Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 12:12 AM JST

PDB ID	:	8J90
EMDB ID	:	EMD-36083
Title	:	Cryo-EM structure of DDM1-nucleosome complex
Authors	:	Osakabe, A.; Takizawa, Y.; Horikoshi, N.; Hatazawa, S.; Berger, F.; Kurumizaka, H.; Kakutani, T.
Deposited on	:	2023-05-02
Resolution	:	4.71 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:

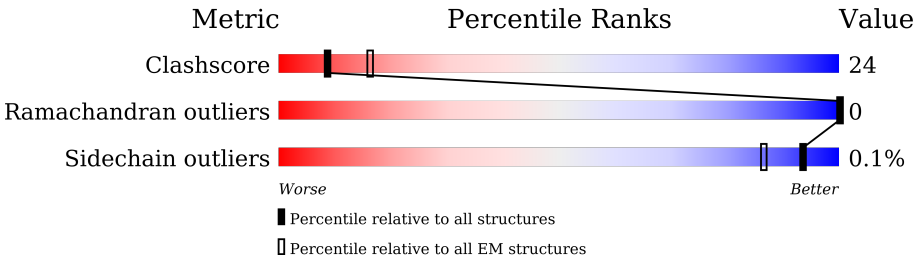
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 4.71 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.



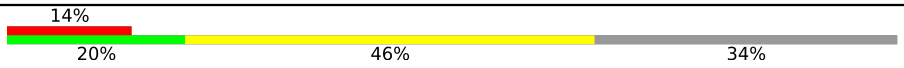
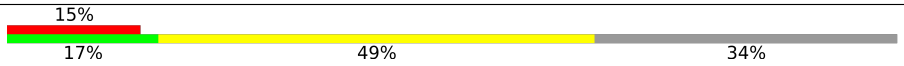
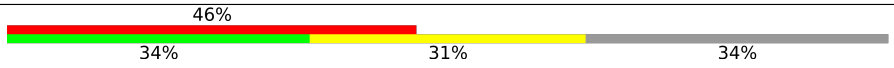
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	139	31% 22% 47%
1	E	139	8% 35% 21% 45%
2	B	106	9% 43% 31% 25%
2	F	106	13% 51% 28% 21%
3	C	153	24% 39% 18% 42%
3	G	153	21% 27% 25% 46%
4	D	153	20% 35% 24% 41%
4	H	153	15% 34% 25% 41%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	169	
6	J	169	
7	K	767	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13881 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 H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	74	Total	C	N	O	S	0	0
			598	379	113	104	2		
1	E	77	Total	C	N	O	S	0	0
			621	393	116	110	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P59226
A	-2	SER	-	expression tag	UNP P59226
A	-1	HIS	-	expression tag	UNP P59226
E	-3	GLY	-	expression tag	UNP P59226
E	-2	SER	-	expression tag	UNP P59226
E	-1	HIS	-	expression tag	UNP P59226

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			636	400	126	109	1		
2	F	84	Total	C	N	O	S	0	0
			676	425	135	115	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P59259
B	-2	SER	-	expression tag	UNP P59259
B	-1	HIS	-	expression tag	UNP P59259
F	-3	GLY	-	expression tag	UNP P59259
F	-2	SER	-	expression tag	UNP P59259
F	-1	HIS	-	expression tag	UNP P59259

- Molecule 3 is a protein called HTA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	88	Total	C	N	O	S	0	0
			676	431	128	115	2		
3	G	82	Total	C	N	O	S	0	0
			635	406	120	108	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9FJE8
C	-2	SER	-	expression tag	UNP Q9FJE8
C	-1	HIS	-	expression tag	UNP Q9FJE8
G	-3	GLY	-	expression tag	UNP Q9FJE8
G	-2	SER	-	expression tag	UNP Q9FJE8
G	-1	HIS	-	expression tag	UNP Q9FJE8

- Molecule 4 is a protein called HTB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	90	Total	C	N	O	S	0	0
			703	451	119	131	2		
4	H	90	Total	C	N	O	S	0	0
			703	451	119	131	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP O23629
D	-2	SER	-	expression tag	UNP O23629
D	-1	HIS	-	expression tag	UNP O23629
H	-3	GLY	-	expression tag	UNP O23629
H	-2	SER	-	expression tag	UNP O23629
H	-1	HIS	-	expression tag	UNP O23629

- Molecule 5 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	111	Total	C	N	O	P	0	0
			2260	1072	410	667	111		

- Molecule 6 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	111	Total	C	N	O	P	0	0
			2291	1082	433	665	111		

- Molecule 7 is a protein called ATP-dependent DNA helicase DDM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	504	Total	C	N	O	S	0	0
			4082	2603	724	735	20		

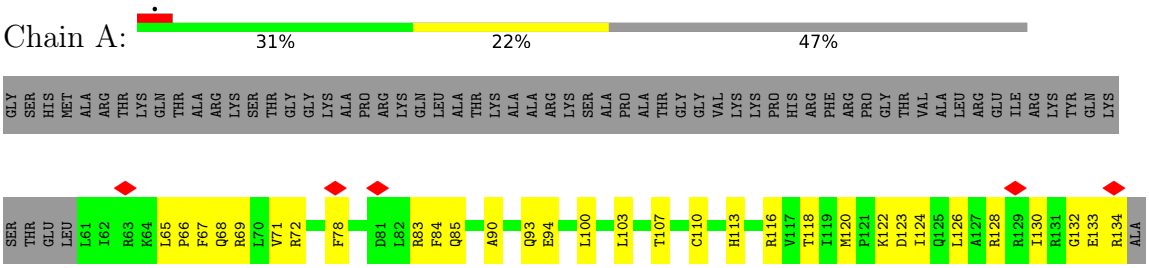
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP Q9XFH4
K	-1	PRO	-	expression tag	UNP Q9XFH4
K	0	HIS	-	expression tag	UNP Q9XFH4

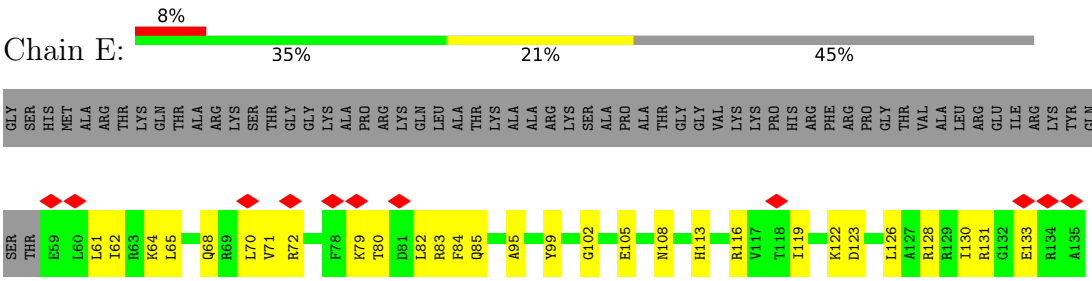
3 Residue-property plots (i)

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.

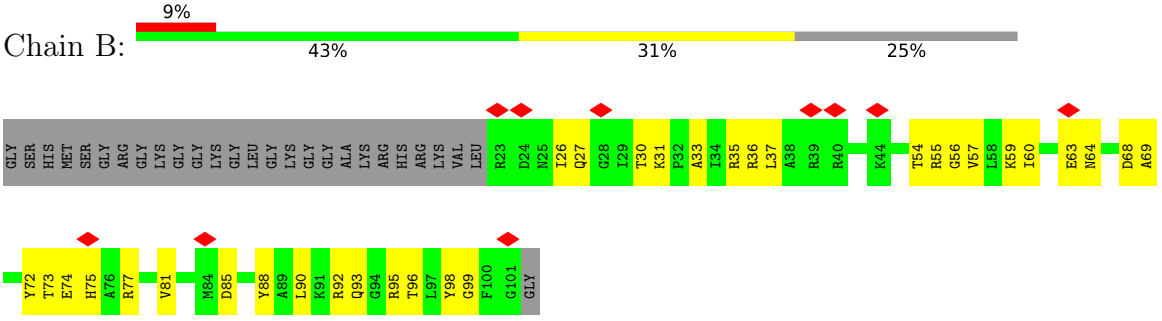
• Molecule 1: Histone H3.1



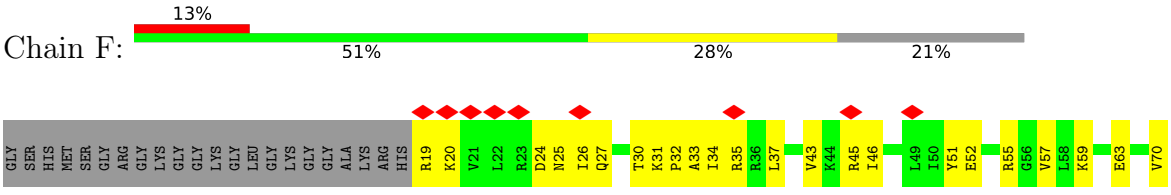
• Molecule 1: Histone H3.1

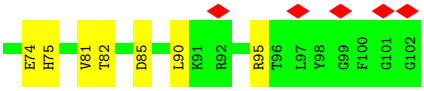


• Molecule 2: Histone H4



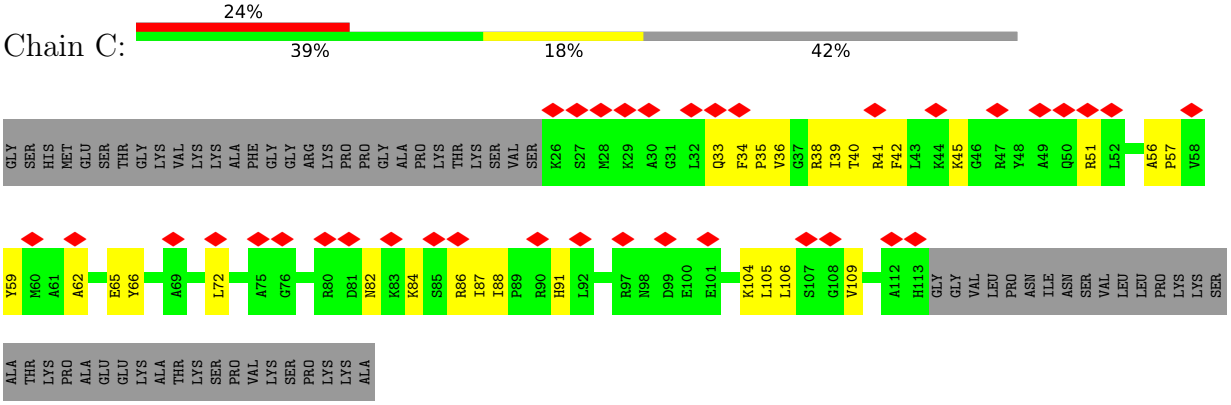
• Molecule 2: Histone H4





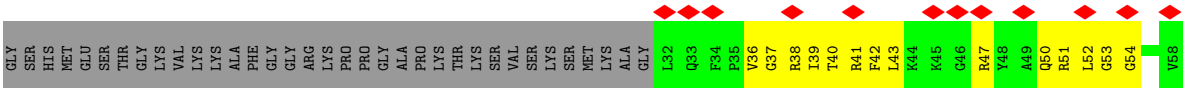
• Molecule 3: HTA6

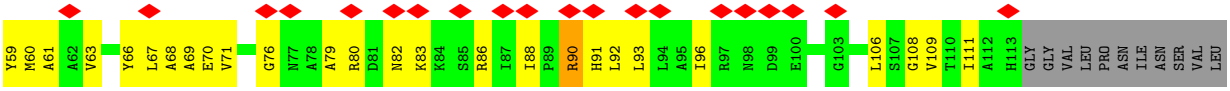
Chain C:

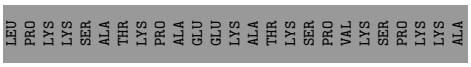


• Molecule 3: HTA6

Chain G:

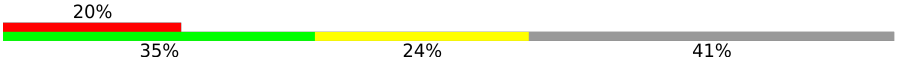


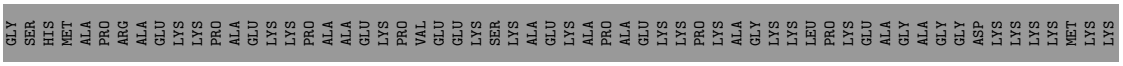


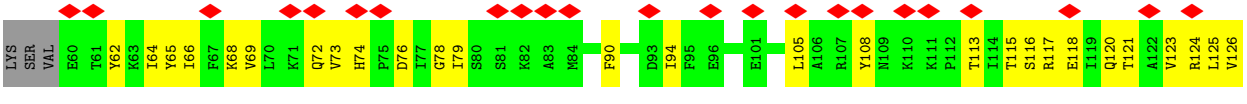


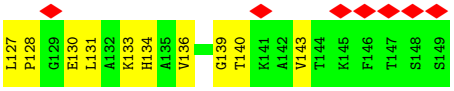
• Molecule 4: HTB9

Chain D:



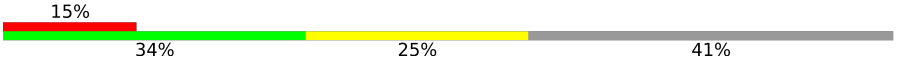


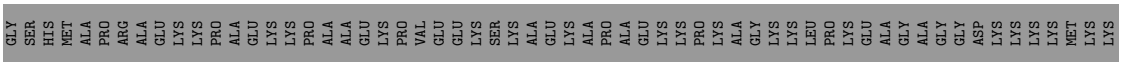


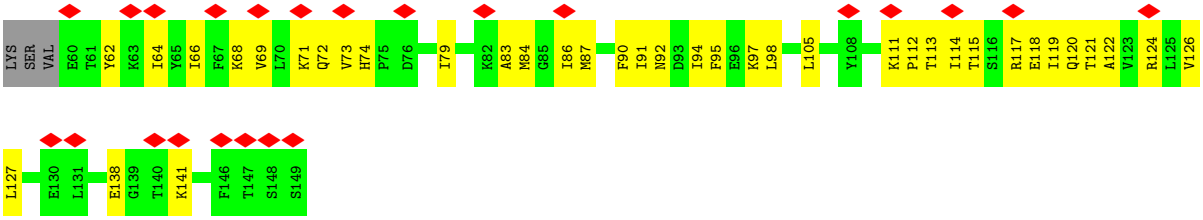


• Molecule 4: HTB9

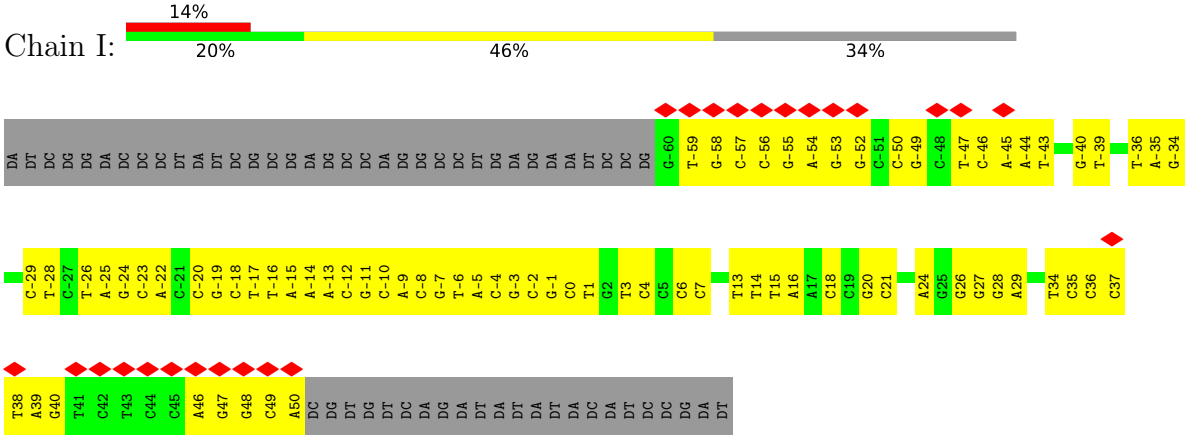
Chain H:



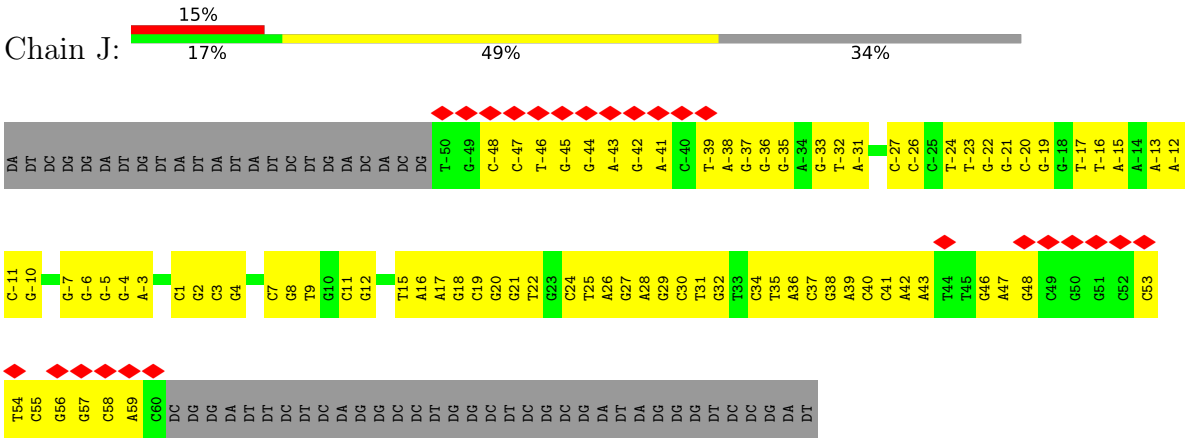




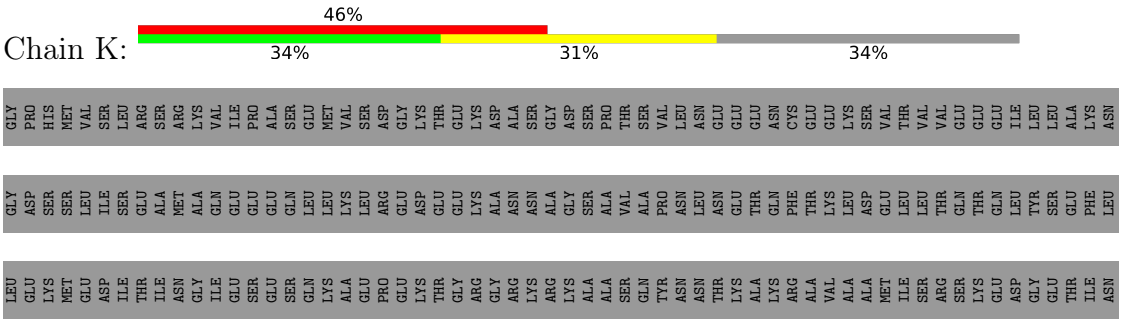
• Molecule 5: DNA (169-MER)

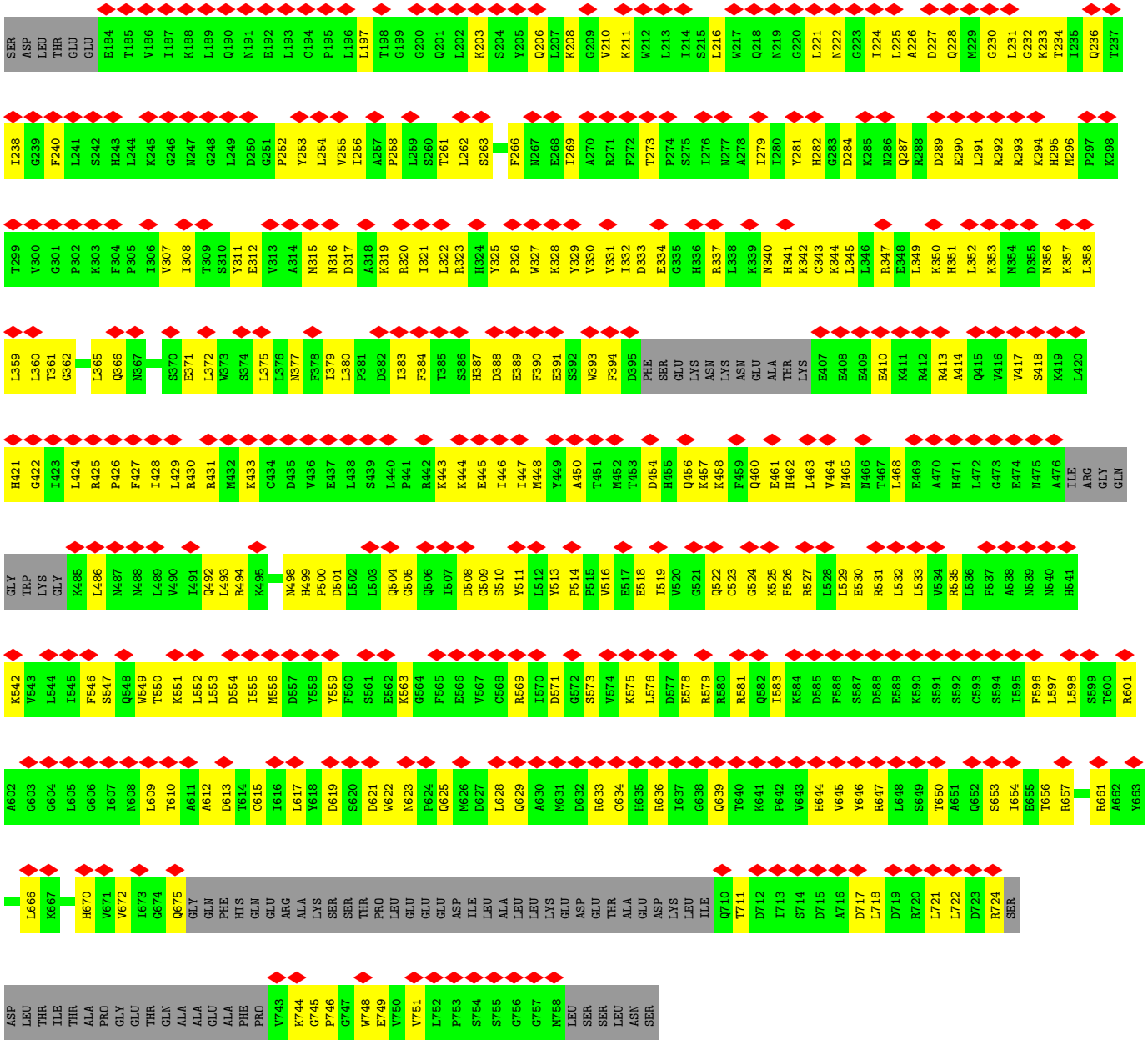


• Molecule 6: DNA (169-MER)



• Molecule 7: ATP-dependent DNA helicase DDM1




SER ASP LEU THR GLU GLU E184 T185 V186 I187 K188 L189 Q190 N191 E192 L193 C194 P195 L196 L197 T198 G199 G200 Q201 L202 K203 S204 Y205 Q206 L207 K208 G209 V210 K211 W212 L213 I214 S215 L216 W217 Q218 N219 G220 L221 N222 G223 I224 L225 A226 D227 Q228 M229 G230 L231 G232 K233 T234 I235 Q236 T237
I238 G239 F240 L241 S242 H243 L244 K245 G246 N247 G248 L249 D250 G251 P252 Y253 L254 V255 T256 A257 P258 L259 S260 T261 L262 S263 F266 N267 E268 I269 A270 R271 F272 T273 P274 S275 I276 N277 A278 I279 I280 Y281 H282 G283 D284 K285 N286 Q287 R288 D289 E290 L291 R292 R293 K294 H295 M296 P297 K298
T299 V300 G301 P302 K303 F304 P305 I306 V307 I308 T309 S310 Y311 E312 V313 A314 M315 N316 D317 A318 K319 R320 I321 L322 R323 H324 Y325 P326 W327 K328 Y329 V330 V331 I332 D333 E334 G335 H336 R337 L338 K339 N340 H341 K342 C343 K344 L345 L346 R347 E348 L349 K350 H351 L352 K353 M354 D355 N356 K357 L358
L359 L360 T361 G362 L365 Q366 N367 S370 E371 L372 W373 S374 L375 L376 N377 F378 I379 L380 P381 D382 I383 F384 T385 S386 H387 D388 E389 F390 E391 S392 W393 F394 D395 PHE SER GLU LYS ASN LYS ASN GLU ALA THR LYS E407 E408 E409 E410 K411 R412 R413 A414 Q415 V416 V417 S418 K419 L420
H421 G422 I423 L424 R425 P426 F427 I428 L429 R430 R431 M432 K433 C434 D435 V436 E437 L438 S439 L440 P441 R442 K443 K444 E445 I446 I447 M448 Y449 A450 T451 M452 T453 D454 H455 Q456 K457 K458 F459 Q460 E461 H462 L463 V464 N465 N466 T467 L468 E469 A470 H471 L472 G473 E474 N475 A476 ILE ARG GLY GLN
GLY TRP LYS GLY K485 L486 N487 N488 L489 V490 I491 Q492 L493 R494 K495 N498 H499 P500 D501 L502 L503 Q504 G505 Q506 I507 D508 G509 S510 Y511 L512 Y513 P514 P515 V516 E517 E518 I519 V520 G521 Q522 C523 G524 K525 F526 R527 L528 L529 E530 R531 L532 L533 V534 R535 L536 F537 A538 N539 N540 H541
K542 V543 L544 I545 F546 S547 Q548 W549 T550 K551 L552 L553 D554 I555 M556 D557 Y558 Y559 F560 S561 E562 K563 G564 F565 E566 V567 C568 R569 I570 D571 G572 S573 V574 K575 L576 D577 E578 R579 R580 R581 Q582 I583 K584 D585 F586 S587 D588 E589 K590 S591 S592 C593 S594 I595 F596 L597 L598 S599 T600 R601
A602 G603 G604 L605 G606 I607 N608 L609 T610 A611 A612 D613 T614 C615 I616 L617 Y618 D619 S620 D621 W622 N623 P624 Q625 M626 D627 L628 Q629 A630 M631 D632 R633 C634 H635 R636 I637 G638 Q639 T640 K641 P642 V643 H644 V645 Y646 R647 L648 S649 T650 A651 Q652 S653 I654 E655 T656 R657 R661 A662 Y663
L666 K667 H670 V671 V672 I673 G674 Q675 GLY GLN PHE HIS GLN GLU GLU ARG ALA LYS SER SER THR PRO LEU GLU GLU GLU ASP ILE LEU LEU ALA LEU LEU LYS GLU ASP GLU THR ALA GLU ASP LYS LEU ILE Q710 T711 D712 I713 S714 D715 A716 D717 L718 D719 R720 L721 L722 D723 R724 SER
ASP LEU THR ILE THR ALA PRO GLY GLU THR GLN ALA ALA GLU ALA PHE PRO V743 K744 G745 P746 G747 W748 E749 V750 V751 L752 P753 S754 S755 G756 G757 M758 LEU SER SER LEU ASN SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34559	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	10000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	211.99998, 211.99998, 211.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.33	0/605	0.66	0/812
1	E	0.27	0/628	0.62	0/842
2	B	0.33	0/643	0.67	0/861
2	F	0.30	0/683	0.67	0/912
3	C	0.26	0/685	0.55	0/918
3	G	0.29	0/644	0.60	0/866
4	D	0.27	0/714	0.54	0/959
4	H	0.25	0/714	0.54	0/959
5	I	0.59	0/2531	0.93	0/3900
6	J	0.56	0/2573	0.90	0/3973
7	K	0.30	0/4162	0.62	2/5611 (0.0%)
All	All	0.41	0/14582	0.74	2/20613 (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})
7	K	509	GLY	N-CA-C	-8.13	92.78	113.10
7	K	232	GLY	N-CA-C	-6.08	97.89	113.10

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	598	0	628	39	0
1	E	621	0	650	39	0
2	B	636	0	675	40	0
2	F	676	0	724	30	0
3	C	676	0	723	33	0
3	G	635	0	675	60	0
4	D	703	0	740	39	0
4	H	703	0	740	40	0
5	I	2260	0	1245	82	0
6	J	2291	0	1244	85	0
7	K	4082	0	4157	243	0
All	All	13881	0	12201	615	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 24.

All (615) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:47:ARG:NH2	3:G:51:ARG:HD2	1.32	1.43
3:G:47:ARG:HH22	3:G:51:ARG:CD	1.34	1.39
3:G:51:ARG:NH1	5:I:39:DA:H3'	1.41	1.35
7:K:505:GLY:HA2	7:K:508:ASP:OD2	1.22	1.31
7:K:505:GLY:CA	7:K:508:ASP:OD2	1.90	1.18
7:K:233:LYS:HD3	7:K:360:LEU:HD11	1.26	1.14
7:K:456:GLN:HG3	7:K:500:PRO:HG3	1.20	1.13
2:B:96:THR:HG22	3:G:108:GLY:O	1.50	1.12
1:A:85:GLN:HG2	5:I:-24:DG:H5"	1.39	1.04
7:K:456:GLN:HE21	7:K:500:PRO:CG	1.70	1.03
2:B:96:THR:HG23	3:G:109:VAL:HA	1.36	1.02
7:K:456:GLN:CG	7:K:500:PRO:HG3	1.88	1.02
7:K:233:LYS:NZ	7:K:361:THR:O	1.93	1.01
2:B:96:THR:CG2	3:G:108:GLY:O	2.12	0.96
2:B:90:LEU:O	2:B:95:ARG:O	1.84	0.95
1:A:85:GLN:HG2	5:I:-24:DG:C5'	1.94	0.95
3:G:51:ARG:NH1	5:I:39:DA:C3'	2.30	0.95
3:G:50:GLN:O	3:G:51:ARG:HG2	1.65	0.94
7:K:228:GLN:NE2	7:K:433:LYS:HE2	1.82	0.94
7:K:456:GLN:NE2	7:K:500:PRO:HG2	1.83	0.92
7:K:456:GLN:HE21	7:K:500:PRO:CD	1.84	0.90
7:K:228:GLN:HG3	7:K:231:LEU:HD22	1.53	0.89
7:K:456:GLN:NE2	7:K:500:PRO:CG	2.34	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:421:HIS:HA	7:K:424:LEU:HB2	1.56	0.88
3:G:51:ARG:HH12	5:I:39:DA:H3'	1.05	0.88
2:B:96:THR:HG23	3:G:109:VAL:CA	2.08	0.84
7:K:505:GLY:HA2	7:K:508:ASP:CG	1.98	0.82
3:G:51:ARG:HH12	5:I:39:DA:C3'	1.91	0.81
7:K:505:GLY:N	7:K:508:ASP:OD2	2.12	0.81
7:K:228:GLN:NE2	7:K:433:LYS:CE	2.45	0.79
7:K:454:ASP:OD1	7:K:457:LYS:NZ	2.16	0.79
7:K:498:ASN:HB3	7:K:552:LEU:HD22	1.63	0.79
7:K:203:LYS:HB2	7:K:206:GLN:HE22	1.48	0.78
7:K:238:ILE:HD11	7:K:269:ILE:HG22	1.66	0.78
7:K:233:LYS:HD3	7:K:360:LEU:CD1	2.11	0.77
2:B:73:THR:HG21	2:B:81:VAL:HG22	1.66	0.77
6:J:-17:DT:H5"	7:K:312:GLU:HG3	1.67	0.77
3:G:50:GLN:O	3:G:51:ARG:CG	2.32	0.76
3:G:47:ARG:HH22	3:G:51:ARG:HD2	0.60	0.76
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.17	0.76
4:H:64:ILE:HD13	5:I:48:DG:H3'	1.66	0.75
7:K:227:ASP:HA	7:K:430:ARG:HD3	1.67	0.75
7:K:456:GLN:HE21	7:K:500:PRO:HG2	1.43	0.75
3:G:38:ARG:HG3	3:G:42:PHE:HE2	1.52	0.74
7:K:317:ASP:HB3	7:K:321:ILE:HD13	1.70	0.73
7:K:230:GLY:O	7:K:636:ARG:NH2	2.22	0.73
1:A:116:ARG:HE	5:I:-3:DG:H3'	1.52	0.72
1:A:69:ARG:NH2	6:J:17:DA:OP1	2.22	0.72
1:E:61:LEU:HD23	2:F:37:LEU:HD23	1.70	0.72
3:C:106:LEU:HD21	4:D:90:PHE:HE1	1.54	0.71
7:K:228:GLN:HG3	7:K:231:LEU:CD2	2.20	0.71
7:K:228:GLN:NE2	7:K:431:ARG:O	2.24	0.71
2:B:74:GLU:O	4:D:117:ARG:NH2	2.24	0.71
7:K:227:ASP:O	7:K:233:LYS:HE2	1.90	0.71
1:A:116:ARG:HD3	1:A:120:MET:HE1	1.74	0.70
7:K:252:PRO:HG2	7:K:328:LYS:H	1.55	0.69
7:K:575:LYS:N	7:K:578:GLU:OE2	2.25	0.69
7:K:612:ALA:O	7:K:639:GLN:NE2	2.23	0.69
7:K:525:LYS:HE2	7:K:650:THR:HA	1.74	0.68
3:G:51:ARG:O	4:H:113:THR:OG1	2.10	0.68
6:J:-20:DC:H2'	6:J:-19:DG:C8	2.28	0.68
7:K:233:LYS:CD	7:K:360:LEU:HD11	2.16	0.68
7:K:377:ASN:ND2	7:K:384:PHE:O	2.26	0.68
2:B:99:GLY:HA2	4:H:86:ILE:HG22	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ARG:NH2	5:I:-13:DA:OP1	2.26	0.68
2:F:20:LYS:HB2	7:K:511:TYR:HA	1.77	0.67
2:F:74:GLU:O	4:H:117:ARG:NH2	2.27	0.67
1:A:107:THR:HG21	1:A:124:ILE:HG13	1.77	0.66
5:I:-47:DT:H2"	5:I:-46:DC:C5	2.30	0.66
7:K:203:LYS:HB2	7:K:206:GLN:NE2	2.10	0.66
7:K:425:ARG:HB2	7:K:675:GLN:HE22	1.59	0.66
7:K:527:ARG:HH11	7:K:531:ARG:HH22	1.42	0.66
2:B:60:ILE:O	2:B:64:ASN:ND2	2.29	0.65
7:K:625:GLN:HA	7:K:628:LEU:HD12	1.78	0.65
3:G:59:TYR:OH	4:H:120:GLN:NE2	2.30	0.65
7:K:319:LYS:HE3	7:K:319:LYS:HA	1.79	0.65
7:K:431:ARG:NH1	7:K:431:ARG:HA	2.12	0.64
7:K:461:GLU:O	7:K:465:ASN:ND2	2.29	0.64
7:K:504:GLN:OE1	7:K:504:GLN:N	2.31	0.64
6:J:30:DC:H2'	6:J:31:DT:H71	1.79	0.64
1:E:128:ARG:HH22	2:F:57:VAL:HG13	1.63	0.64
2:B:90:LEU:C	2:B:95:ARG:O	2.35	0.64
7:K:366:GLN:HB2	7:K:371:GLU:HG3	1.79	0.64
7:K:504:GLN:HB3	7:K:508:ASP:OD1	1.96	0.64
6:J:-24:DT:C2	6:J:-23:DT:N3	2.65	0.64
7:K:424:LEU:HA	7:K:427:PHE:HB3	1.79	0.64
7:K:254:LEU:N	7:K:329:TYR:O	2.31	0.63
3:G:47:ARG:NH2	3:G:51:ARG:CD	2.16	0.63
7:K:456:GLN:CG	7:K:500:PRO:CG	2.73	0.63
7:K:717:ASP:O	7:K:721:LEU:HG	1.99	0.63
3:C:33:GLN:NE2	4:D:72:GLN:OE1	2.31	0.63
3:G:79:ALA:O	3:G:83:LYS:N	2.31	0.63
5:I:21:DC:H5"	7:K:337:ARG:HH12	1.63	0.63
5:I:26:DG:H2"	5:I:27:DG:N7	2.13	0.63
7:K:316:ASN:O	7:K:320:ARG:NH2	2.31	0.63
7:K:504:GLN:C	7:K:508:ASP:OD1	2.37	0.63
6:J:28:DA:H2"	6:J:29:DG:C8	2.34	0.62
7:K:262:LEU:HD12	7:K:263:SER:N	2.13	0.62
7:K:224:ILE:HD11	7:K:379:ILE:HG21	1.81	0.62
7:K:253:TYR:HA	7:K:329:TYR:HB2	1.81	0.62
3:C:66:TYR:HE2	4:D:131:LEU:HG	1.64	0.62
5:I:35:DC:H2"	5:I:36:DC:C5	2.33	0.62
1:E:95:ALA:HB2	2:F:90:LEU:HD21	1.80	0.62
7:K:445:GLU:HB2	7:K:647:ARG:HH12	1.63	0.62
7:K:294:LYS:HE3	7:K:295:HIS:CE1	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:NH1	1:A:118:THR:O	2.33	0.62
2:F:75:HIS:O	4:H:117:ARG:NH1	2.28	0.62
6:J:-39:DT:H2"	6:J:-38:DA:N7	2.14	0.62
7:K:365:LEU:O	7:K:625:GLN:NE2	2.32	0.62
3:C:38:ARG:O	3:C:41:ARG:HG2	2.00	0.62
3:C:105:LEU:HD13	4:D:128:PRO:HD3	1.81	0.62
7:K:255:VAL:HG23	7:K:331:VAL:HG23	1.80	0.62
1:E:65:LEU:O	1:E:68:GLN:HG3	2.01	0.61
7:K:292:ARG:HA	7:K:296:MET:HG2	1.82	0.61
1:A:85:GLN:HG2	5:I:-24:DG:H5'	1.78	0.61
4:D:126:VAL:HG13	4:D:127:LEU:HD12	1.82	0.61
1:E:72:ARG:HH22	1:E:84:PHE:H	1.47	0.61
6:J:15:DT:H2"	6:J:16:DA:C8	2.36	0.61
4:D:118:GLU:HA	4:D:121:THR:HG22	1.82	0.60
7:K:529:LEU:HD12	7:K:532:LEU:HD11	1.81	0.60
7:K:281:TYR:CD1	7:K:291:LEU:HD13	2.37	0.60
5:I:0:DC:H2'	5:I:1:DT:H71	1.82	0.60
7:K:443:LYS:NZ	7:K:444:LYS:O	2.34	0.60
2:B:75:HIS:O	4:D:117:ARG:NH1	2.27	0.60
7:K:255:VAL:HA	7:K:331:VAL:O	2.01	0.60
7:K:431:ARG:HA	7:K:431:ARG:HH11	1.65	0.60
1:E:85:GLN:HE22	2:F:82:THR:HA	1.65	0.60
6:J:37:DC:H2"	6:J:38:DG:C8	2.37	0.60
1:A:130:ILE:HG22	1:E:131:ARG:NH2	2.15	0.60
6:J:41:DC:N3	6:J:42:DA:N6	2.50	0.59
7:K:578:GLU:HA	7:K:581:ARG:HG2	1.83	0.59
2:B:96:THR:CG2	3:G:108:GLY:C	2.70	0.59
6:J:-32:DT:H2"	6:J:-31:DA:H8	1.66	0.59
2:B:96:THR:HG23	2:B:96:THR:O	2.01	0.59
7:K:486:LEU:HB3	7:K:492:GLN:NE2	2.17	0.59
1:E:99:TYR:HB2	2:F:95:ARG:HH12	1.66	0.59
7:K:252:PRO:HB2	7:K:327:TRP:CE3	2.38	0.59
7:K:417:VAL:O	7:K:422:GLY:N	2.32	0.59
7:K:569:ARG:HG3	7:K:597:LEU:HD22	1.84	0.59
7:K:206:GLN:O	7:K:210:VAL:HG23	2.03	0.59
7:K:505:GLY:CA	7:K:508:ASP:CG	2.62	0.59
7:K:446:ILE:HD11	7:K:748:TRP:HB2	1.85	0.59
6:J:28:DA:H2"	6:J:29:DG:H8	1.65	0.59
1:E:116:ARG:HH12	1:E:122:LYS:NZ	2.01	0.59
3:G:86:ARG:NH1	4:H:79:ILE:O	2.35	0.59
5:I:7:DC:H5"	5:I:7:DC:H6	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:505:GLY:N	7:K:508:ASP:CG	2.56	0.59
3:C:33:GLN:O	4:D:68:LYS:NZ	2.36	0.58
4:H:111:LYS:HD2	4:H:112:PRO:HD2	1.85	0.58
6:J:20:DG:H2"	6:J:21:DG:H5"	1.84	0.58
7:K:504:GLN:C	7:K:508:ASP:CG	2.62	0.58
3:C:41:ARG:NE	5:I:-44:DA:OP1	2.37	0.58
7:K:216:LEU:HD12	7:K:221:LEU:HB2	1.85	0.58
5:I:-8:DC:H2"	5:I:-7:DG:C8	2.38	0.58
5:I:-44:DA:H1'	5:I:-43:DT:H5'	1.85	0.58
7:K:225:LEU:N	7:K:359:LEU:O	2.32	0.58
7:K:516:VAL:HA	7:K:519:ILE:HD13	1.85	0.58
4:H:94:ILE:HA	4:H:97:LYS:HG2	1.86	0.58
7:K:296:MET:HB2	7:K:325:TYR:OH	2.03	0.58
1:A:67:PHE:O	1:A:71:VAL:HG23	2.04	0.57
7:K:425:ARG:HB2	7:K:675:GLN:NE2	2.19	0.57
1:A:83:ARG:HH11	5:I:-23:DC:H5"	1.68	0.57
7:K:456:GLN:HE22	7:K:522:GLN:C	2.08	0.57
2:F:82:THR:HG23	2:F:85:ASP:H	1.69	0.57
6:J:-7:DG:H2"	6:J:-6:DG:C8	2.40	0.57
1:A:66:PRO:HG3	1:A:69:ARG:NH2	2.20	0.57
7:K:347:ARG:HA	7:K:350:LYS:NZ	2.19	0.57
4:D:116:SER:O	4:D:120:GLN:NE2	2.38	0.57
1:A:90:ALA:O	1:A:94:GLU:HG3	2.04	0.56
7:K:513:TYR:CE2	7:K:519:ILE:HD11	2.40	0.56
1:A:130:ILE:O	1:E:131:ARG:NH1	2.37	0.56
1:E:126:LEU:O	1:E:130:ILE:HD12	2.05	0.56
4:H:73:VAL:HG22	4:H:74:HIS:CD2	2.40	0.56
5:I:15:DT:H1'	5:I:16:DA:C8	2.40	0.56
7:K:456:GLN:HG3	7:K:500:PRO:CG	2.14	0.56
3:C:35:PRO:HD3	4:D:65:TYR:CE1	2.40	0.56
4:H:138:GLU:HA	4:H:141:LYS:HD2	1.87	0.56
2:B:60:ILE:O	2:B:63:GLU:HG3	2.05	0.56
2:F:19:ARG:NH2	7:K:511:TYR:O	2.39	0.56
7:K:228:GLN:HE22	7:K:433:LYS:HE2	1.67	0.56
7:K:629:GLN:HB3	7:K:633:ARG:HH12	1.68	0.56
7:K:316:ASN:OD1	7:K:317:ASP:N	2.39	0.56
7:K:458:LYS:O	7:K:462:HIS:ND1	2.34	0.55
7:K:575:LYS:HG2	7:K:576:LEU:H	1.71	0.55
3:C:38:ARG:HA	3:C:41:ARG:HE	1.72	0.55
7:K:553:LEU:HA	7:K:556:MET:SD	2.46	0.55
6:J:24:DC:H2"	6:J:25:DT:C6	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:666:LEU:O	7:K:670:HIS:ND1	2.39	0.55
1:A:130:ILE:HG22	1:E:131:ARG:HH22	1.72	0.55
4:H:69:VAL:O	4:H:73:VAL:HG12	2.06	0.55
5:I:-36:DT:H2"	5:I:-35:DA:N7	2.22	0.55
7:K:508:ASP:HB3	7:K:510:SER:H	1.71	0.55
7:K:226:ALA:HB1	7:K:362:GLY:O	2.06	0.55
7:K:529:LEU:HA	7:K:532:LEU:HG	1.88	0.55
2:B:72:TYR:OH	2:B:92:ARG:HG3	2.07	0.55
5:I:-59:DT:H2"	5:I:-58:DG:C8	2.41	0.55
1:A:120:MET:CG	1:A:122:LYS:HG2	2.37	0.55
2:F:24:ASP:HB2	2:F:27:GLN:HG3	1.89	0.55
5:I:-26:DT:H2"	5:I:-25:DA:N7	2.22	0.55
5:I:-2:DC:H2"	5:I:-1:DG:C8	2.41	0.54
7:K:513:TYR:HE2	7:K:519:ILE:HD11	1.72	0.54
5:I:49:DC:H2"	5:I:50:DA:C8	2.42	0.54
3:G:51:ARG:HH11	5:I:39:DA:H3'	1.60	0.54
1:A:67:PHE:HE2	1:A:93:GLN:HA	1.72	0.54
1:A:78:PHE:HZ	2:B:63:GLU:HB2	1.73	0.54
7:K:417:VAL:HG13	7:K:421:HIS:HB3	1.89	0.54
5:I:46:DA:H2"	5:I:47:DG:N7	2.23	0.54
6:J:-4:DG:H2"	6:J:-3:DA:C8	2.43	0.54
7:K:553:LEU:HB3	7:K:597:LEU:HD21	1.88	0.54
4:D:64:ILE:HG13	4:D:65:TYR:HD2	1.73	0.54
7:K:504:GLN:O	7:K:508:ASP:N	2.41	0.54
7:K:546:PHE:HE1	7:K:598:LEU:HD23	1.71	0.54
7:K:372:LEU:HD13	7:K:375:LEU:HD21	1.90	0.54
7:K:610:THR:HA	7:K:634:CYS:HA	1.89	0.54
6:J:-13:DA:H2"	6:J:-12:DA:C8	2.43	0.53
7:K:463:LEU:HD11	7:K:492:GLN:HB3	1.91	0.53
5:I:20:DG:H3'	7:K:344:LYS:HD3	1.90	0.53
3:G:50:GLN:O	3:G:51:ARG:CD	2.57	0.53
7:K:711:THR:OG1	7:K:746:PRO:O	2.27	0.53
6:J:1:DC:H2"	6:J:2:DG:C8	2.42	0.53
4:D:73:VAL:HG12	4:D:74:HIS:CD2	2.44	0.53
7:K:292:ARG:HH21	7:K:293:ARG:NH1	2.06	0.53
7:K:387:HIS:O	7:K:391:GLU:HB2	2.09	0.53
2:B:77:ARG:HE	4:D:117:ARG:NH2	2.07	0.53
3:C:84:LYS:HE2	6:J:58:DC:OP1	2.09	0.53
6:J:35:DT:H2"	6:J:36:DA:C8	2.44	0.53
1:A:130:ILE:C	1:E:131:ARG:HH22	2.12	0.53
6:J:7:DC:H2"	6:J:8:DG:C8	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:745:GLY:HA3	7:K:748:TRP:CZ2	2.44	0.53
1:A:85:GLN:CG	5:I:-24:DG:H5"	2.24	0.53
1:A:67:PHE:CE2	1:A:93:GLN:HA	2.45	0.52
3:G:47:ARG:NH2	3:G:50:GLN:O	2.42	0.52
7:K:287:GLN:HA	7:K:290:GLU:HG3	1.91	0.52
7:K:527:ARG:HH11	7:K:531:ARG:NH2	2.07	0.52
7:K:266:PHE:HA	7:K:269:ILE:HG12	1.92	0.52
7:K:312:GLU:OE2	7:K:316:ASN:ND2	2.42	0.52
7:K:317:ASP:HB3	7:K:321:ILE:CD1	2.40	0.52
1:E:68:GLN:HA	1:E:71:VAL:HG12	1.91	0.52
6:J:21:DG:H2"	6:J:22:DT:H5'	1.90	0.52
7:K:417:VAL:HA	7:K:421:HIS:HB3	1.91	0.52
2:F:74:GLU:OE1	4:H:124:ARG:NH1	2.42	0.52
3:G:88:ILE:HD12	3:G:90:ARG:HE	1.75	0.52
5:I:-50:DC:H2"	5:I:-49:DG:C8	2.44	0.52
5:I:-14:DA:H2"	5:I:-13:DA:C8	2.44	0.52
5:I:28:DG:H2"	5:I:29:DA:H8	1.74	0.52
7:K:226:ALA:HA	7:K:361:THR:O	2.09	0.52
7:K:262:LEU:HD22	7:K:282:HIS:CD2	2.45	0.52
7:K:617:LEU:O	7:K:647:ARG:HA	2.10	0.52
3:G:88:ILE:HG12	3:G:91:HIS:ND1	2.24	0.52
4:H:69:VAL:O	4:H:72:GLN:HG3	2.10	0.52
7:K:326:PRO:HA	7:K:353:LYS:HD2	1.92	0.52
3:G:54:GLY:HA3	5:I:38:DT:OP1	2.10	0.52
7:K:228:GLN:H	7:K:430:ARG:HD3	1.75	0.52
2:B:85:ASP:HA	2:B:88:TYR:HD2	1.74	0.51
3:C:62:ALA:O	3:C:65:GLU:HG3	2.09	0.51
1:E:119:ILE:HD13	2:F:43:VAL:HG11	1.91	0.51
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.45	0.51
6:J:-27:DC:H2"	6:J:-26:DC:C5	2.45	0.51
1:E:83:ARG:HD3	1:E:84:PHE:N	2.26	0.51
7:K:333:ASP:HA	7:K:360:LEU:HB3	1.91	0.51
7:K:527:ARG:HD3	7:K:531:ARG:HH12	1.75	0.51
3:G:53:GLY:HA3	4:H:115:THR:HA	1.92	0.51
7:K:425:ARG:HB3	7:K:426:PRO:HD3	1.93	0.51
3:C:35:PRO:HD3	4:D:65:TYR:CD1	2.46	0.51
6:J:-23:DT:H2"	6:J:-22:DG:N7	2.26	0.51
7:K:208:LYS:HA	7:K:211:LYS:HE3	1.93	0.51
7:K:334:GLU:OE1	7:K:337:ARG:HB2	2.11	0.51
3:C:33:GLN:HB3	4:D:68:LYS:HZ3	1.76	0.51
6:J:-38:DA:H2'	6:J:-37:DG:C8	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:56:DG:H2"	6:J:57:DG:N7	2.26	0.51
4:H:115:THR:HG23	4:H:117:ARG:H	1.75	0.51
3:G:52:LEU:HD11	4:H:119:ILE:HD11	1.93	0.50
6:J:-21:DG:H2'	6:J:-20:DC:C6	2.45	0.50
7:K:323:ARG:HH12	7:K:351:HIS:C	2.14	0.50
7:K:254:LEU:HD22	7:K:327:TRP:CD1	2.46	0.50
7:K:535:ARG:NH1	7:K:722:LEU:HD12	2.26	0.50
7:K:583:ILE:HG23	7:K:609:LEU:HD21	1.92	0.50
4:H:94:ILE:HG23	4:H:98:LEU:HD23	1.92	0.50
5:I:21:DC:P	7:K:344:LYS:HG2	2.52	0.50
2:B:54:THR:HA	2:B:57:VAL:HG22	1.93	0.50
7:K:345:LEU:O	7:K:349:LEU:HG	2.12	0.50
3:G:106:LEU:HD11	4:H:90:PHE:CE1	2.47	0.50
1:E:72:ARG:HH12	1:E:83:ARG:HA	1.77	0.50
2:F:31:LYS:HG2	2:F:35:ARG:NH1	2.26	0.50
3:G:96:ILE:HG12	3:G:106:LEU:HD12	1.93	0.50
6:J:54:DT:H2"	6:J:55:DC:C6	2.46	0.50
7:K:493:LEU:HD13	7:K:654:ILE:HD13	1.94	0.50
4:D:130:GLU:O	4:D:134:HIS:ND1	2.35	0.50
2:F:31:LYS:HG3	2:F:51:TYR:CE2	2.47	0.50
6:J:3:DC:H2"	6:J:4:DG:C8	2.46	0.50
3:G:37:GLY:O	3:G:40:THR:OG1	2.27	0.49
6:J:-24:DT:C4	6:J:-23:DT:O4	2.65	0.49
6:J:25:DT:H2"	6:J:26:DA:N7	2.27	0.49
7:K:234:THR:O	7:K:238:ILE:HD12	2.11	0.49
7:K:524:GLY:HA2	7:K:527:ARG:HE	1.77	0.49
1:A:72:ARG:CZ	1:A:84:PHE:HB2	2.42	0.49
7:K:390:PHE:HA	7:K:393:TRP:CZ3	2.48	0.49
2:B:74:GLU:HG3	4:D:124:ARG:HH12	1.76	0.49
6:J:31:DT:H2"	6:J:32:DG:C8	2.47	0.49
7:K:519:ILE:HD12	7:K:519:ILE:H	1.77	0.49
1:A:69:ARG:HH22	6:J:17:DA:P	2.35	0.49
4:H:83:ALA:HA	4:H:86:ILE:HG12	1.94	0.49
7:K:225:LEU:HD11	7:K:429:LEU:HD23	1.95	0.49
2:B:56:GLY:O	2:B:60:ILE:HD12	2.12	0.49
2:B:96:THR:CG2	3:G:109:VAL:CA	2.86	0.49
5:I:-10:DC:H2"	5:I:-9:DA:C8	2.48	0.49
5:I:-7:DG:H2"	5:I:-6:DT:C6	2.48	0.49
5:I:3:DT:H2"	5:I:4:DC:C5	2.47	0.49
6:J:19:DC:C2	6:J:20:DG:N7	2.81	0.49
7:K:332:ILE:HD11	7:K:359:LEU:HD23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-29:DC:H2'	5:I:-28:DT:H72	1.95	0.49
6:J:-21:DG:H2'	6:J:-20:DC:H6	1.77	0.49
7:K:366:GLN:H	7:K:371:GLU:CD	2.14	0.49
7:K:424:LEU:O	7:K:428:ILE:N	2.39	0.49
1:E:83:ARG:HD3	1:E:84:PHE:H	1.78	0.49
4:H:126:VAL:HG23	4:H:127:LEU:HD22	1.93	0.49
6:J:-44:DG:H2"	6:J:-43:DA:H8	1.76	0.49
6:J:-32:DT:H2"	6:J:-31:DA:C8	2.45	0.49
5:I:-55:DG:H2"	5:I:-54:DA:C8	2.48	0.48
5:I:27:DG:H2"	5:I:28:DG:C8	2.47	0.48
2:F:24:ASP:O	2:F:26:ILE:N	2.43	0.48
4:D:62:TYR:O	4:D:66:ILE:HD12	2.12	0.48
7:K:622:TRP:CZ3	7:K:661:ARG:HD2	2.49	0.48
1:A:65:LEU:HA	1:A:68:GLN:HB3	1.95	0.48
5:I:34:DT:H2"	5:I:35:DC:C6	2.49	0.48
7:K:380:LEU:HD13	7:K:383:ILE:HD12	1.94	0.48
1:E:62:ILE:HD11	2:F:37:LEU:HD11	1.94	0.48
6:J:-43:DA:H2"	6:J:-42:DG:C8	2.48	0.48
7:K:535:ARG:NH1	7:K:718:LEU:HD13	2.29	0.48
2:B:31:LYS:HE2	2:B:35:ARG:HH21	1.79	0.48
7:K:233:LYS:O	7:K:236:GLN:HG2	2.14	0.48
2:B:27:GLN:HA	2:B:55:ARG:CZ	2.44	0.48
7:K:228:GLN:CB	7:K:231:LEU:HB2	2.44	0.48
7:K:256:ILE:HB	7:K:332:ILE:HG22	1.95	0.48
3:C:51:ARG:HD3	6:J:39:DA:H5'	1.95	0.47
2:F:32:PRO:HB3	2:F:35:ARG:NH2	2.28	0.47
7:K:646:TYR:HE1	7:K:722:LEU:HD11	1.78	0.47
3:C:87:ILE:HB	4:D:79:ILE:HD12	1.96	0.47
2:F:52:GLU:HA	2:F:55:ARG:HD3	1.96	0.47
3:C:36:VAL:HG13	3:C:57:PRO:HB2	1.97	0.47
3:G:76:GLY:HA3	4:H:74:HIS:ND1	2.28	0.47
7:K:331:VAL:HG12	7:K:358:LEU:HD12	1.96	0.47
3:C:59:TYR:CE2	4:D:139:GLY:HA3	2.49	0.47
3:C:106:LEU:HB3	3:C:109:VAL:HB	1.96	0.47
7:K:330:VAL:HB	7:K:356:ASN:O	2.14	0.47
1:E:99:TYR:OH	1:E:133:GLU:OE2	2.32	0.47
4:H:73:VAL:HG22	4:H:74:HIS:HD2	1.79	0.47
7:K:341:HIS:CD2	7:K:342:LYS:HZ2	2.33	0.47
7:K:494:ARG:CZ	7:K:622:TRP:HE1	2.28	0.47
7:K:550:THR:HA	7:K:553:LEU:HD12	1.97	0.47
7:K:389:GLU:HG2	7:K:390:PHE:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:ILE:HG22	1:E:131:ARG:HH21	1.80	0.47
3:G:60:MET:HA	3:G:63:VAL:HG12	1.96	0.47
3:G:92:LEU:O	3:G:96:ILE:HD12	2.15	0.47
5:I:-6:DT:H2"	5:I:-5:DA:N7	2.29	0.47
6:J:55:DC:H2"	6:J:56:DG:N7	2.30	0.47
7:K:227:ASP:CB	7:K:430:ARG:HA	2.45	0.47
7:K:255:VAL:HG12	7:K:308:ILE:HA	1.97	0.47
5:I:-19:DG:H2"	5:I:-18:DC:C6	2.50	0.47
5:I:-16:DT:H2"	5:I:-15:DA:N7	2.30	0.47
6:J:46:DG:H2"	6:J:47:DA:C8	2.50	0.47
7:K:448:MET:HE1	7:K:450:ALA:HB3	1.96	0.47
2:B:75:HIS:ND1	4:D:121:THR:HG21	2.30	0.47
7:K:292:ARG:HE	7:K:293:ARG:NH1	2.13	0.47
7:K:347:ARG:HA	7:K:350:LYS:HZ3	1.80	0.47
2:B:96:THR:CG2	3:G:109:VAL:HA	2.25	0.47
3:C:33:GLN:HB3	4:D:68:LYS:NZ	2.29	0.47
7:K:414:ALA:O	7:K:418:SER:N	2.47	0.47
1:E:99:TYR:CB	2:F:95:ARG:HH12	2.26	0.46
7:K:527:ARG:HB2	7:K:531:ARG:HH12	1.80	0.46
1:A:66:PRO:HD3	6:J:17:DA:H3'	1.97	0.46
4:H:92:ASN:O	4:H:95:PHE:HB3	2.16	0.46
5:I:34:DT:H2"	5:I:35:DC:C5	2.50	0.46
2:B:56:GLY:O	2:B:59:LYS:HG2	2.16	0.46
3:G:43:LEU:HD13	3:G:52:LEU:HD22	1.97	0.46
5:I:-59:DT:H3	6:J:59:DA:H61	1.64	0.46
5:I:39:DA:H8	5:I:39:DA:P	2.38	0.46
6:J:37:DC:H2"	6:J:38:DG:H8	1.81	0.46
7:K:530:GLU:O	7:K:533:LEU:HG	2.16	0.46
4:D:123:VAL:HG13	4:D:127:LEU:HD13	1.96	0.46
5:I:-54:DA:H2"	5:I:-53:DG:C8	2.51	0.46
5:I:-5:DA:H2"	5:I:-4:DC:C5	2.50	0.46
6:J:-46:DT:H2"	6:J:-45:DG:O4'	2.16	0.46
2:B:72:TYR:HE1	4:D:125:LEU:HD22	1.81	0.46
3:C:56:ALA:HB3	3:C:57:PRO:HD3	1.96	0.46
3:C:88:ILE:H	3:C:91:HIS:HB2	1.80	0.46
4:H:115:THR:O	4:H:119:ILE:HG12	2.15	0.46
7:K:344:LYS:HB2	7:K:347:ARG:HG2	1.97	0.46
5:I:-20:DC:H2'	5:I:-19:DG:H8	1.81	0.46
6:J:8:DG:C2'	6:J:9:DT:H71	2.46	0.46
7:K:208:LYS:HA	7:K:211:LYS:HG2	1.97	0.46
3:G:36:VAL:O	3:G:40:THR:HG23	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:82:ASN:HB2	3:G:91:HIS:HE2	1.80	0.46
5:I:-35:DA:H2"	5:I:-34:DG:C8	2.50	0.46
5:I:34:DT:O2	6:J:-33:DG:N2	2.49	0.46
6:J:21:DG:H2'	6:J:22:DT:H71	1.97	0.46
7:K:527:ARG:CD	7:K:531:ARG:HH22	2.29	0.46
7:K:625:GLN:HA	7:K:628:LEU:CD1	2.46	0.46
1:A:84:PHE:HD1	2:B:81:VAL:HB	1.81	0.46
2:F:33:ALA:O	2:F:37:LEU:HG	2.15	0.46
4:H:62:TYR:O	4:H:66:ILE:HG12	2.15	0.46
4:H:118:GLU:HA	4:H:121:THR:HG22	1.97	0.46
7:K:644:HIS:ND1	7:K:722:LEU:HD22	2.31	0.46
7:K:340:ASN:OD1	7:K:343:CYS:N	2.49	0.46
7:K:499:HIS:CE1	7:K:523:CYS:HG	2.29	0.46
7:K:526:PHE:HZ	7:K:559:TYR:CG	2.34	0.46
1:A:130:ILE:HG22	1:E:131:ARG:CZ	2.45	0.46
3:G:67:LEU:HD21	4:H:94:ILE:HG21	1.98	0.46
6:J:39:DA:H2"	6:J:40:DC:H5'	1.98	0.46
7:K:322:LEU:HD12	7:K:352:LEU:HD23	1.97	0.46
7:K:554:ASP:OD1	7:K:555:ILE:N	2.49	0.46
7:K:629:GLN:HB3	7:K:633:ARG:NH1	2.31	0.46
6:J:40:DC:C2	6:J:41:DC:C5	3.05	0.45
3:G:38:ARG:HG3	3:G:42:PHE:CE2	2.42	0.45
4:H:79:ILE:HD12	4:H:84:MET:HB2	1.99	0.45
5:I:6:DC:H1'	5:I:7:DC:C5	2.51	0.45
6:J:-11:DC:C2	6:J:-10:DG:N7	2.84	0.45
7:K:228:GLN:NE2	7:K:433:LYS:HE3	2.31	0.45
7:K:421:HIS:HE1	7:K:672:VAL:O	1.98	0.45
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.50	0.45
3:C:86:ARG:CZ	4:D:78:GLY:HA3	2.47	0.45
3:G:68:ALA:HA	3:G:71:VAL:HG22	1.98	0.45
7:K:596:PHE:HE2	7:K:598:LEU:HD22	1.82	0.45
6:J:-48:DC:H2"	6:J:-47:DC:C5	2.52	0.45
6:J:58:DC:H1'	6:J:59:DA:C8	2.51	0.45
3:G:41:ARG:NE	6:J:-44:DG:OP2	2.45	0.45
3:G:53:GLY:N	4:H:114:ILE:O	2.49	0.45
5:I:-17:DT:H2"	5:I:-16:DT:C6	2.52	0.45
7:K:222:ASN:ND2	7:K:357:LYS:HE3	2.31	0.45
7:K:547:SER:HB2	7:K:553:LEU:HD21	1.98	0.45
1:A:130:ILE:HG22	1:E:131:ARG:NH1	2.31	0.45
7:K:448:MET:HG3	7:K:647:ARG:O	2.17	0.45
7:K:609:LEU:HD23	7:K:609:LEU:HA	1.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:LYS:HD2	4:D:128:PRO:HB3	1.98	0.45
1:E:64:LYS:HG2	5:I:18:DC:OP1	2.17	0.45
7:K:619:ASP:OD1	7:K:619:ASP:N	2.48	0.45
5:I:38:DT:O2	6:J:-37:DG:N2	2.50	0.45
7:K:330:VAL:H	7:K:356:ASN:HB3	1.82	0.45
7:K:456:GLN:NE2	7:K:523:CYS:HB3	2.32	0.45
7:K:601:ARG:NH1	7:K:621:ASP:OD2	2.50	0.45
7:K:722:LEU:O	7:K:724:ARG:NE	2.46	0.45
4:D:65:TYR:OH	6:J:48:DG:OP1	2.22	0.45
5:I:-56:DC:H2"	5:I:-55:DG:C8	2.52	0.45
7:K:391:GLU:HG2	7:K:394:PHE:HE2	1.81	0.45
2:F:45:ARG:NH2	5:I:7:DC:O4'	2.50	0.44
7:K:258:PRO:HG2	7:K:261:THR:HG22	1.98	0.44
7:K:646:TYR:CE1	7:K:722:LEU:HD11	2.51	0.44
5:I:-59:DT:H2"	5:I:-58:DG:N7	2.32	0.44
6:J:20:DG:C4	6:J:21:DG:C8	3.06	0.44
7:K:410:GLU:HA	7:K:413:ARG:HH11	1.82	0.44
7:K:654:ILE:HG13	7:K:657:ARG:HH21	1.83	0.44
1:A:124:ILE:HD12	1:A:124:ILE:H	1.82	0.44
5:I:-40:DG:H2'	5:I:-39:DT:H71	1.99	0.44
5:I:28:DG:H2"	5:I:29:DA:C8	2.52	0.44
7:K:208:LYS:O	7:K:211:LYS:HG2	2.17	0.44
3:C:42:PHE:HA	3:C:45:LYS:HG2	1.98	0.44
4:H:68:LYS:HA	4:H:71:LYS:HG2	2.00	0.44
5:I:-50:DC:H2"	5:I:-49:DG:H8	1.82	0.44
6:J:-16:DT:H2"	6:J:-15:DA:O4'	2.17	0.44
7:K:650:THR:O	7:K:653:SER:OG	2.24	0.44
2:F:30:THR:O	2:F:34:ILE:HD12	2.18	0.44
5:I:-46:DC:H2"	5:I:-45:DA:N7	2.32	0.44
6:J:-36:DG:H2"	6:J:-35:DG:N7	2.32	0.44
6:J:-22:DG:C4	6:J:-21:DG:C8	3.05	0.44
2:B:30:THR:HG23	2:B:33:ALA:H	1.82	0.44
4:D:90:PHE:O	4:D:94:ILE:HG12	2.18	0.44
1:E:108:ASN:HB2	2:F:43:VAL:HG22	1.99	0.44
6:J:-13:DA:H2"	6:J:-12:DA:H8	1.82	0.44
7:K:457:LYS:HA	7:K:460:GLN:HG3	1.99	0.44
7:K:744:LYS:HA	7:K:749:GLU:OE1	2.18	0.44
1:A:132:GLY:O	1:A:134:ARG:NH1	2.51	0.44
1:E:128:ARG:NE	1:E:133:GLU:OE2	2.51	0.44
3:G:39:ILE:HA	3:G:42:PHE:HD2	1.83	0.44
5:I:-52:DG:N2	6:J:53:DC:O2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:365:LEU:HD12	7:K:372:LEU:HD23	2.00	0.44
7:K:553:LEU:C	7:K:569:ARG:HH12	2.21	0.44
1:A:100:LEU:HD23	2:B:37:LEU:HD13	1.99	0.44
3:C:84:LYS:HZ2	3:C:86:ARG:N	2.15	0.44
1:A:120:MET:HG2	1:A:122:LYS:H	1.83	0.44
3:C:38:ARG:HH21	6:J:48:DG:H5"	1.83	0.44
3:C:72:LEU:HD12	4:D:69:VAL:HG12	2.00	0.44
1:E:133:GLU:OE1	1:E:133:GLU:N	2.39	0.44
4:H:122:ALA:O	4:H:126:VAL:HG22	2.18	0.44
7:K:513:TYR:CG	7:K:514:PRO:HD2	2.53	0.44
7:K:623:ASN:OD1	7:K:625:GLN:HG2	2.18	0.44
1:A:128:ARG:HD2	1:A:133:GLU:HG2	1.99	0.43
3:C:51:ARG:HB3	4:D:113:THR:HG22	1.98	0.43
1:E:85:GLN:NE2	2:F:82:THR:HA	2.32	0.43
3:C:34:PHE:HB3	3:C:35:PRO:HD2	1.99	0.43
4:D:76:ASP:OD1	4:D:76:ASP:N	2.51	0.43
1:E:102:GLY:O	1:E:105:GLU:HG3	2.18	0.43
5:I:6:DC:H1'	5:I:7:DC:C4	2.53	0.43
6:J:-45:DG:H2"	6:J:-44:DG:H8	1.82	0.43
7:K:424:LEU:HD13	7:K:427:PHE:HD2	1.83	0.43
7:K:559:TYR:CE2	7:K:563:LYS:HD2	2.53	0.43
3:C:36:VAL:O	3:C:40:THR:OG1	2.27	0.43
6:J:-42:DG:C2	6:J:-41:DA:C5	3.05	0.43
7:K:315:MET:SD	7:K:345:LEU:HD13	2.59	0.43
7:K:542:LYS:N	7:K:613:ASP:OD1	2.48	0.43
3:C:82:ASN:HD21	3:C:91:HIS:CE1	2.36	0.43
3:G:36:VAL:HA	3:G:39:ILE:HG12	2.01	0.43
7:K:535:ARG:HH12	7:K:722:LEU:HD12	1.83	0.43
2:B:33:ALA:HA	2:B:36:ARG:CZ	2.48	0.43
7:K:456:GLN:HE21	7:K:500:PRO:HD3	1.76	0.43
6:J:40:DC:H5'	6:J:40:DC:H6	1.84	0.43
7:K:311:TYR:OH	7:K:334:GLU:HB3	2.18	0.43
5:I:21:DC:H5"	7:K:337:ARG:HH22	1.82	0.43
7:K:255:VAL:CG1	7:K:308:ILE:HA	2.49	0.43
7:K:447:ILE:HD11	7:K:751:VAL:HG23	2.01	0.43
7:K:745:GLY:HA3	7:K:748:TRP:CE2	2.54	0.43
3:G:66:TYR:O	3:G:69:ALA:HB3	2.19	0.43
7:K:356:ASN:O	7:K:357:LYS:HG3	2.18	0.43
7:K:552:LEU:HD12	7:K:555:ILE:HB	2.00	0.43
7:K:231:LEU:HD12	7:K:231:LEU:HA	1.64	0.43
7:K:460:GLN:O	7:K:464:VAL:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:571:ASP:OD1	7:K:573:SER:OG	2.31	0.43
7:K:323:ARG:HH21	7:K:353:LYS:HG3	1.84	0.42
1:A:103:LEU:O	1:A:107:THR:HG23	2.19	0.42
4:D:133:LYS:HA	4:D:136:VAL:HG12	2.01	0.42
1:E:79:LYS:HD3	1:E:80:THR:O	2.19	0.42
3:G:51:ARG:HH11	5:I:39:DA:C3'	2.25	0.42
7:K:463:LEU:HD12	7:K:468:LEU:HD22	2.01	0.42
2:B:96:THR:O	3:G:109:VAL:HA	2.19	0.42
3:G:50:GLN:C	3:G:51:ARG:HG2	2.35	0.42
5:I:-23:DC:H2"	5:I:-22:DA:C8	2.55	0.42
5:I:26:DG:H2"	5:I:27:DG:C8	2.55	0.42
5:I:-20:DC:H2'	5:I:-19:DG:C8	2.54	0.42
6:J:-12:DA:C4	6:J:-11:DC:C5	3.07	0.42
7:K:240:PHE:CD2	7:K:358:LEU:HD11	2.54	0.42
1:E:70:LEU:HD22	2:F:25:ASN:OD1	2.19	0.42
3:G:38:ARG:O	3:G:42:PHE:CD2	2.72	0.42
3:G:67:LEU:HA	3:G:70:GLU:OE1	2.20	0.42
3:G:39:ILE:HD13	3:G:61:ALA:HB2	2.02	0.42
4:H:105:LEU:HD21	4:H:122:ALA:HB2	2.00	0.42
6:J:-44:DG:H2"	6:J:-43:DA:C8	2.54	0.42
6:J:26:DA:H2"	6:J:27:DG:C8	2.54	0.42
7:K:615:CYS:O	7:K:645:VAL:HA	2.20	0.42
2:B:26:ILE:HG12	2:B:55:ARG:HD3	2.02	0.42
3:G:80:ARG:HH12	4:H:74:HIS:CE1	2.38	0.42
5:I:-12:DC:H1'	5:I:-11:DG:H5'	2.01	0.42
6:J:-21:DG:OP1	7:K:549:TRP:HB3	2.20	0.42
6:J:18:DG:C4	6:J:19:DC:C5	3.08	0.42
7:K:227:ASP:HA	7:K:430:ARG:CD	2.43	0.42
7:K:289:ASP:HA	7:K:292:ARG:NH1	2.35	0.42
7:K:366:GLN:HA	7:K:625:GLN:NE2	2.34	0.42
7:K:511:TYR:HD2	7:K:511:TYR:H	1.68	0.42
7:K:526:PHE:O	7:K:529:LEU:HB3	2.20	0.42
2:B:56:GLY:HA2	2:B:59:LYS:NZ	2.35	0.42
4:D:117:ARG:HA	4:D:120:GLN:NE2	2.34	0.42
5:I:38:DT:H2"	5:I:39:DA:N7	2.35	0.42
7:K:284:ASP:N	7:K:287:GLN:OE1	2.50	0.42
7:K:653:SER:O	7:K:656:THR:OG1	2.30	0.42
5:I:13:DT:C2'	5:I:14:DT:H71	2.49	0.41
6:J:34:DC:H2"	6:J:35:DT:OP2	2.19	0.41
7:K:518:GLU:O	7:K:522:GLN:HG2	2.20	0.41
4:D:105:LEU:HA	4:D:108:TYR:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:PHE:CE2	2:F:81:VAL:HG21	2.55	0.41
2:F:59:LYS:O	2:F:63:GLU:OE1	2.38	0.41
4:H:105:LEU:HD11	4:H:118:GLU:HB3	2.02	0.41
6:J:8:DG:H2'	6:J:9:DT:H71	2.01	0.41
7:K:499:HIS:CD2	7:K:501:ASP:HB2	2.55	0.41
1:E:116:ARG:HH12	1:E:122:LYS:HZ1	1.64	0.41
1:A:110:CYS:SG	1:A:126:LEU:HD23	2.61	0.41
4:D:140:THR:HA	4:D:143:VAL:HG12	2.03	0.41
3:G:51:ARG:NH1	5:I:40:DG:OP2	2.53	0.41
6:J:57:DG:H2"	6:J:58:DC:OP2	2.20	0.41
7:K:254:LEU:HB3	7:K:330:VAL:HG22	2.02	0.41
7:K:454:ASP:O	7:K:457:LYS:HG2	2.20	0.41
2:B:98:TYR:HE2	4:H:90:PHE:HD1	1.69	0.41
3:G:50:GLN:O	3:G:51:ARG:HD2	2.20	0.41
3:G:60:MET:O	3:G:63:VAL:HG12	2.21	0.41
6:J:11:DC:H2"	6:J:12:DG:C8	2.56	0.41
7:K:579:ARG:O	7:K:583:ILE:HG13	2.20	0.41
7:K:514:PRO:HB2	7:K:518:GLU:OE1	2.21	0.41
7:K:749:GLU:OE1	7:K:749:GLU:HA	2.19	0.41
1:A:72:ARG:NH2	5:I:-23:DC:OP2	2.54	0.41
5:I:14:DT:H2'	5:I:15:DT:H71	2.02	0.41
5:I:24:DA:H5"	7:K:622:TRP:CZ3	2.55	0.41
6:J:29:DG:C4	6:J:30:DC:C5	3.08	0.41
7:K:197:LEU:HA	7:K:273:THR:HG22	2.03	0.41
7:K:279:ILE:HD11	7:K:307:VAL:HG22	2.01	0.41
7:K:456:GLN:CD	7:K:500:PRO:CG	2.88	0.41
2:B:69:ALA:O	2:B:73:THR:HG23	2.21	0.41
3:C:38:ARG:NH2	6:J:48:DG:H5"	2.36	0.41
3:C:39:ILE:HG13	3:C:57:PRO:HB3	2.02	0.41
3:G:53:GLY:CA	4:H:115:THR:HA	2.51	0.41
4:H:87:MET:O	4:H:91:ILE:HG12	2.21	0.41
6:J:15:DT:H6	6:J:15:DT:H2'	1.69	0.41
6:J:55:DC:OP2	6:J:55:DC:H2'	2.20	0.41
7:K:333:ASP:OD1	7:K:334:GLU:N	2.50	0.41
7:K:457:LYS:O	7:K:461:GLU:HG3	2.20	0.41
1:E:119:ILE:HD11	2:F:46:ILE:HG22	2.03	0.41
1:E:131:ARG:NE	1:E:131:ARG:HA	2.32	0.41
5:I:-59:DT:H3	6:J:59:DA:N6	2.18	0.41
6:J:41:DC:C2	6:J:42:DA:N7	2.90	0.40
4:D:115:THR:N	4:D:118:GLU:OE2	2.53	0.40
6:J:42:DA:H2"	6:J:43:DA:C8	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:388:ASP:N	7:K:388:ASP:OD1	2.54	0.40
7:K:527:ARG:HD2	7:K:531:ARG:HH22	1.86	0.40
7:K:654:ILE:H	7:K:654:ILE:HD12	1.87	0.40
4:D:130:GLU:HA	4:D:133:LYS:NZ	2.37	0.40
1:E:82:LEU:HD21	2:F:70:VAL:HG23	2.02	0.40
3:G:66:TYR:O	3:G:70:GLU:OE1	2.38	0.40
4:H:117:ARG:O	4:H:120:GLN:HB2	2.22	0.40
5:I:-57:DC:H2"	5:I:-56:DC:C5	2.56	0.40
5:I:47:DG:H2"	5:I:48:DG:N7	2.36	0.40
6:J:-6:DG:H2"	6:J:-5:DG:C8	2.56	0.40
3:G:93:LEU:HD12	3:G:111:ILE:HB	2.04	0.40
6:J:-21:DG:OP1	7:K:551:LYS:N	2.42	0.40
7:K:366:GLN:HG3	7:K:625:GLN:NE2	2.36	0.40
1:A:120:MET:O	1:A:123:ASP:HB2	2.22	0.40
2:B:75:HIS:HB2	4:D:121:THR:OG1	2.22	0.40
4:H:94:ILE:O	4:H:98:LEU:HD23	2.22	0.40
5:I:37:DC:H6	5:I:37:DC:H2'	1.68	0.40
6:J:39:DA:C4	6:J:40:DC:C5	3.09	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	72/139 (52%)	70 (97%)	2 (3%)	0	100	100
1	E	75/139 (54%)	73 (97%)	2 (3%)	0	100	100
2	B	77/106 (73%)	74 (96%)	3 (4%)	0	100	100
2	F	82/106 (77%)	80 (98%)	2 (2%)	0	100	100
3	C	86/153 (56%)	85 (99%)	1 (1%)	0	100	100
3	G	80/153 (52%)	78 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	88/153 (58%)	87 (99%)	1 (1%)	0	100	100
4	H	88/153 (58%)	87 (99%)	1 (1%)	0	100	100
7	K	494/767 (64%)	459 (93%)	35 (7%)	0	100	100
All	All	1142/1869 (61%)	1093 (96%)	49 (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	62/111 (56%)	62 (100%)	0	100	100
1	E	64/111 (58%)	64 (100%)	0	100	100
2	B	65/81 (80%)	65 (100%)	0	100	100
2	F	69/81 (85%)	69 (100%)	0	100	100
3	C	67/119 (56%)	67 (100%)	0	100	100
3	G	63/119 (53%)	62 (98%)	1 (2%)	62	79
4	D	79/126 (63%)	79 (100%)	0	100	100
4	H	79/126 (63%)	79 (100%)	0	100	100
7	K	454/679 (67%)	454 (100%)	0	100	100
All	All	1002/1553 (64%)	1001 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	90	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	64	ASN
3	C	33	GLN
4	D	88	ASN
4	D	120	GLN
4	H	120	GLN
7	K	228	GLN
7	K	282	HIS
7	K	366	GLN
7	K	377	ASN
7	K	421	HIS
7	K	456	GLN
7	K	465	ASN
7	K	675	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.

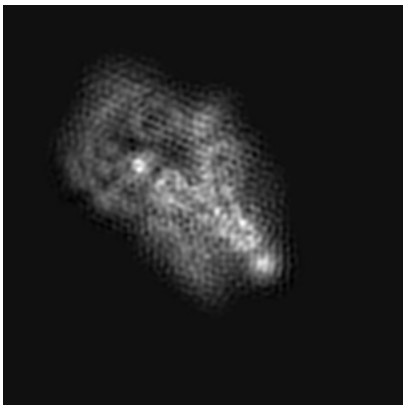
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36083. These allow visual inspection of the internal detail of the map and identification of artifacts.

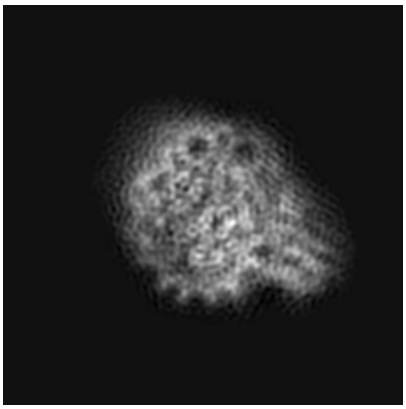
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

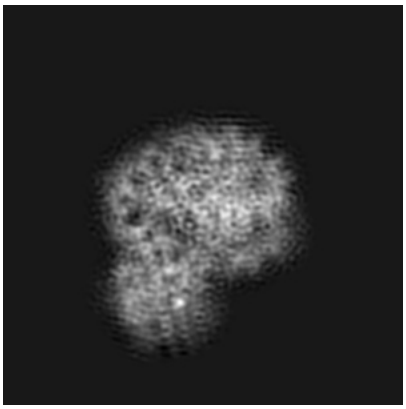
6.1.1 Primary map



X

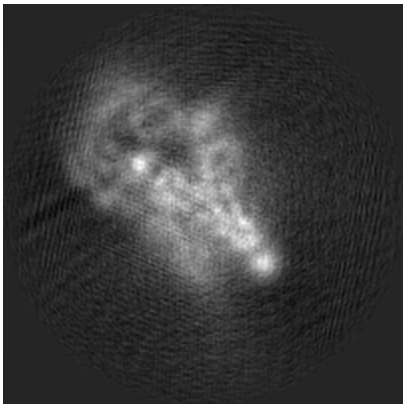


Y

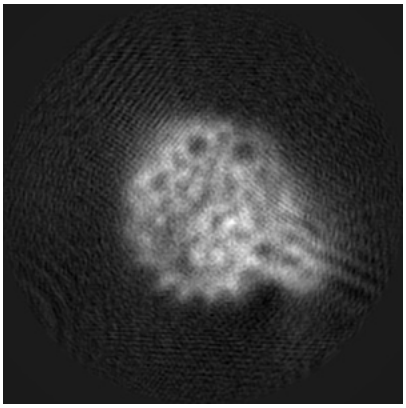


Z

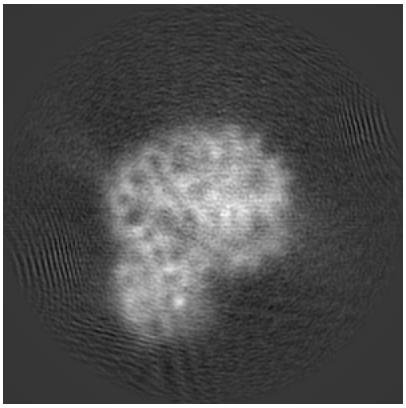
6.1.2 Raw map



X



Y

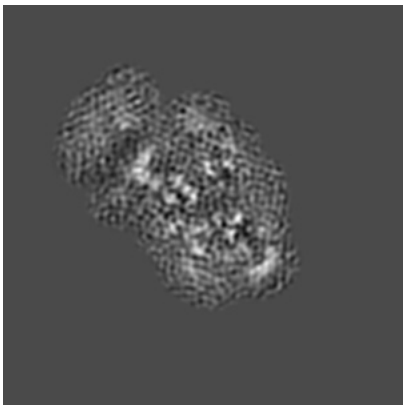


Z

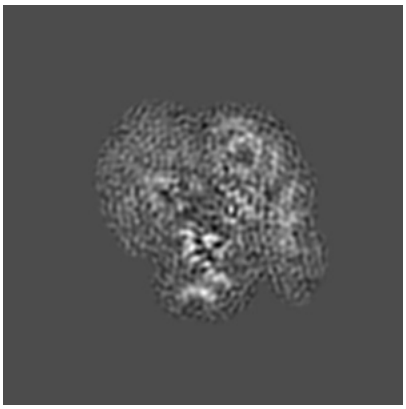
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

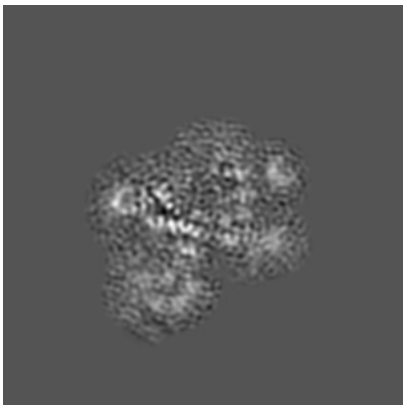
6.2.1 Primary map



X Index: 100

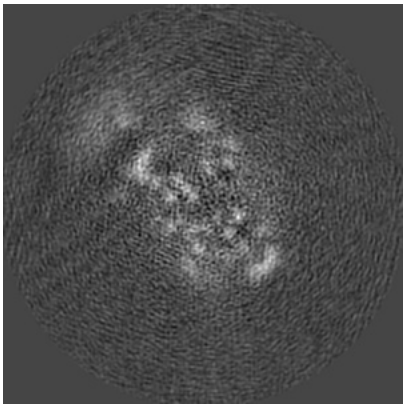


Y Index: 100

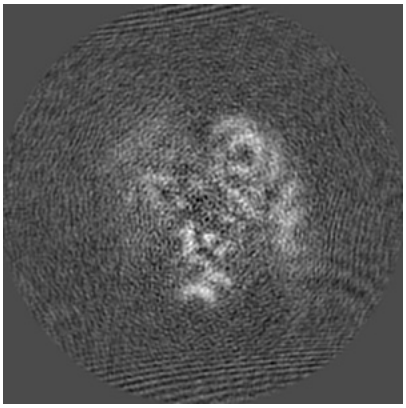


Z Index: 100

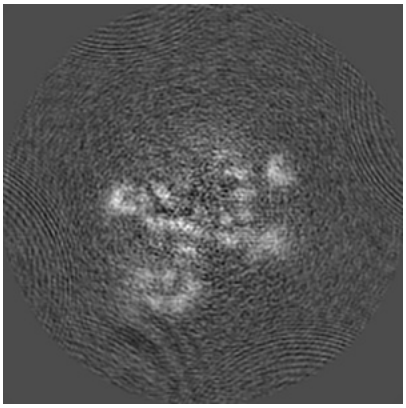
6.2.2 Raw map



X Index: 100



Y Index: 100

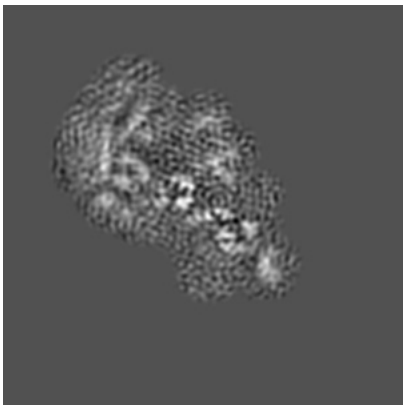


Z Index: 100

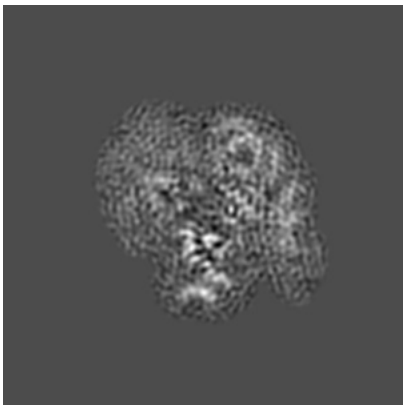
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

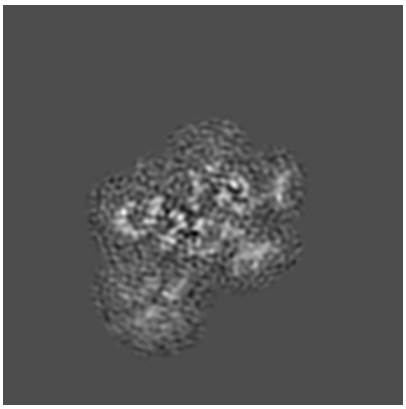
6.3.1 Primary map



X Index: 89

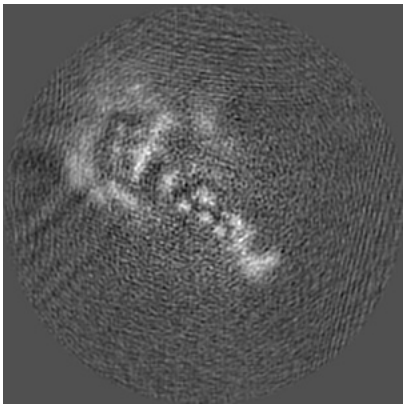


Y Index: 100

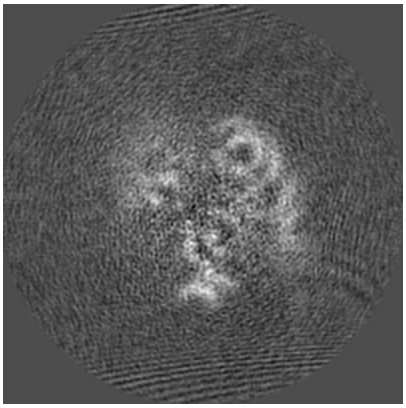


Z Index: 109

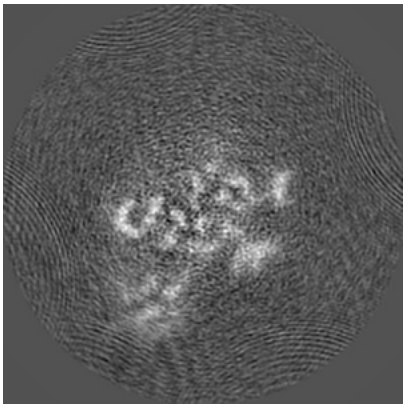
6.3.2 Raw map



X Index: 82



Y Index: 99

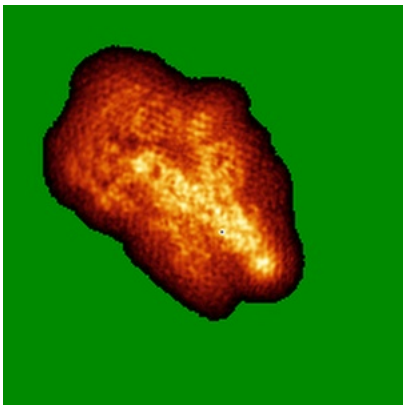


Z Index: 109

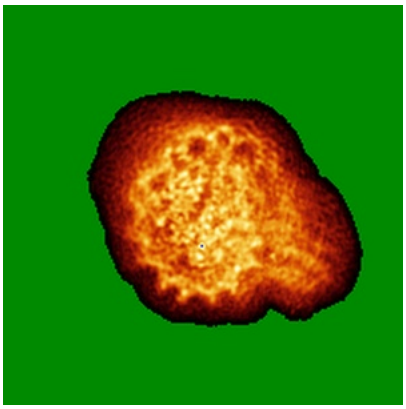
The images above show the largest variance slices of the map in three orthogonal directions.

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

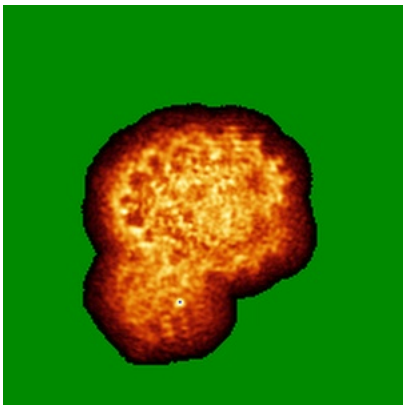
6.4.1 Primary map



X

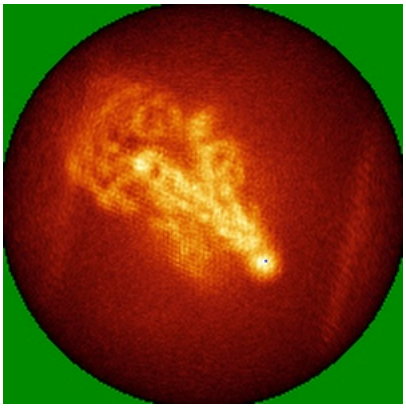


Y

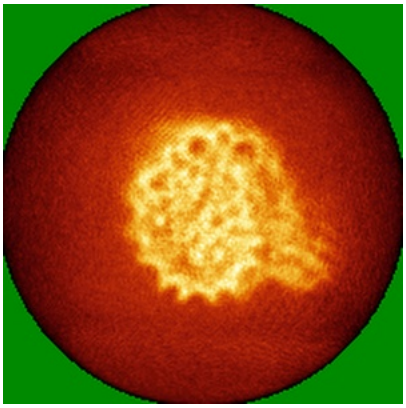


Z

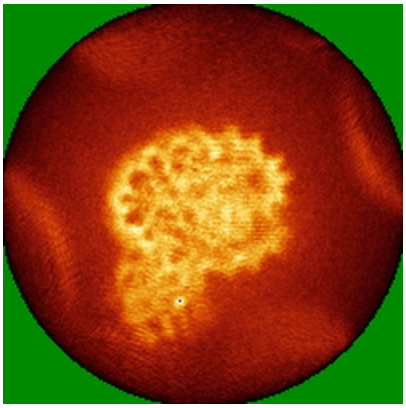
6.4.2 Raw map



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 0.0115. 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.

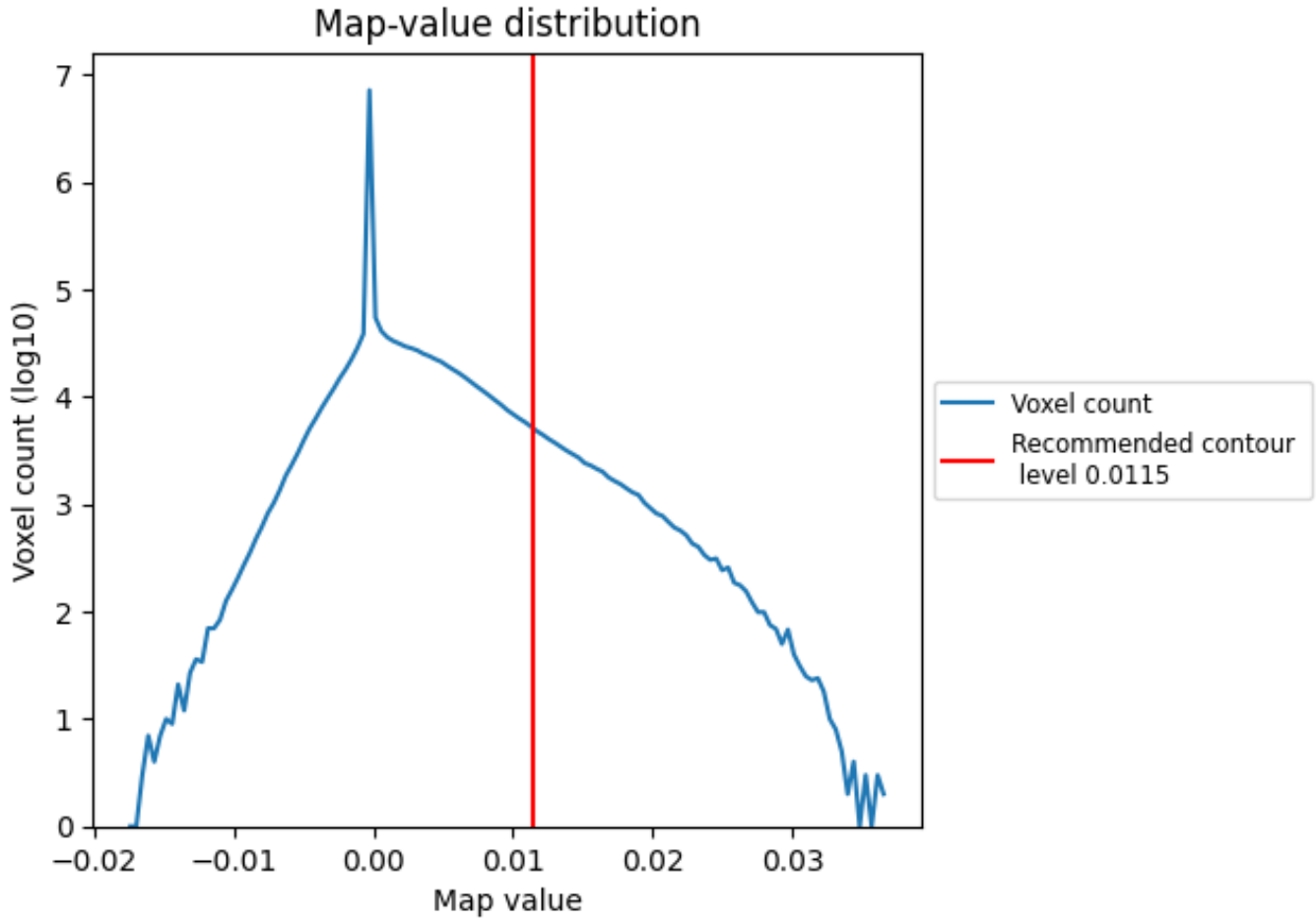
6.6 Mask visualisation (i)

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

7 Map analysis

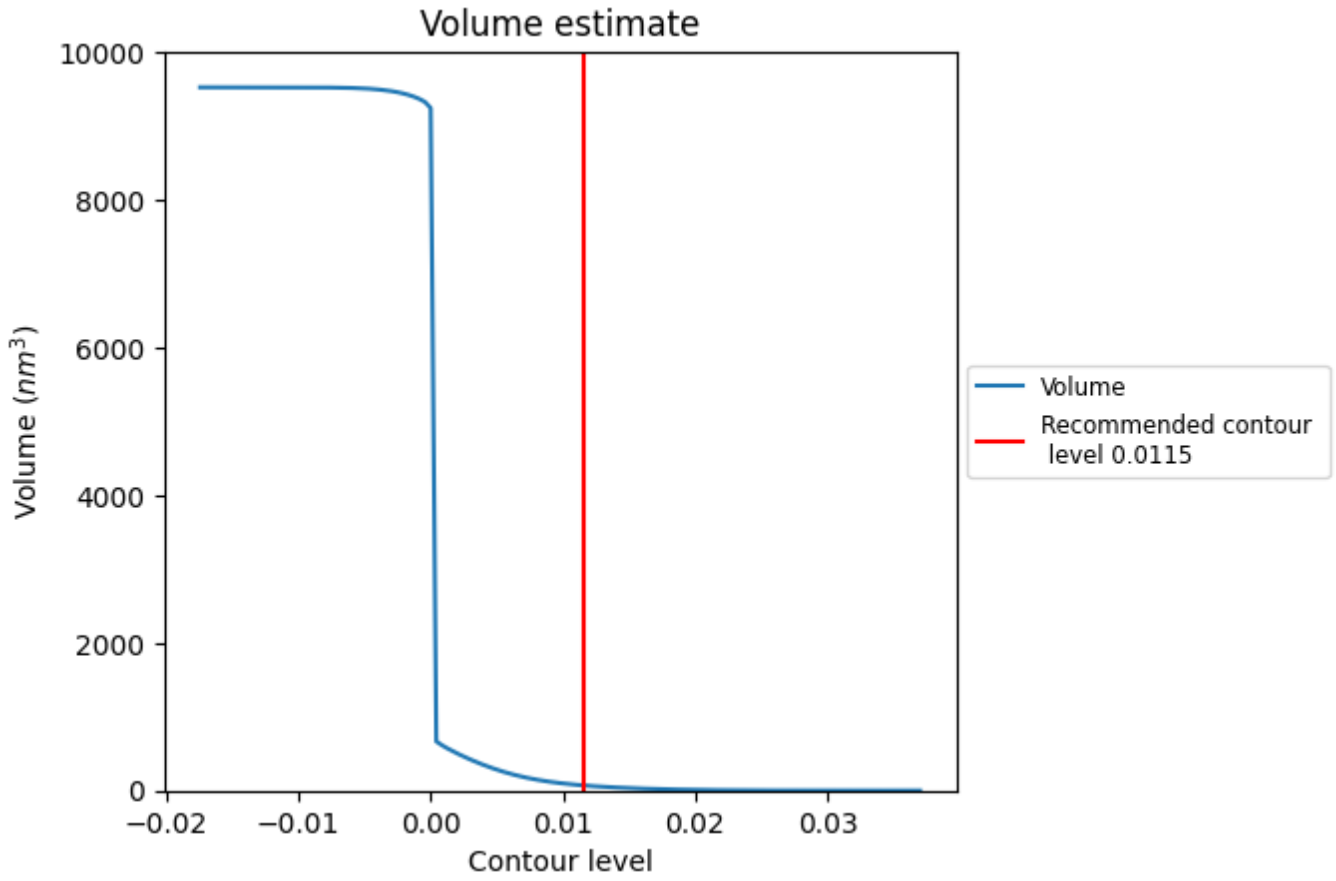
This section contains the results of statistical analysis of the map.

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.

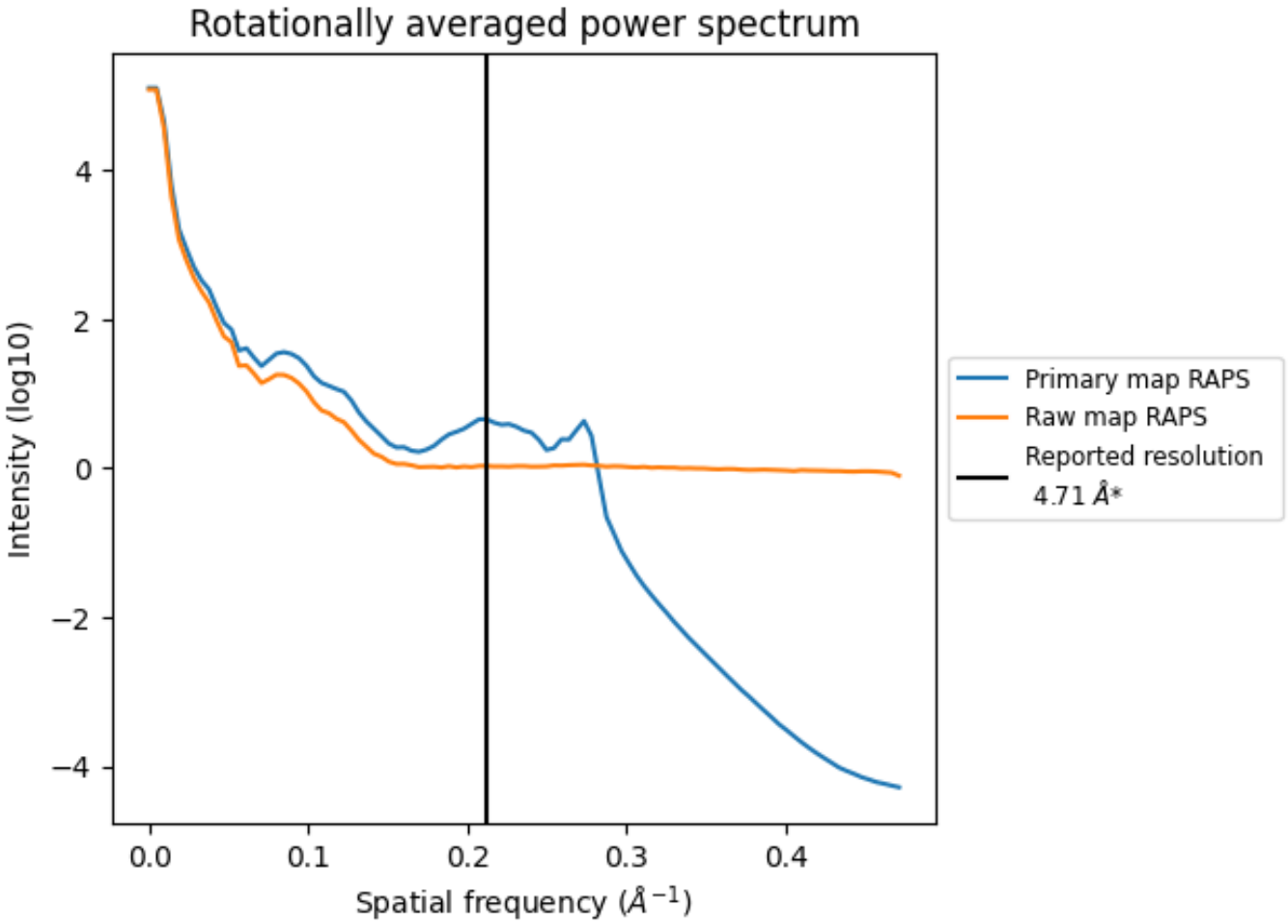
7.2 Volume estimate



The volume at the recommended contour level is 70 nm^3; this corresponds to an approximate mass of 64 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)

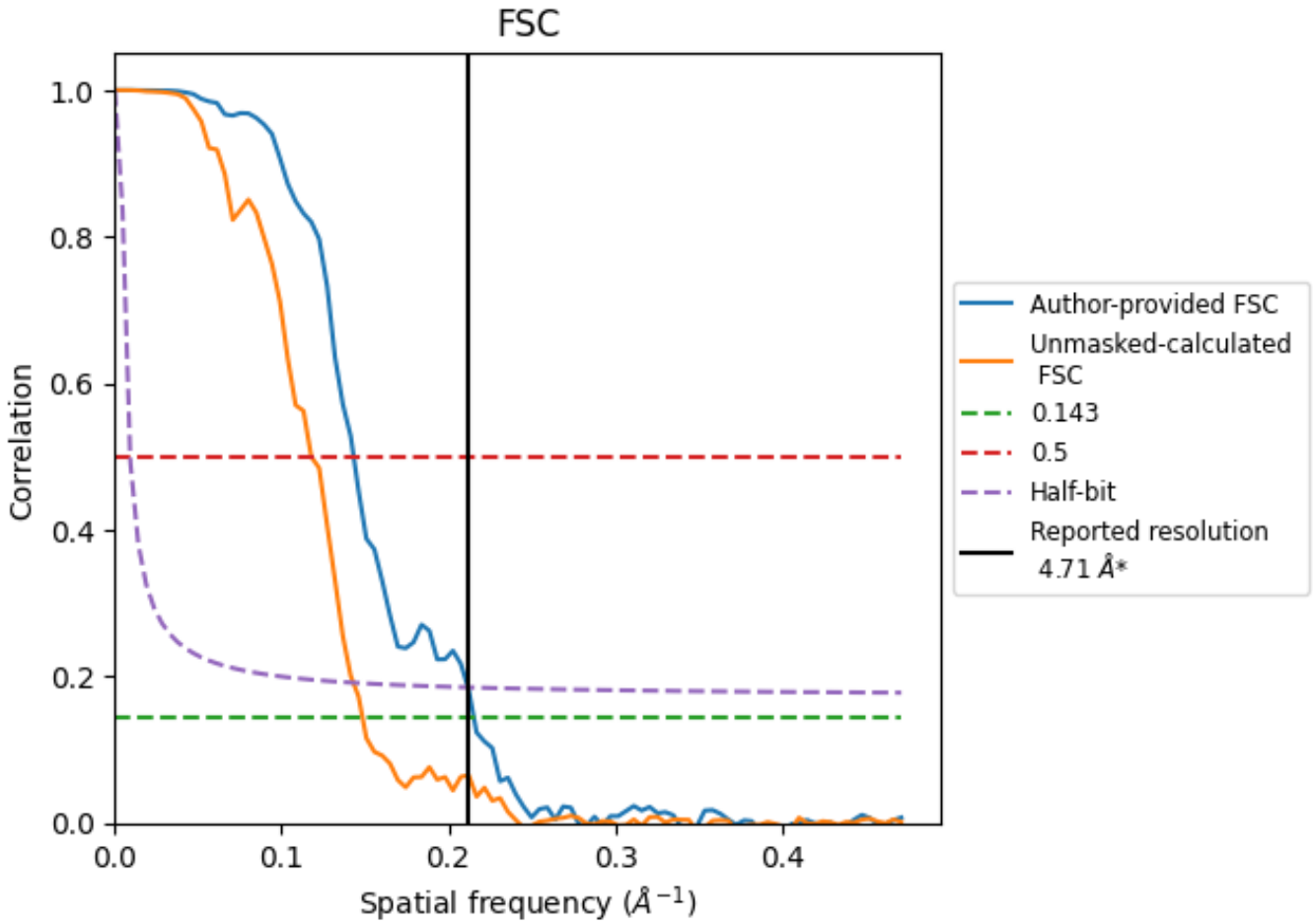


*Reported resolution corresponds to spatial frequency of 0.212 $Å^{-1}$

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 0.212 Å^{-1}

8.2 Resolution estimates (i)

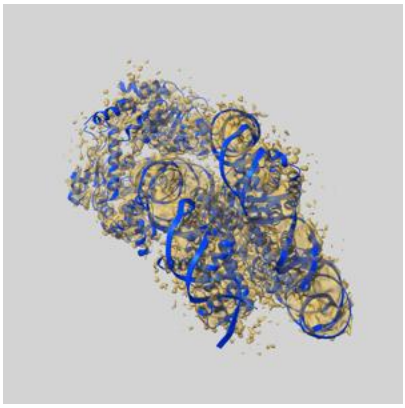
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.71	-	-
Author-provided FSC curve	4.64	6.98	4.72
Unmasked-calculated*	6.72	8.48	6.99

*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 6.72 differs from the reported value 4.71 by more than 10 %

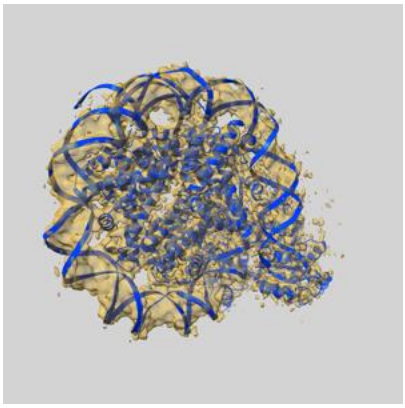
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36083 and PDB model 8J90. Per-residue inclusion information can be found in section 3 on page 7.

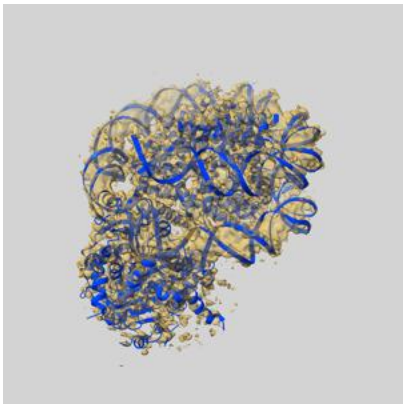
9.1 Map-model overlay



X



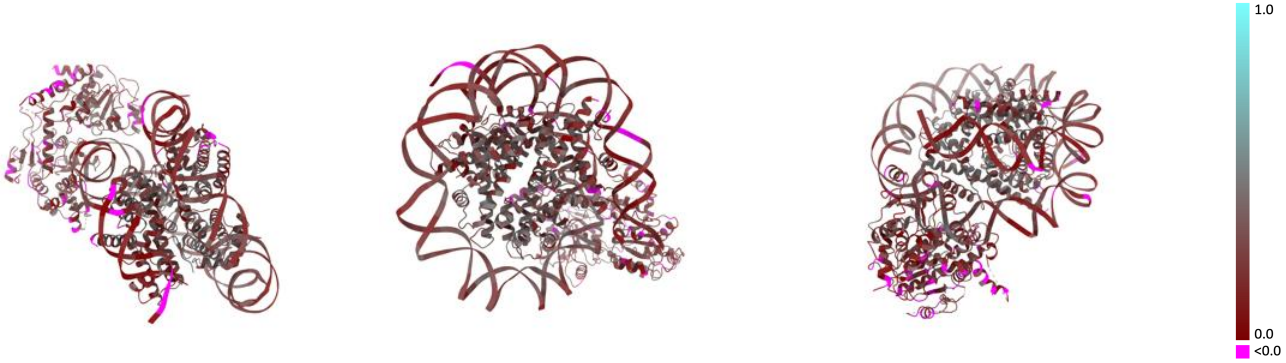
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115 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.

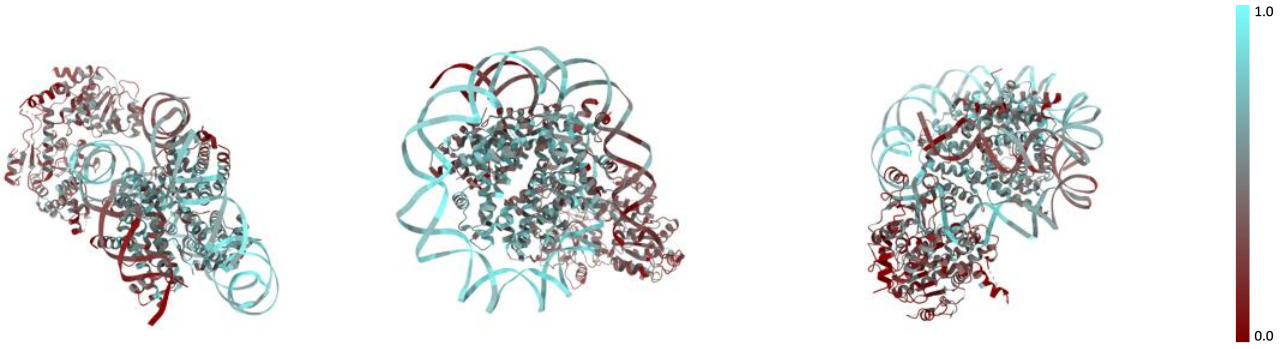
9.2 Q-score mapped to coordinate model



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.

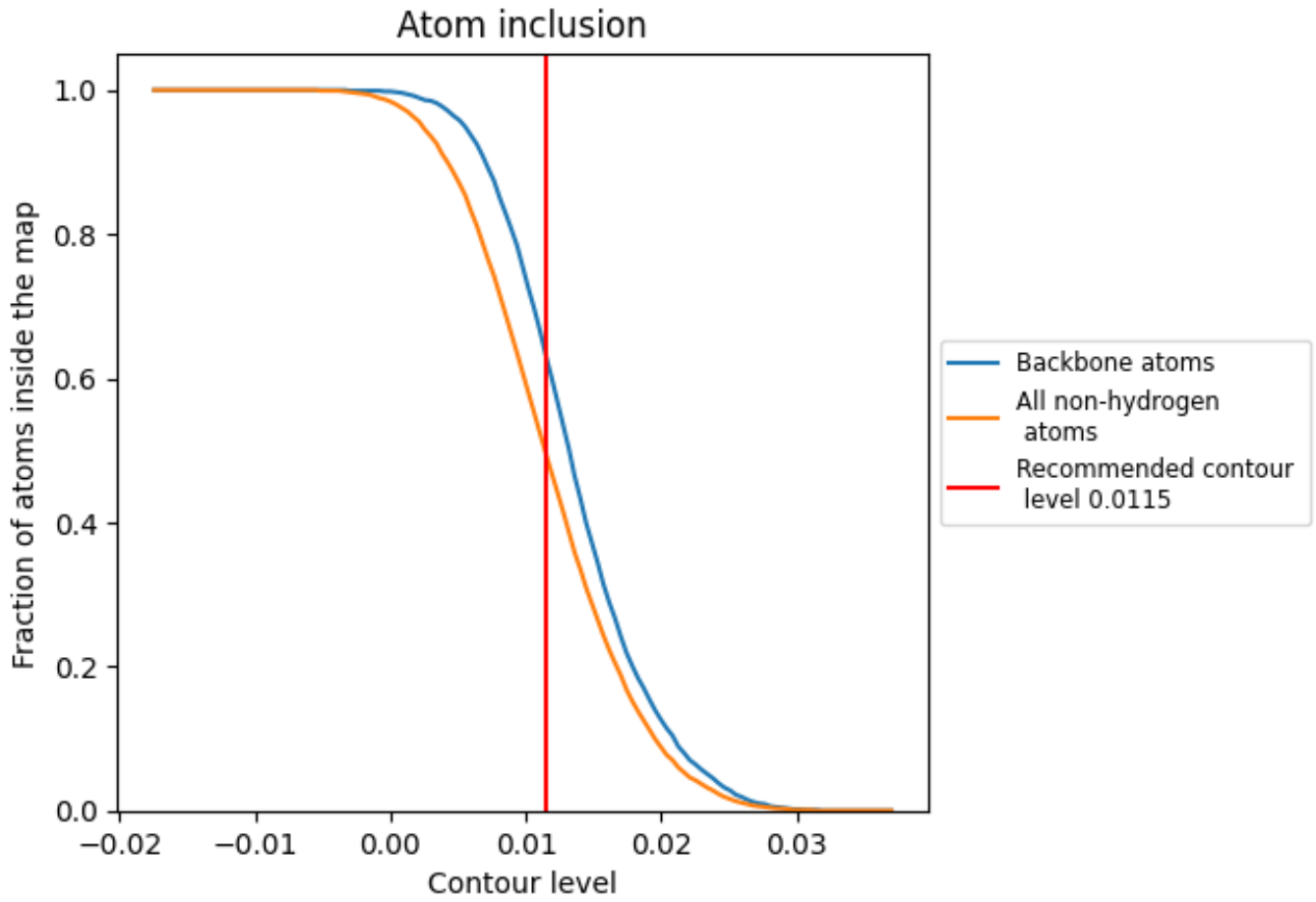
9.3 Atom inclusion mapped to coordinate model



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 (0.0115).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 49% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.2430
A	0.6320	0.3540
B	0.6180	0.3480
C	0.4760	0.2630
D	0.4990	0.2700
E	0.5780	0.3240
F	0.5870	0.3220
G	0.4760	0.2500
H	0.5060	0.2590
I	0.6200	0.2310
J	0.6040	0.2260
K	0.2950	0.1890