0.42
7:K:438:HIS:HB2	7:K:489:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:455:ALA:HB2	7:K:815:PHE:HB3	2.01	0.42
1:A:89:VAL:HA	1:A:92:LEU:HD12	2.01	0.42
7:K:237:LEU:HD22	7:K:314:MET:HB3	2.02	0.42
2:B:31:LYS:HG3	2:B:32:PRO:HD3	2.01	0.42
2:B:91:LYS:HZ1	4:D:80:TYR:HH	1.58	0.42
3:C:18:SER:O	3:C:22:GLY:N	2.52	0.42
7:K:412:ASP:OD1	7:K:614:ARG:N	2.45	0.42
3:C:78:ILE:HB	4:D:51:ILE:HG13	2.01	0.42
7:K:312:GLU:HA	7:K:315:ARG:HG2	2.01	0.42
5:J:95:DG:N2	6:I:53:DC:O2	2.53	0.42
1:E:49:ARG:NH1	6:I:8:DT:O3'	2.52	0.42
7:K:457:PHE:HE1	7:K:845:LEU:HD23	1.84	0.42
1:A:70:LEU:HA	2:B:25:ASN:HB3	2.02	0.42
2:F:35:ARG:NH1	6:I:82:DG:OP2	2.36	0.42
3:C:38:ASN:ND2	3:G:39:TYR:O	2.52	0.42
4:H:43:LYS:NZ	4:H:49:THR:O	2.42	0.42
7:K:414:MET:HB3	7:K:865:GLN:HA	2.01	0.42
2:F:99:GLY:HA3	4:D:58:ILE:HD13	2.00	0.41
7:K:306:LEU:HD23	7:K:306:LEU:HA	1.77	0.41
7:K:693:MET:HA	7:K:697:ILE:HD11	2.02	0.41
7:K:726:PHE:O	7:K:730:GLN:N	2.50	0.41
7:K:473:ARG:HH22	7:K:496:LEU:HD22	1.85	0.41
7:K:478:GLU:O	7:K:482:SER:OG	2.38	0.41
2:F:30:THR:HG21	5:J:60:DA:H5"	2.00	0.41
3:G:20:ARG:HH11	4:H:118:TYR:HE1	1.68	0.41
7:K:284:GLN:CB	7:K:302:LEU:HD13	2.50	0.41
7:K:526:ARG:HH21	7:K:573:LEU:HB2	1.84	0.41
7:K:719:LYS:H	7:K:719:LYS:HG2	1.59	0.41
7:K:753:LYS:HD3	7:K:753:LYS:HA	1.87	0.41
4:D:87:THR:H	4:D:90:GLU:CD	2.23	0.41
1:A:63:ARG:NE	5:J:90:DA:O3'	2.52	0.41
1:A:101:VAL:O	1:A:105:GLU:HG2	2.21	0.41
1:E:51:ILE:HG12	2:F:42:GLY:HA2	2.02	0.41
2:B:79:LYS:N	5:J:101:DG:OP1	2.54	0.41
3:C:74:LYS:HE3	3:C:74:LYS:HB3	1.94	0.41
4:H:43:LYS:HD3	4:H:47:PRO:HA	2.03	0.41
7:K:392:ILE:HA	7:K:395:ILE:HG12	2.01	0.41
7:K:466:TYR:H	7:K:491:LEU:N	2.19	0.41
3:C:42:ARG:HG2	5:J:112:DG:H5"	2.02	0.41
7:K:849:ASN:HD22	7:K:879:VAL:HA	1.85	0.41
7:K:868:ASP:N	7:K:868:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:GLU:OE2	3:C:41:GLU:N	2.54	0.41
7:K:385:ILE:HD13	7:K:385:ILE:HA	1.92	0.41
2:F:39:ARG:HA	2:F:39:ARG:HD3	1.92	0.41
2:F:65:VAL:O	2:F:68:ASP:HB2	2.21	0.41
4:D:65:ASP:OD1	4:D:69:ARG:NE	2.53	0.41
4:H:63:VAL:O	4:H:67:PHE:HB3	2.21	0.41
5:J:122:DG:H1'	5:J:123:DC:H5'	2.03	0.41
7:K:302:LEU:HG	7:K:305:ARG:NE	2.35	0.41
7:K:456:LYS:HD3	7:K:845:LEU:HG	2.03	0.41
7:K:765:LYS:HA	7:K:765:LYS:HD3	1.87	0.41
7:K:646:PHE:CE2	7:K:650:GLN:HB2	2.56	0.41
7:K:709:LYS:HB3	7:K:709:LYS:HE2	1.87	0.41
1:A:73:GLU:HB2	2:B:25:ASN:HD22	1.86	0.40
2:B:61:PHE:HA	2:B:64:ASN:HD22	1.86	0.40
1:A:57:SER:HB2	1:A:59:GLU:OE1	2.21	0.40
1:E:124:ILE:H	1:E:124:ILE:HG13	1.71	0.40
7:K:305:ARG:CG	7:K:306:LEU:N	2.82	0.40
1:A:128:ARG:NE	1:A:133:GLU:OE1	2.42	0.40
7:K:793:LEU:HA	7:K:796:VAL:HG22	2.02	0.40
1:A:76:GLN:NE2	1:A:80:THR:OG1	2.55	0.40
2:B:26:ILE:HD13	2:B:59:LYS:HD2	2.03	0.40
4:D:102:GLU:OE2	4:D:106:HIS:NE2	2.55	0.40
1:A:120:MET:HB2	1:A:122:LYS:HZ1	1.87	0.40
2:B:75:HIS:HB2	4:D:93:THR:HG21	2.04	0.40
2:F:34:ILE:HA	2:F:37:LEU:HD12	2.02	0.40
5:J:129:DC:H1'	5:J:130:DG:C5	2.55	0.40
7:K:440:VAL:HG22	7:K:491:LEU:HD13	2.03	0.40
7:K:818:ASP:O	7:K:822:GLN:NE2	2.54	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	96/135 (71%)	93 (97%)	3 (3%)	0	100	100
1	E	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
2	B	79/103 (77%)	75 (95%)	4 (5%)	0	100	100
2	F	84/103 (82%)	78 (93%)	6 (7%)	0	100	100
3	C	104/123 (85%)	103 (99%)	1 (1%)	0	100	100
3	G	103/123 (84%)	97 (94%)	6 (6%)	0	100	100
4	D	93/123 (76%)	89 (96%)	4 (4%)	0	100	100
4	H	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
7	K	634/922 (69%)	570 (90%)	64 (10%)	0	100	100
All	All	1380/1890 (73%)	1286 (93%)	94 (7%)	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	85/110 (77%)	84 (99%)	1 (1%)	71	84
1	E	85/110 (77%)	84 (99%)	1 (1%)	71	84
2	B	66/79 (84%)	66 (100%)	0	100	100
2	F	71/79 (90%)	70 (99%)	1 (1%)	67	81
3	C	82/93 (88%)	81 (99%)	1 (1%)	71	84
3	G	81/93 (87%)	81 (100%)	0	100	100
4	D	82/104 (79%)	81 (99%)	1 (1%)	71	84
4	H	80/104 (77%)	78 (98%)	2 (2%)	47	68
7	K	577/815 (71%)	569 (99%)	8 (1%)	67	81
All	All	1209/1587 (76%)	1194 (99%)	15 (1%)	72	84

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	E	67	PHE
2	F	17	ARG
3	C	74	LYS
4	D	31	LYS
4	H	40	LYS
4	H	67	PHE
7	K	243	LYS
7	K	501	LYS
7	K	504	ARG
7	K	508	ARG
7	K	532	ARG
7	K	662	LYS
7	K	765	LYS
7	K	832	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	76	GLN
1	E	113	HIS
2	B	25	ASN
2	B	64	ASN
2	B	93	GLN
2	F	64	ASN
3	C	19	ASN
3	C	38	ASN
3	C	84	GLN
3	G	31	HIS
4	H	81	ASN
7	K	438	HIS
7	K	449	ASN
7	K	483	ASN
7	K	513	ASN
7	K	533	HIS
7	K	598	GLN
7	K	730	GLN
7	K	772	ASN
7	K	817	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

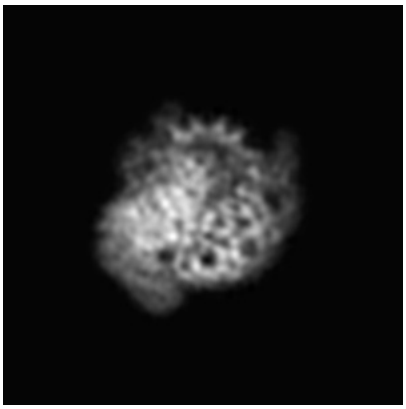
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33521. These allow visual inspection of the internal detail of the map and identification of artifacts.

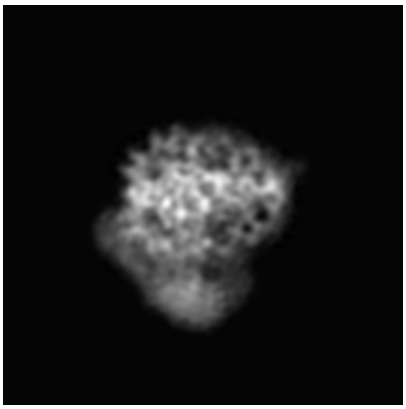
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

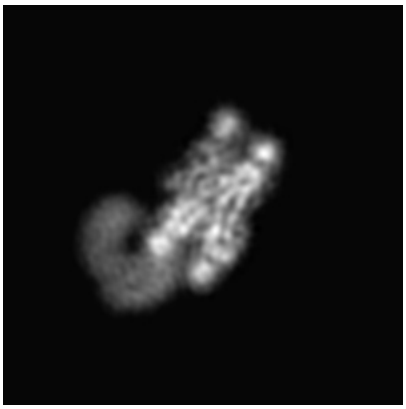
6.1.1 Primary map



X

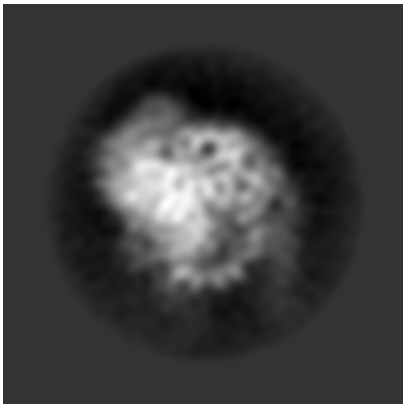


Y

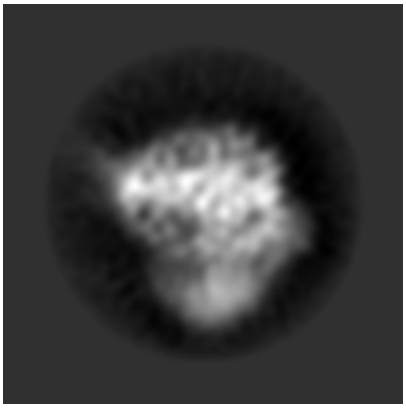


Z

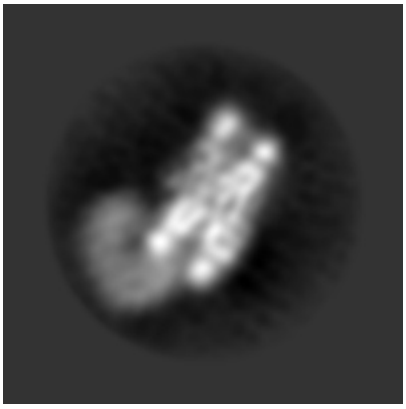
6.1.2 Raw map



X



Y



Z

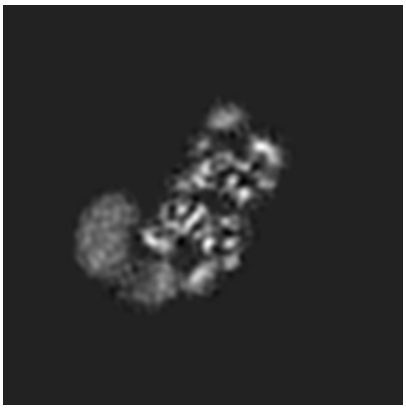
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 112

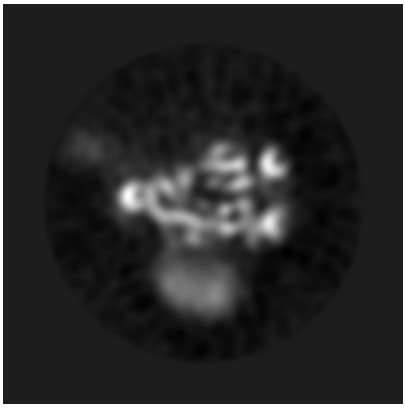
Y Index: 112



Z Index: 112

6.2.2 Raw map

X Index: 112



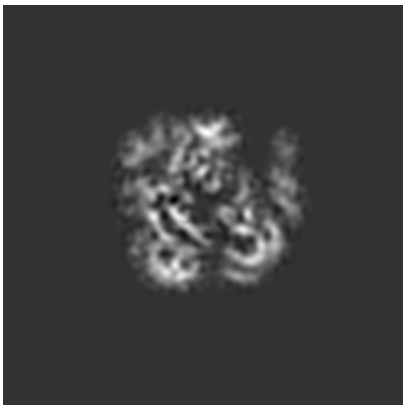
Y Index: 112

Z Index: 112

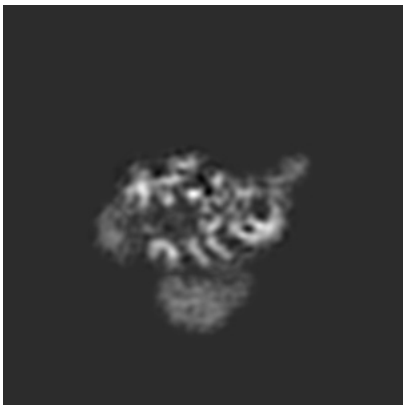
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

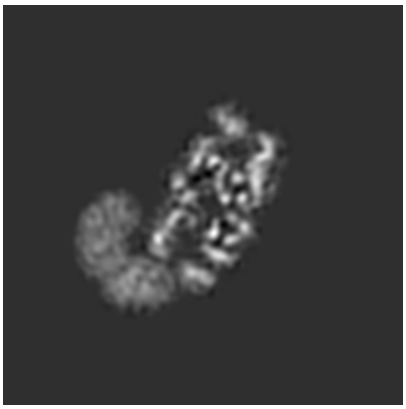
6.3.1 Primary map



X Index: 119



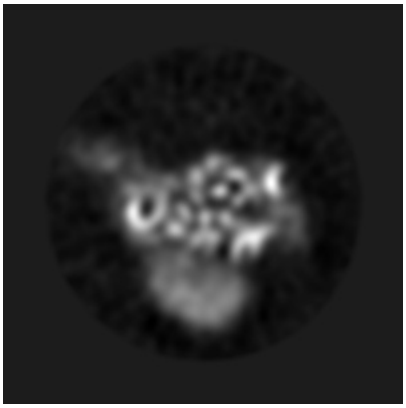
Y Index: 96



Z Index: 106

6.3.2 Raw map

X Index: 120



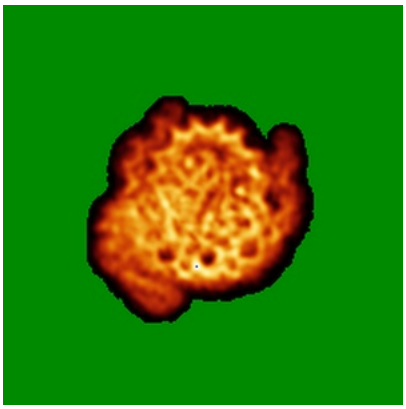
Y Index: 101

Z Index: 117

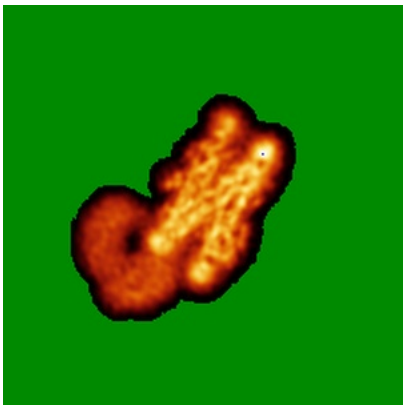
The images above show the largest variance slices of the map in three orthogonal directions.

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

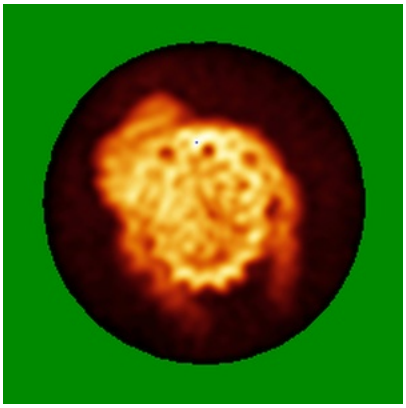
6.4.1 Primary map

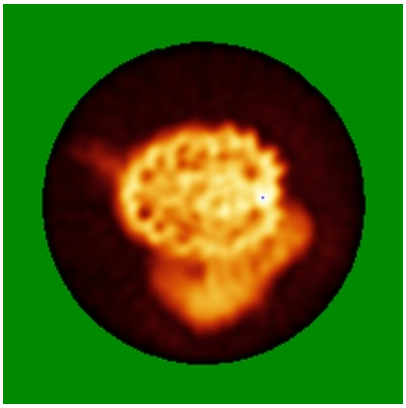

X

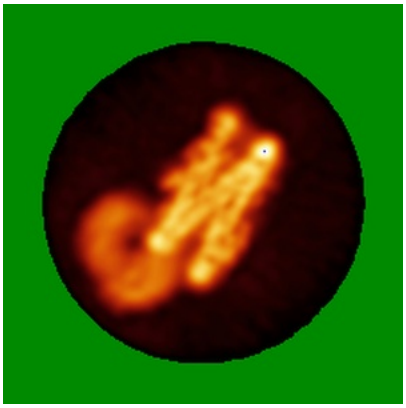

Y


Z

6.4.2 Raw map


X

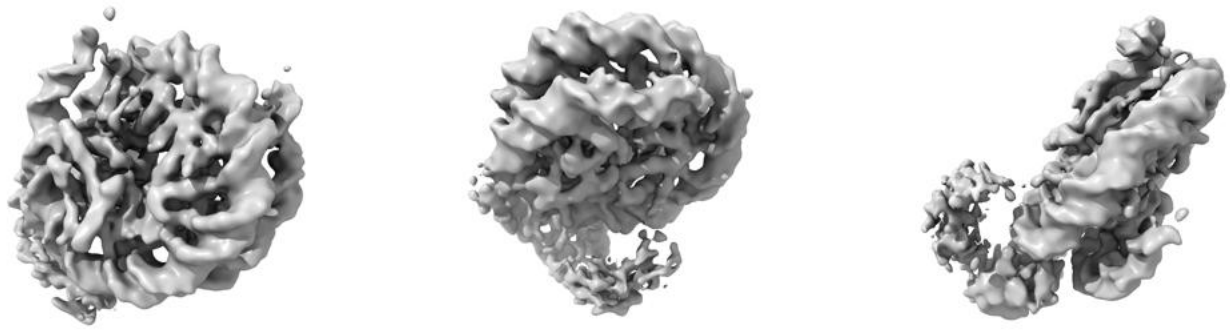

Y


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)

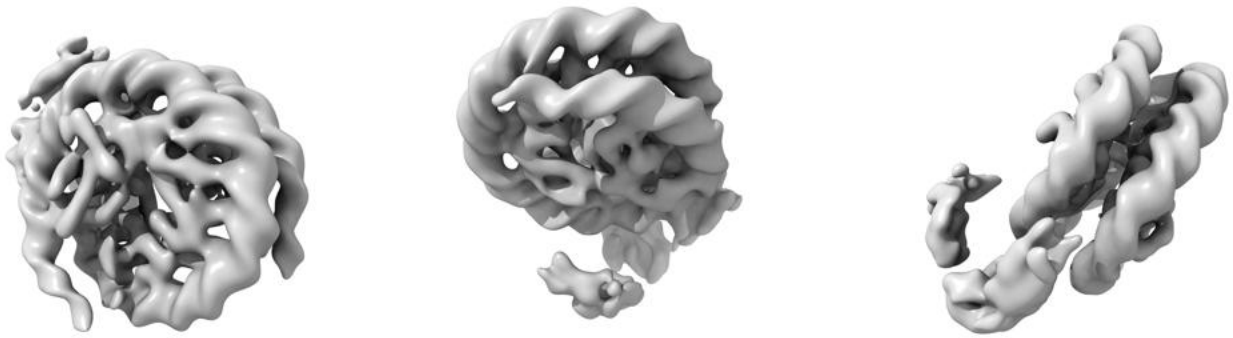
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

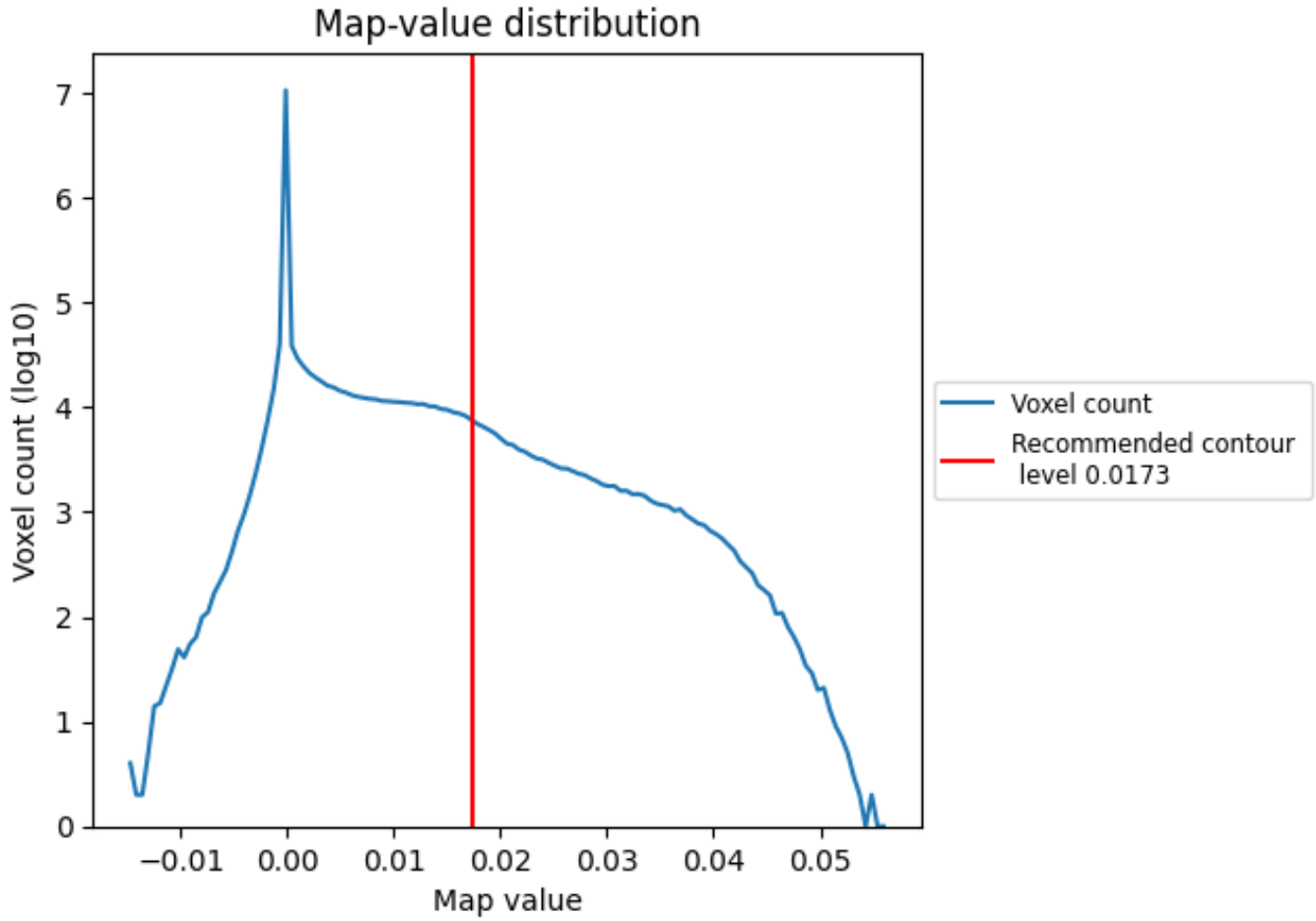
6.6 Mask visualisation (i)

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

7 Map analysis

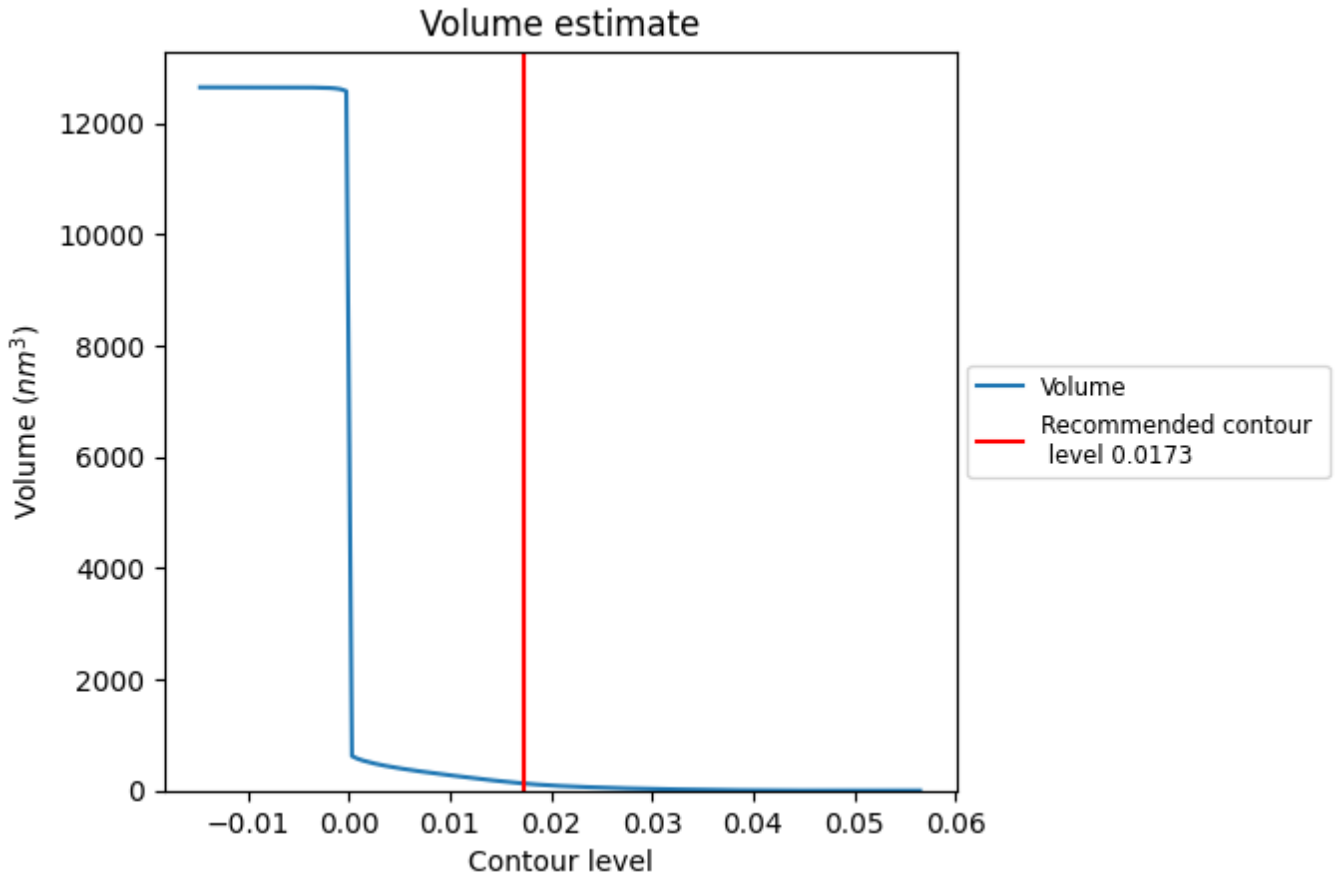
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

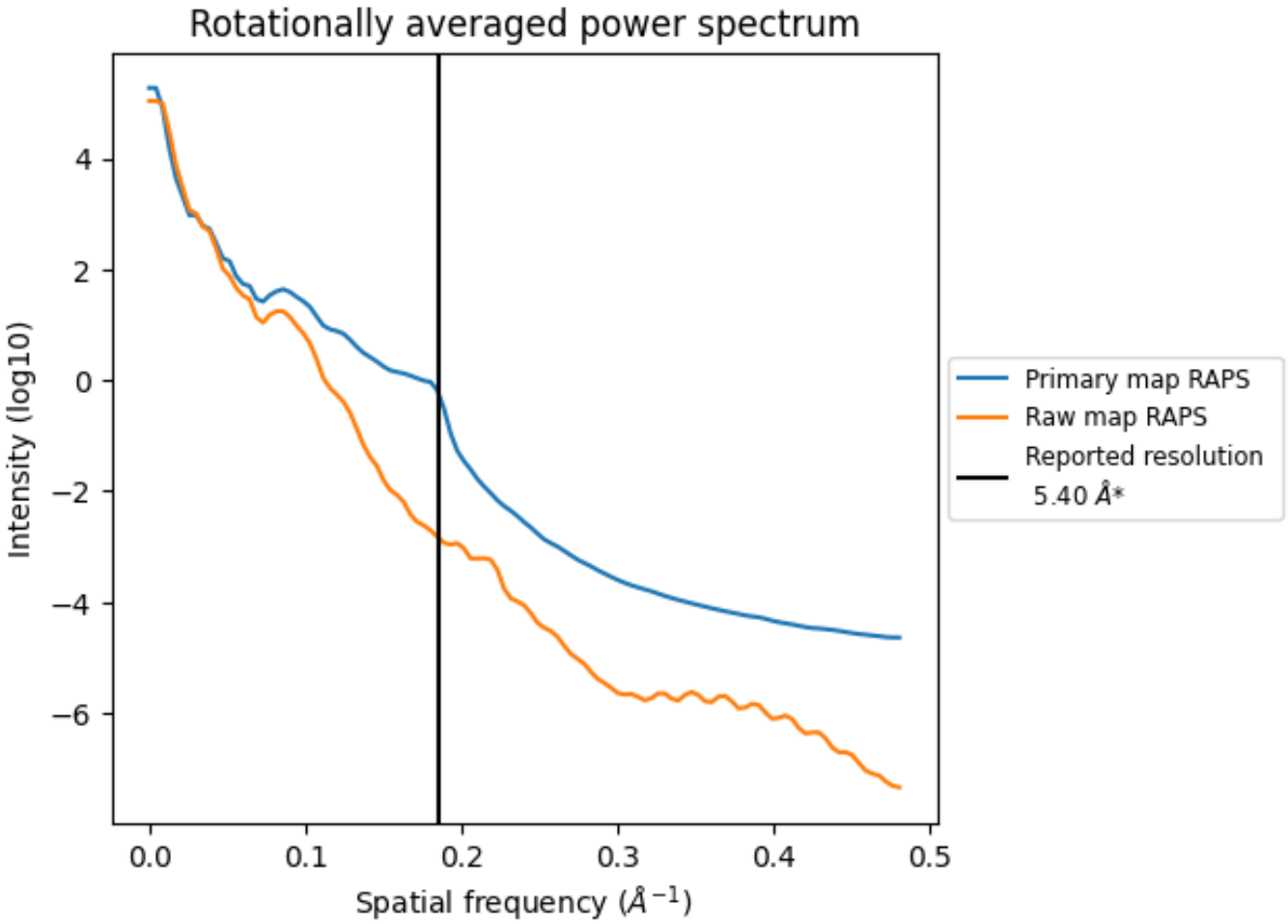
7.2 Volume estimate



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 115 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)

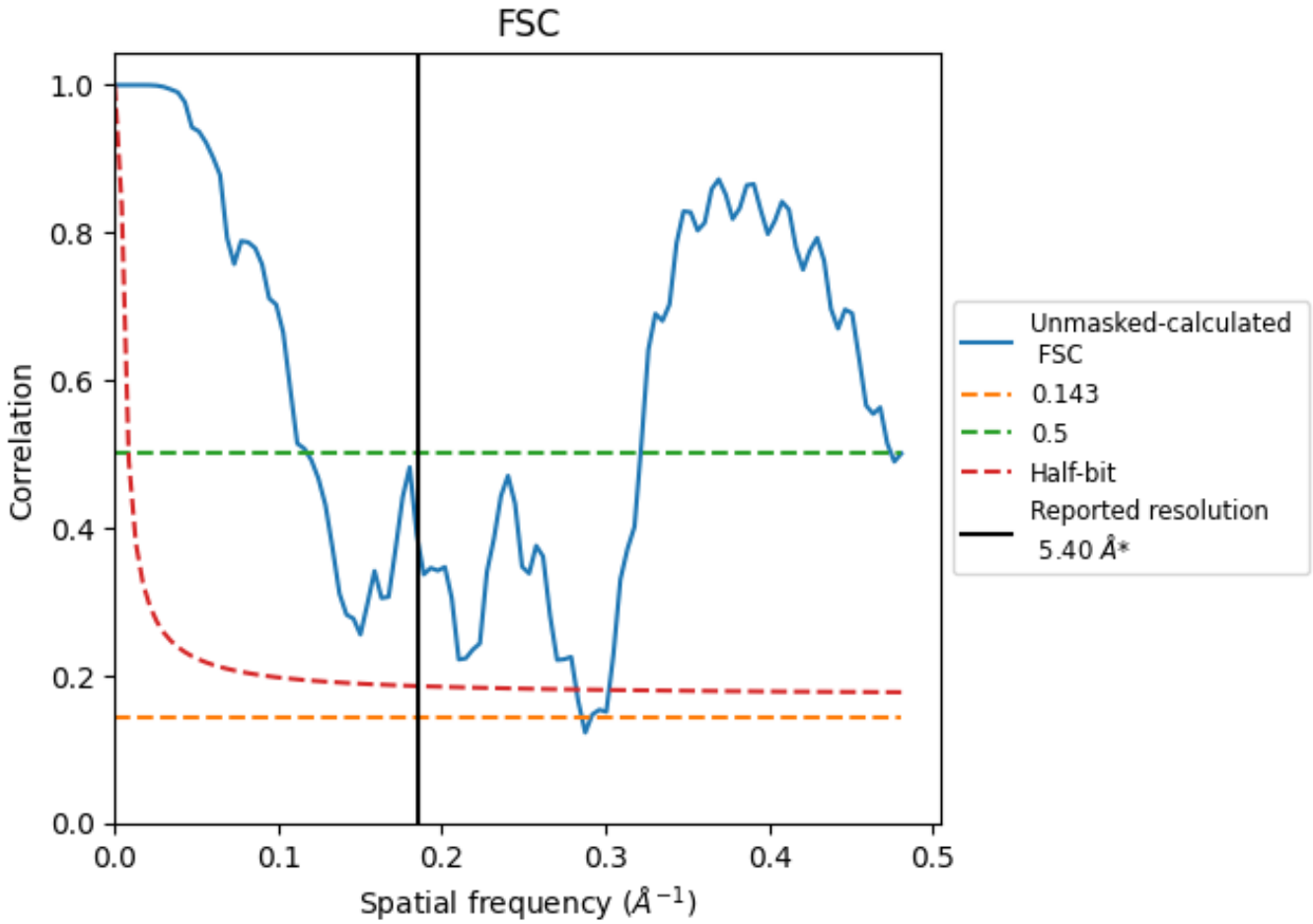


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

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 0.185 Å^{-1}

8.2 Resolution estimates (i)

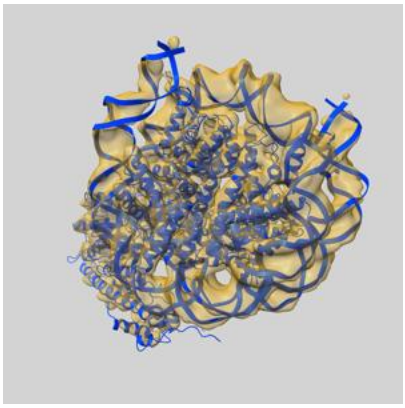
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	8.49	3.54

*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 3.50 differs from the reported value 5.4 by more than 10 %

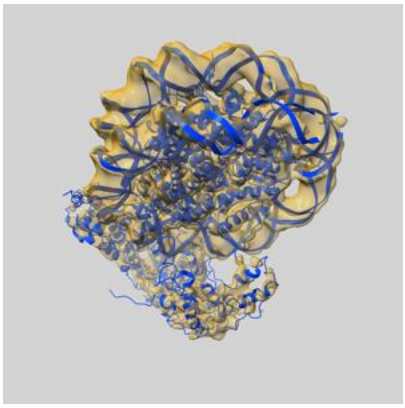
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33521 and PDB model 7XYG. Per-residue inclusion information can be found in section 3 on page 6.

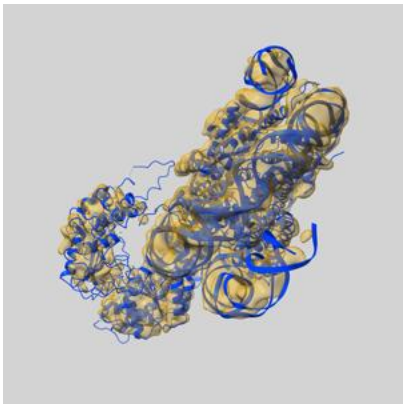
9.1 Map-model overlay



X



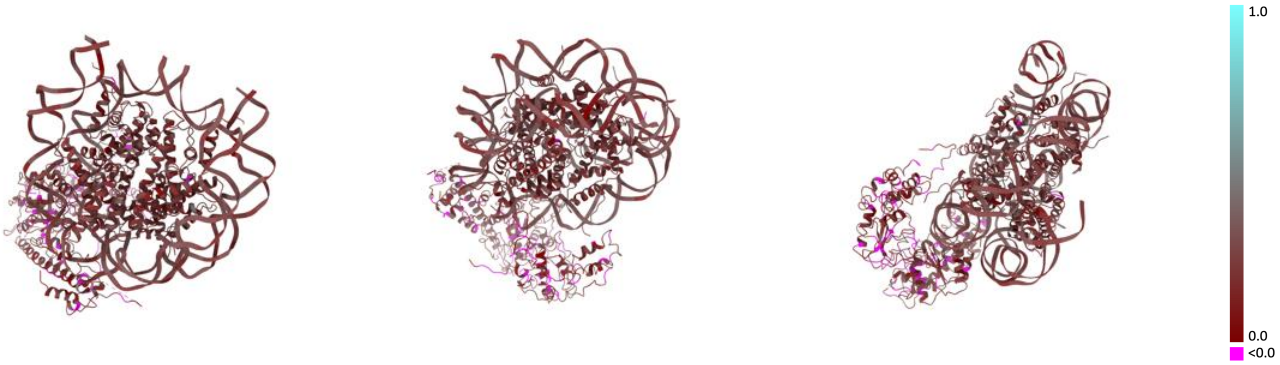
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

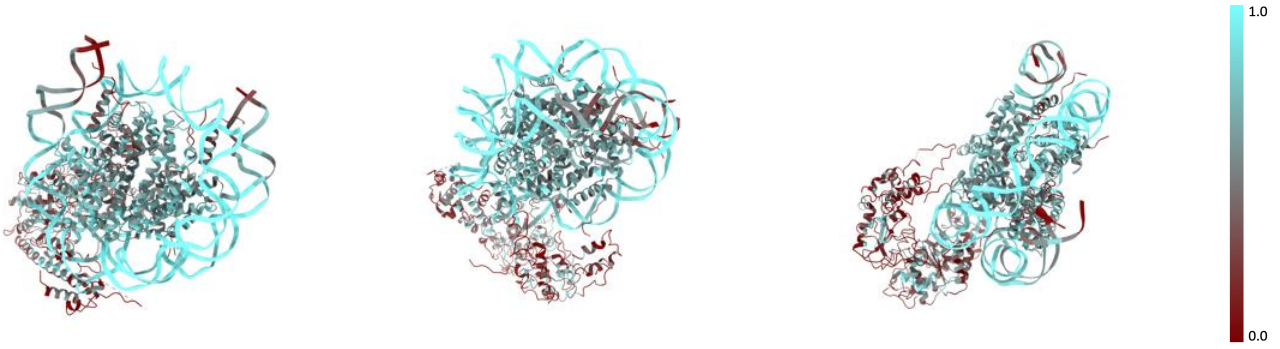
9.2 Q-score mapped to coordinate model



X Y Z

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

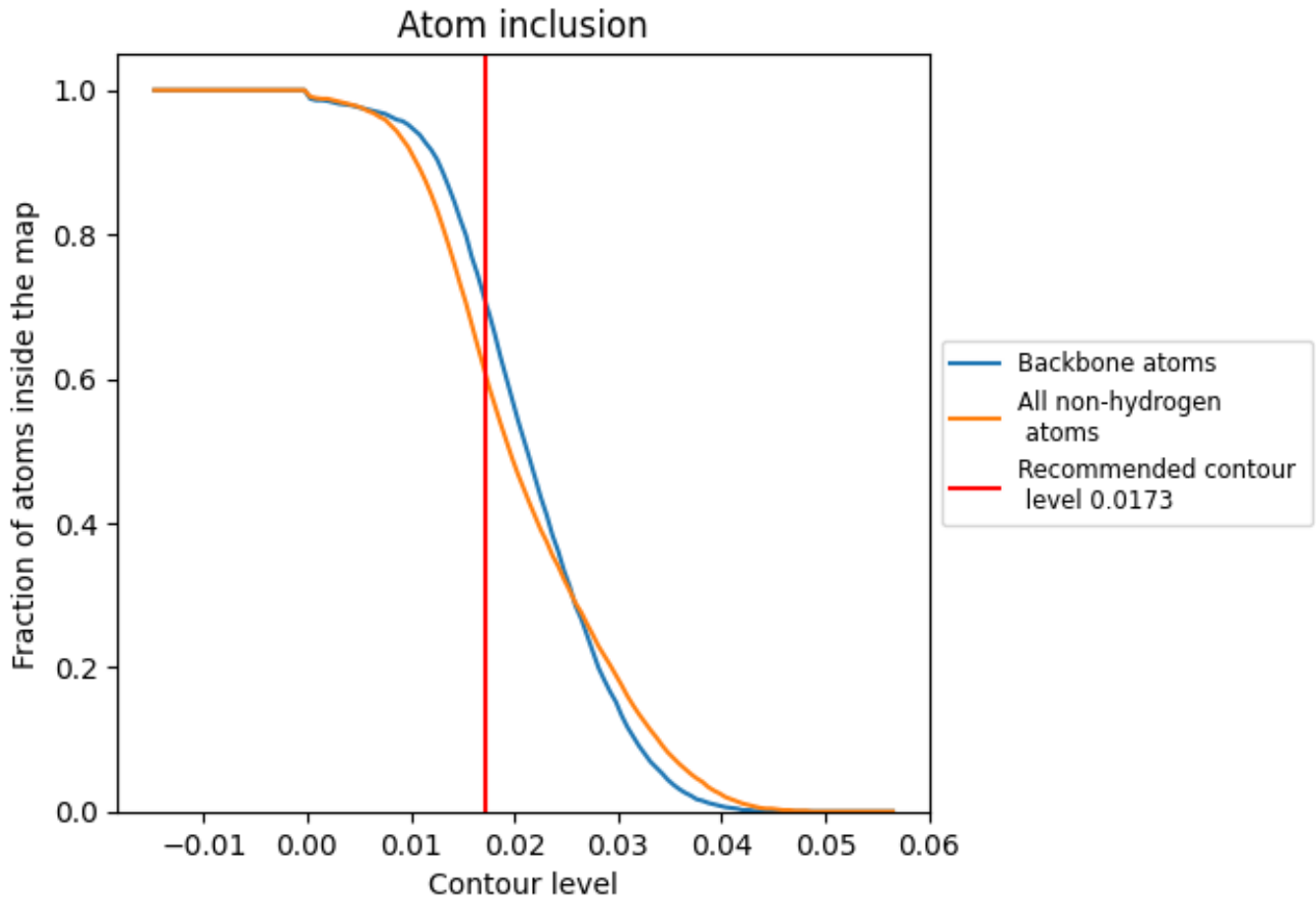
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0173).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 60% 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 (0.0173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.2190
A	0.6080	0.2290
B	0.6760	0.2390
C	0.5930	0.2340
D	0.6140	0.2340
E	0.5950	0.2220
F	0.6280	0.2470
G	0.6000	0.2240
H	0.6730	0.2360
I	0.8520	0.2810
J	0.8450	0.2720
K	0.2910	0.1360