Full wwPDB EM Validation Report ⓘ

Jun 10, 2025 – 11:11 PM JST

PDB ID	:	7EVN / pdb_00007evn
EMDB ID	:	EMD-31330
Title	:	The cryo-EM structure of the DDX42-SF3b complex
Authors	:	Zhang, X.; Zhan, X.; Shi, Y.
Deposited on	:	2021-05-21
Resolution	:	2.60 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:

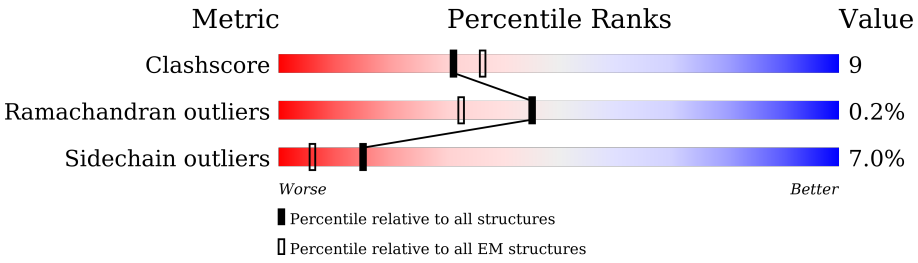
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	86	80% 8% • 9%
2	C	872	69% 23% • 7%
3	D	110	5% 75% 9% • 15%
4	A	1250	5% 73% 19% • 6%
5	E	958	47% 47% • • 49%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19668 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 Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	78	Total	C	N	O	S	0	0
			646	409	114	118	5		

- Molecule 2 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	815	Total	C	N	O	S	0	0
			6487	4163	1121	1164	39		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	433	MET	-	initiating methionine	UNP O75533
C	434	ALA	-	expression tag	UNP O75533
C	435	SER	-	expression tag	UNP O75533
C	436	ASP	-	expression tag	UNP O75533
C	437	TYR	-	expression tag	UNP O75533
C	438	LYS	-	expression tag	UNP O75533
C	439	ASP	-	expression tag	UNP O75533
C	440	ASP	-	expression tag	UNP O75533
C	441	ASP	-	expression tag	UNP O75533
C	442	ASP	-	expression tag	UNP O75533
C	443	LYS	-	expression tag	UNP O75533
C	444	ALA	-	expression tag	UNP O75533
C	445	SER	-	expression tag	UNP O75533
C	446	ASP	-	expression tag	UNP O75533
C	447	GLU	-	expression tag	UNP O75533
C	448	VAL	-	expression tag	UNP O75533
C	449	ASP	-	expression tag	UNP O75533
C	450	ALA	-	expression tag	UNP O75533
C	451	GLY	-	expression tag	UNP O75533

- Molecule 3 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			700	429	123	135	13		

- Molecule 4 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1177	Total	C	N	O	S	0	0
			9227	5858	1568	1756	45		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	TRP	-	expression tag	UNP Q15393
A	-31	SER	-	expression tag	UNP Q15393
A	-30	HIS	-	expression tag	UNP Q15393
A	-29	PRO	-	expression tag	UNP Q15393
A	-28	GLN	-	expression tag	UNP Q15393
A	-27	PHE	-	expression tag	UNP Q15393
A	-26	GLU	-	expression tag	UNP Q15393
A	-25	LYS	-	expression tag	UNP Q15393
A	-24	GLY	-	expression tag	UNP Q15393
A	-23	GLY	-	expression tag	UNP Q15393
A	-22	GLY	-	expression tag	UNP Q15393
A	-21	SER	-	expression tag	UNP Q15393
A	-20	GLY	-	expression tag	UNP Q15393
A	-19	GLY	-	expression tag	UNP Q15393
A	-18	GLY	-	expression tag	UNP Q15393
A	-17	SER	-	expression tag	UNP Q15393
A	-16	GLY	-	expression tag	UNP Q15393
A	-15	GLY	-	expression tag	UNP Q15393
A	-14	SER	-	expression tag	UNP Q15393
A	-13	ALA	-	expression tag	UNP Q15393
A	-12	TRP	-	expression tag	UNP Q15393
A	-11	SER	-	expression tag	UNP Q15393
A	-10	HIS	-	expression tag	UNP Q15393
A	-9	PRO	-	expression tag	UNP Q15393
A	-8	GLN	-	expression tag	UNP Q15393
A	-7	PHE	-	expression tag	UNP Q15393
A	-6	GLU	-	expression tag	UNP Q15393
A	-5	LYS	-	expression tag	UNP Q15393
A	-4	GLY	-	expression tag	UNP Q15393
A	-3	SER	-	expression tag	UNP Q15393
A	-2	ALA	-	expression tag	UNP Q15393

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q15393
A	0	ALA	-	expression tag	UNP Q15393

- Molecule 5 is a protein called ATP-dependent RNA helicase DDX42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	486	Total	C	N	O	S	0	0
			2605	1555	505	542	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP Q86XP3
E	-18	ALA	-	expression tag	UNP Q86XP3
E	-17	SER	-	expression tag	UNP Q86XP3
E	-16	ASP	-	expression tag	UNP Q86XP3
E	-15	TYR	-	expression tag	UNP Q86XP3
E	-14	LYS	-	expression tag	UNP Q86XP3
E	-13	ASP	-	expression tag	UNP Q86XP3
E	-12	ASP	-	expression tag	UNP Q86XP3
E	-11	ASP	-	expression tag	UNP Q86XP3
E	-10	ASP	-	expression tag	UNP Q86XP3
E	-9	LYS	-	expression tag	UNP Q86XP3
E	-8	ALA	-	expression tag	UNP Q86XP3
E	-7	SER	-	expression tag	UNP Q86XP3
E	-6	ASP	-	expression tag	UNP Q86XP3
E	-5	GLU	-	expression tag	UNP Q86XP3
E	-4	VAL	-	expression tag	UNP Q86XP3
E	-3	ASP	-	expression tag	UNP Q86XP3
E	-2	ALA	-	expression tag	UNP Q86XP3
E	-1	GLY	-	expression tag	UNP Q86XP3
E	0	THR	-	expression tag	UNP Q86XP3

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	D	3	Total	Zn	0
			3	3	

3 Residue-property plots (i)

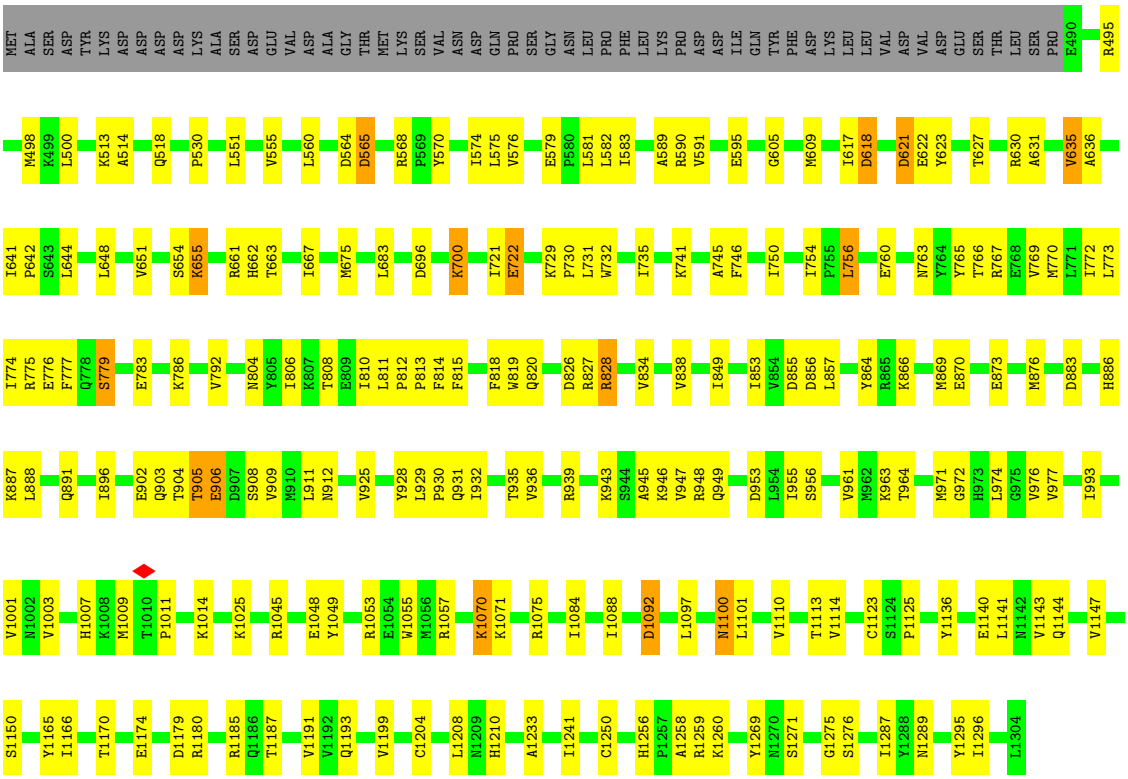
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Splicing factor 3B subunit 5

Chain B:

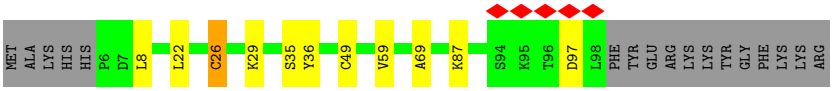
• Molecule 2: Splicing factor 3B subunit 1

Chain C:



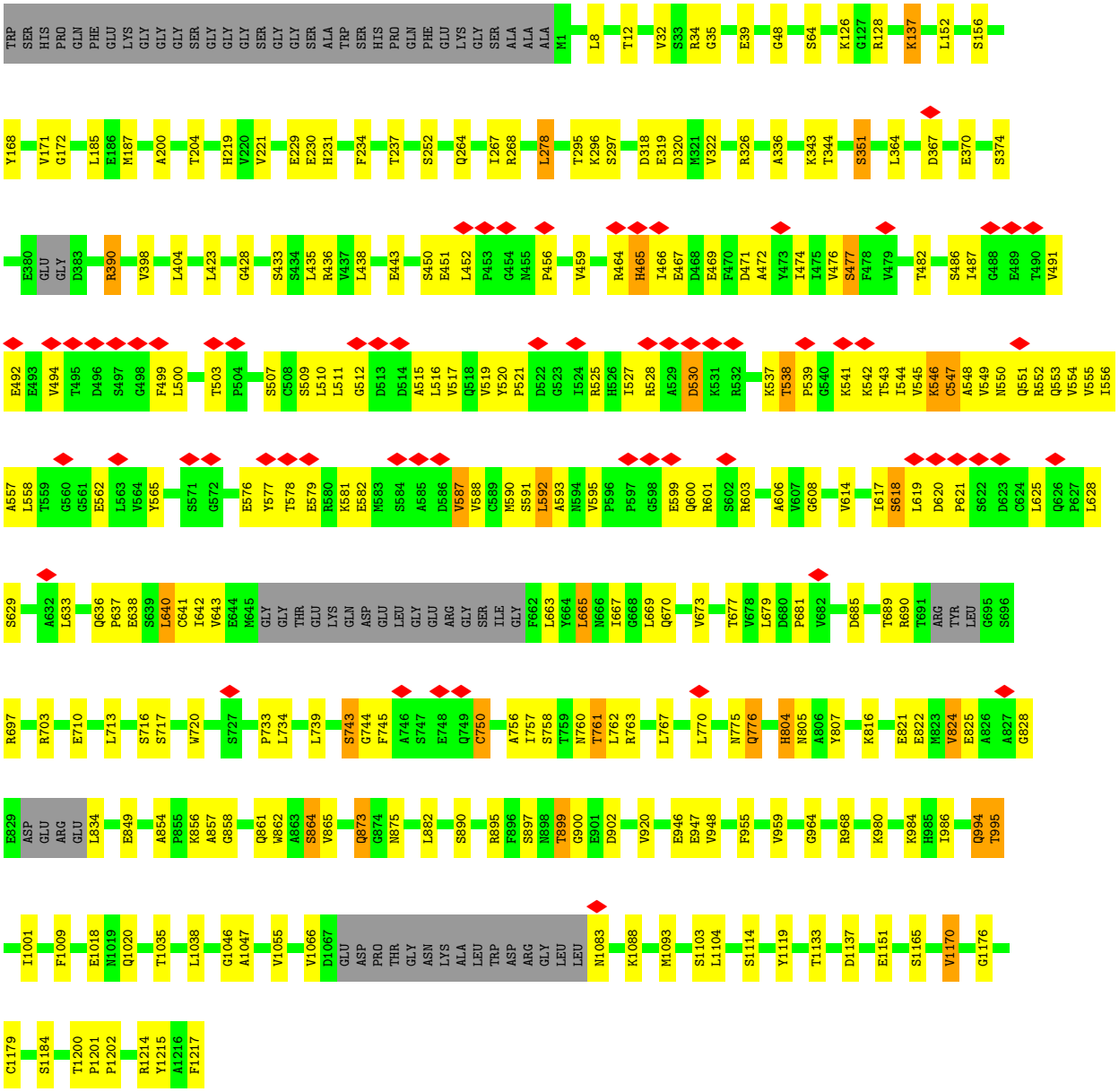
• Molecule 3: PHD finger-like domain-containing protein 5A

Chain D:



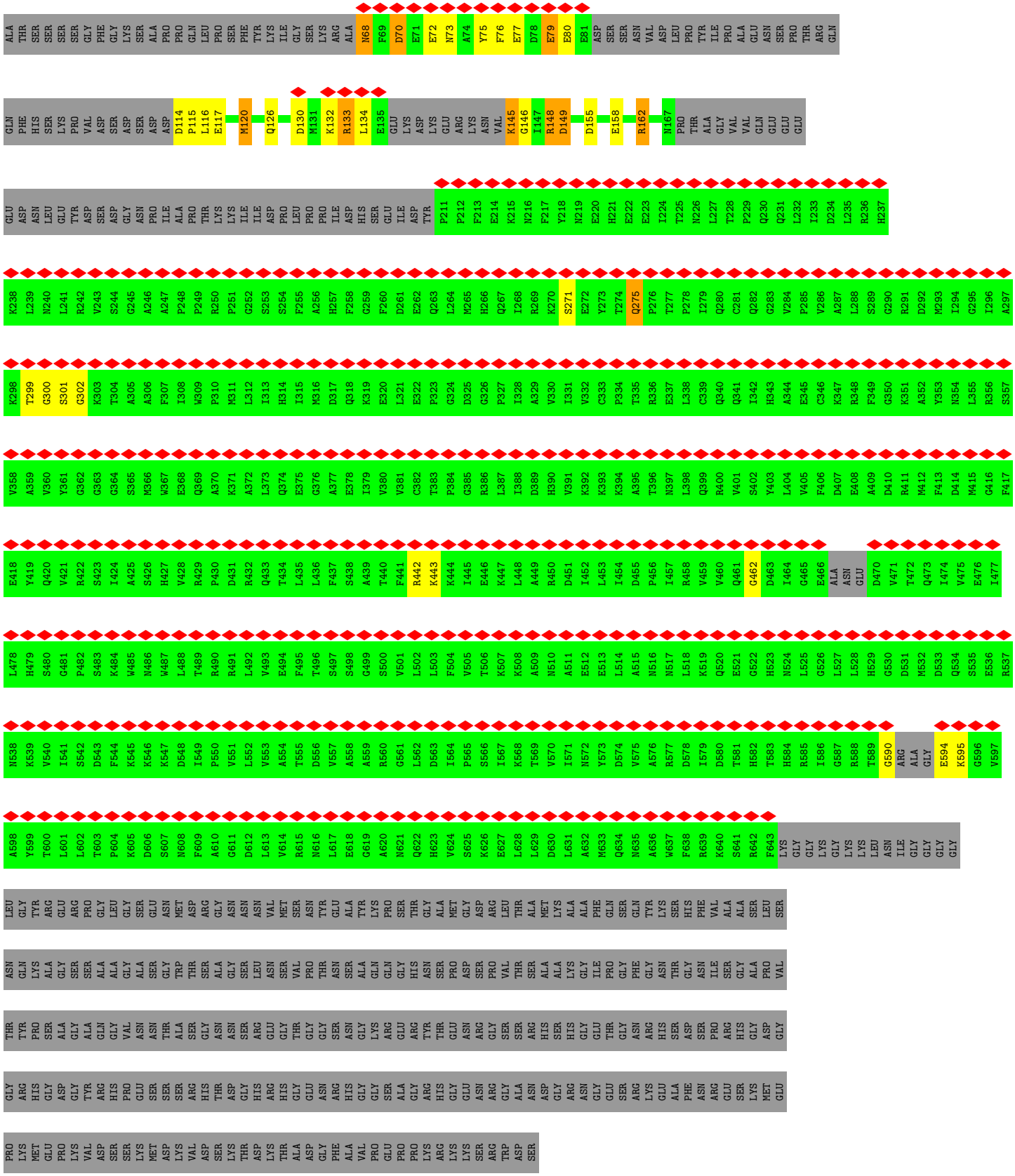
• Molecule 4: Splicing factor 3B subunit 3

Chain A:



• Molecule 5: ATP-dependent RNA helicase DDX42

Chain E:


ALA THR SER SER SER SER GLY PHE GLY LYS SER ALA PRO PRO GLN LEU PRO SER PHE TYR LYS ILE GLY SER LYS ARG ALA N68 F69 D70 E71 E72 N73 A74 Y75 F76 E77 D78 E79 E80 E81 ASP SER SER ASN VAL ASP LEU PRO TYR ILE PRO ALA GLU ASN SER PRO THR ARG GLN
GLN PHE HIS SER LYS PRO VAL ASP SER ASP SER ASP ASP D114 P115 L116 E117 M120 Q126 D130 M131 K132 R133 L134 E135 GLU LYS ASP LYS GLU ARG LYS ASN VAL K145 G146 I147 R148 D149 D155 E158 R162 N167 PRO THR ALA GLY VAL VAL GLN GLU GLU GLU
GLU ASP ASN LEU GLU TYR ASP SER ASP GLY ASN PRO ILE ALA PRO THR LYS LYS ILE ILE ASP PRO LEU PRO PRO ILE ASP HIS SER GLU ILE ASP TYR P211 P212 F213 E214 K215 N216 F217 Y218 N219 E220 H221 E222 E223 I224 T225 N226 L227 T228 P229 Q230 Q231 L232 I233 D234 L235 R236 H237
K238 L239 N240 L241 R242 V243 S244 G245 A246 A247 P248 P249 R250 P251 G252 S253 S254 F255 A256 H257 F258 G259 F260 D261 E262 Q263 L264 M265 H266 Q267 I268 R269 K270 S271 E272 Y273 T274 Q275 P276 T277 P278 I279 Q280 C281 Q282 G283 V284 P285 V286 A287 L288 S289 G290 R291 D292 M293 I294 G295 I296 A297
K298 T299 G300 S301 G302 K303 T304 A305 A306 F307 I308 W309 P310 M311 L312 I313 H314 I315 M316 D317 Q318 K319 E320 L321 E322 P323 G324 D325 G326 P327 I328 A329 V330 I331 V332 C333 P334 T335 R336 E337 L338 C339 Q340 Q341 T342 H343 A344 E345 C346 K347 R348 F349 G350 K351 A352 Y353 N354 L355 R356 S357
V358 A359 V360 Y361 G362 G363 G364 S365 M366 W367 E368 Q369 A370 K371 A372 L373 Q374 E375 G376 A377 E378 I379 V380 V381 C382 T383 P384 G385 R386 L387 I388 D389 H390 V391 K392 K393 K394 A395 T396 N397 L398 Q399 R400 V401 S402 Y403 L404 V405 F406 D407 E408 A409 D410 R411 M412 F413 D414 M415 G416 F417
E418 Y419 Q420 V421 R422 S423 I424 A425 S426 H427 V428 R429 P430 D431 R432 Q433 T434 L435 L436 F437 S438 A439 T440 F441 R442 K443 K444 I445 E446 K447 L448 A449 R450 D451 I452 L453 I454 D455 P456 I457 R458 V459 V460 Q461 G462 D463 I464 G465 E466 ALA ASN GLU D470 V471 T472 Q473 I474 V475 E476 I477
L478 H479 S480 G481 P482 S483 K484 W485 N486 W487 L488 T489 R490 R491 L492 V493 E494 F495 T496 S497 S498 G499 S500 V501 L502 L503 F504 V505 T506 K507 K508 A509 N510 A511 E512 E513 L514 A515 N516 N517 L518 K519 Q520 E521 G522 H523 N524 L525 G526 L527 L528 H529 G530 D531 M532 D533 Q534 S535 E536 R537
N538 K539 V540 I541 S542 D543 F544 K545 K546 K547 D548 I549 P550 V551 L552 V553 A554 T555 D556 V557 A558 A559 R560 G561 L562 D563 I564 P565 S566 I567 K568 T569 V570 I571 N572 Y573 D574 V575 A576 R577 D578 I579 D580 T581 H582 T583 H584 R585 I586 G587 R588 T589 G590 ARG ALA GLY E594 K595 G596 V597
A598 Y599 T600 L601 L602 T603 P604 K605 D606 S607 N608 F609 A610 G611 D612 L613 V614 R615 N616 L617 E618 G619 A620 N621 Q622 H623 V624 S625 K626 E627 L628 L629 D630 L631 A632 M633 Q634 N635 A636 W637 F638 R639 K640 S641 R642 F643 LYS GLY GLY LYS GLY LYS LYS LEU ASN ILE GLY GLY GLY GLY
LEU GLY TYR ARG GLU ARG PRO GLY LEU GLY SER GLU ASN MET ASP ARG GLY ASN ASN ASN VAL MET SER ASN TYR GLU ALA TYR LYS PRO SER THR GLY ALA MET GLY ASP ARG LEU THR ALA MET LYS ALA ALA PHE GLN SER GLN TYR LYS SER HIS PHE VAL ALA ALA SER LEU SER
ASN GLN LYS ALA GLY SER ALA ALA GLY SER GLY TRP THR SER ALA GLY SER LEU ASN SER VAL PRO THR ASN SER ALA GLN GLN GLY HIS ASN SER PRO ASP SER PRO VAL THR SER ALA ALA LYS GLY ILE PRO GLY PHE GLY ASN THR GLY ASN ILE SER GLY ALA ALA PRO VAL
THR TYR PRO SER ALA GLY VAL ASN ASN THR ALA SER GLY ASN ASN SER ARG GLU ARG GLY THR GLY GLY SER ASN SER GLY LYS ARG GLU ARG TYR THR GLU GLY ASN ARG GLY SER SER ARG HIS SER GLY GLU THR GLY ASN ARG HIS SER ASP SER PRO ARG HIS GLY ASP GLY
GLY ARG HIS GLY ASP GLY TYR ARG HIS PRO GLU SER SER ARG HIS THR ASP GLY HIS ARG HIS GLY GLY GLU ASN ARG HIS GLY GLY SER ALA GLY ARG HIS GLY GLU ASN ARG GLY ARG ASN GLY GLU SER ARG LYS GLU ALA PHE ASN ARG GLU SER LYS MET GLU
PRO LYS MET GLU PRO LYS VAL ASP SER LYS THR ASP LYS THR ALA ASP GLY PHE ALA VAL PRO GLU PRO PRO LYS ARG LYS LYS SER ARG TRP ASP SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	234800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.27	0/665	0.50	0/899
2	C	0.25	0/6609	0.48	2/8946 (0.0%)
3	D	0.29	0/709	0.47	0/952
4	A	0.27	1/9415 (0.0%)	0.46	1/12775 (0.0%)
5	E	0.62	0/2607	0.98	5/3593 (0.1%)
All	All	0.34	1/20005 (0.0%)	0.56	8/27165 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	HIS	C-O	6.55	1.32	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	275	GLN	CA-C-N	-8.04	111.73	119.85
5	E	275	GLN	C-N-CA	-8.04	111.73	119.85
5	E	271	SER	CA-C-N	6.98	134.27	121.70
5	E	271	SER	C-N-CA	6.98	134.27	121.70
2	C	565	ASP	N-CA-C	-5.91	104.74	113.61
2	C	564	ASP	O-C-N	-5.79	114.49	122.30
4	A	137	LYS	N-CA-CB	-5.49	107.91	114.17
5	E	462	GLY	N-CA-C	5.11	118.82	112.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	646	0	608	6	0
2	C	6487	0	6700	157	0
3	D	700	0	682	6	0
4	A	9227	0	9154	142	0
5	E	2605	0	1378	67	0
6	D	3	0	0	0	0
All	All	19668	0	18522	330	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 9.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:786:LYS:NZ	5:E:72:GLU:HG3	1.52	1.22
5:E:120:MET:HA	5:E:120:MET:HE2	1.24	1.18
2:C:741:LYS:HE3	5:E:79:GLU:HB2	1.19	1.15
4:A:221:VAL:CG1	5:E:146:GLY:HA3	1.82	1.10
2:C:741:LYS:CE	5:E:79:GLU:HB2	1.87	1.04
2:C:786:LYS:HZ1	5:E:72:GLU:HG3	0.87	1.01
2:C:662:HIS:CE1	2:C:700:LYS:HD2	1.95	1.00
2:C:630:ARG:NH2	5:E:68:ASN:HB2	1.79	0.97
5:E:162:ARG:HH11	5:E:162:ARG:HB3	1.27	0.96
5:E:162:ARG:HB3	5:E:162:ARG:NH1	1.82	0.94
5:E:120:MET:HA	5:E:120:MET:CE	2.00	0.91
2:C:786:LYS:NZ	5:E:72:GLU:CG	2.33	0.90
2:C:786:LYS:HZ1	5:E:72:GLU:CG	1.80	0.89
2:C:662:HIS:HE1	2:C:700:LYS:HD2	1.40	0.87
2:C:783:GLU:CG	5:E:75:TYR:CD2	2.56	0.87
2:C:783:GLU:HG3	5:E:75:TYR:CD2	2.14	0.82
5:E:145:LYS:HB2	5:E:145:LYS:NZ	1.95	0.80
4:A:221:VAL:HG12	5:E:146:GLY:HA3	1.63	0.79
2:C:1180:ARG:CZ	5:E:442:ARG:HA	2.13	0.79
4:A:459:VAL:HG11	4:A:757:ILE:HD13	1.65	0.78
5:E:70:ASP:HB2	5:E:73:ASN:ND2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:221:VAL:HG11	5:E:146:GLY:HA3	1.64	0.77
4:A:264:GLN:HE22	4:A:322:VAL:H	1.31	0.77
5:E:120:MET:HE2	5:E:120:MET:CA	2.12	0.76
2:C:783:GLU:HG2	5:E:75:TYR:CD2	2.20	0.76
2:C:498:MET:HE1	2:C:530:PRO:HB2	1.68	0.76
4:A:486:SER:HB2	4:A:494:VAL:HB	1.68	0.76
2:C:1208:LEU:HB2	2:C:1241:ILE:HD11	1.66	0.76
4:A:221:VAL:CG1	5:E:146:GLY:CA	2.63	0.74
4:A:804:HIS:HD2	4:A:862:TRP:CZ2	2.06	0.74
5:E:149:ASP:N	5:E:149:ASP:OD1	2.20	0.74
4:A:547:CYS:SG	4:A:548:ALA:N	2.61	0.73
4:A:528:ARG:HG3	4:A:530:ASP:H	1.55	0.72
2:C:961:VAL:HA	2:C:964:THR:HG22	1.72	0.71
2:C:1001:VAL:HG12	2:C:1009:MET:HE1	1.71	0.71
4:A:1200:THR:HG22	4:A:1202:PRO:HD2	1.73	0.71
4:A:552:ARG:NH1	4:A:600:GLN:O	2.24	0.70
2:C:655:LYS:NZ	5:E:114:ASP:HB2	2.05	0.70
2:C:963:LYS:HD3	2:C:1003:VAL:HG22	1.73	0.70
4:A:828:GLY:O	4:A:834:LEU:N	2.24	0.70
2:C:568:ARG:NH1	5:E:130:ASP:OD1	2.24	0.69
2:C:783:GLU:OE2	5:E:72:GLU:HG2	1.91	0.69
4:A:507:SER:HB2	4:A:519:VAL:HB	1.73	0.69
2:C:1180:ARG:NH2	5:E:443:LYS:H	1.90	0.69
4:A:1001:ILE:HG13	4:A:1038:LEU:HD21	1.74	0.68
5:E:300:GLY:O	5:E:302:GLY:N	2.21	0.68
2:C:1289:ASN:ND2	2:C:1295:TYR:H	1.93	0.67
4:A:603:ARG:HA	4:A:619:LEU:HB2	1.77	0.66
2:C:662:HIS:HE1	2:C:700:LYS:CD	2.09	0.66
4:A:499:PHE:O	4:A:525:ARG:NH1	2.30	0.65
2:C:622:GLU:OE2	2:C:622:GLU:HA	1.97	0.65
5:E:145:LYS:HB2	5:E:145:LYS:HZ2	1.58	0.65
4:A:550:ASN:ND2	4:A:593:ALA:O	2.30	0.64
4:A:637:PRO:HA	4:A:669:LEU:HA	1.78	0.64
4:A:221:VAL:HG13	5:E:146:GLY:C	2.23	0.64
4:A:558:LEU:HD23	4:A:558:LEU:H	1.63	0.63
2:C:731:LEU:HB3	2:C:750:ILE:HD11	1.80	0.63
2:C:1097:LEU:O	2:C:1100:ASN:ND2	2.32	0.62
2:C:655:LYS:HZ2	5:E:114:ASP:HB2	1.63	0.62
2:C:618:ASP:OD1	2:C:618:ASP:N	2.33	0.62
2:C:621:ASP:OD2	2:C:621:ASP:N	2.30	0.62
5:E:68:ASN:O	5:E:68:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:947:GLU:HG3	4:A:948:VAL:H	1.65	0.61
2:C:769:VAL:O	2:C:773:LEU:HB2	2.00	0.61
2:C:786:LYS:HZ2	5:E:72:GLU:CD	2.09	0.61
4:A:549:VAL:HG13	4:A:554:VAL:HG22	1.83	0.61
4:A:465:HIS:CE1	4:A:467:GLU:HB2	2.36	0.60
4:A:720:TRP:HA	4:A:733:PRO:HA	1.84	0.60
2:C:581:LEU:HD22	2:C:589:ALA:HB1	1.84	0.60
2:C:974:LEU:HA	2:C:977:VAL:HG12	1.83	0.60
2:C:1001:VAL:O	2:C:1045:ARG:NH2	2.34	0.60
2:C:630:ARG:HH21	5:E:68:ASN:HB2	1.67	0.60
4:A:554:VAL:HG12	4:A:556:ILE:HD11	1.84	0.60
4:A:603:ARG:O	4:A:619:LEU:N	2.34	0.60
2:C:1009:MET:HE2	2:C:1011:PRO:HG2	1.83	0.59
4:A:614:VAL:HG13	4:A:633:LEU:HD21	1.85	0.59
4:A:1083:ASN:N	4:A:1088:LYS:HZ1	2.01	0.58
4:A:553:GLN:HE21	4:A:601:ARG:HB2	1.67	0.58
4:A:511:LEU:HD22	4:A:517:VAL:HG21	1.84	0.58
4:A:1055:VAL:HG23	4:A:1093:MET:HE3	1.85	0.58
4:A:343:LYS:O	4:A:344:THR:OG1	2.17	0.57
4:A:466:ILE:HA	4:A:510:LEU:HD21	1.85	0.57
2:C:972:GLY:O	2:C:976:VAL:HG23	2.04	0.57
5:E:117:GLU:OE1	5:E:117:GLU:HA	2.04	0.57
2:C:513:LYS:HE2	5:E:158:GLU:HG3	1.87	0.57
2:C:570:TYR:O	2:C:574:ILE:HG12	2.04	0.57
2:C:786:LYS:HZ2	5:E:72:GLU:CG	2.17	0.57
4:A:126:LYS:HB2	4:A:128:ARG:HE	1.69	0.57
4:A:946:GLU:OE2	4:A:968:ARG:NH2	2.34	0.57
1:B:25:ASP:OD1	2:C:1259:ARG:NH2	2.30	0.56
2:C:903:GLN:HE21	2:C:906:GLU:HA	1.69	0.56
2:C:1113:THR:HG23	2:C:1150:SER:HA	1.87	0.56
4:A:320:ASP:N	4:A:320:ASP:OD1	2.36	0.56
4:A:545:VAL:HG22	4:A:546:LYS:HE2	1.87	0.56
4:A:617:ILE:HG21	4:A:625:LEU:HD13	1.86	0.56
4:A:464:ARG:HE	4:A:472:ALA:HB1	1.71	0.56
2:C:783:GLU:HG2	5:E:75:TYR:CG	2.41	0.55
4:A:562:GLU:HG2	4:A:582:GLU:HG2	1.88	0.55
2:C:722:GLU:CD	2:C:722:GLU:H	2.15	0.55
2:C:1174:GLU:OE1	2:C:1210:HIS:NE2	2.36	0.55
4:A:640:LEU:HD12	4:A:667:ILE:HD12	1.87	0.55
2:C:1289:ASN:HD22	2:C:1295:TYR:H	1.52	0.55
4:A:278:LEU:HD21	4:A:816:LYS:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:739:LEU:HG	4:A:756:ALA:HB1	1.89	0.54
4:A:565:TYR:HD2	4:A:577:TYR:HB2	1.72	0.54
4:A:428:GLY:HA3	4:A:433:SER:HA	1.89	0.54
2:C:581:LEU:O	2:C:590:ARG:HA	2.07	0.54
2:C:1166:ILE:O	2:C:1170:THR:HG23	2.08	0.54
4:A:456:PRO:HB2	4:A:757:ILE:HG21	1.90	0.54
4:A:544:ILE:HA	4:A:558:LEU:HA	1.89	0.54
2:C:741:LYS:HD3	5:E:76:PHE:HA	1.90	0.54
2:C:834:VAL:O	2:C:838:VAL:HG23	2.08	0.54
2:C:655:LYS:NZ	5:E:115:PRO:HD3	2.22	0.53
4:A:955:PHE:HD1	4:A:995:THR:HG21	1.73	0.53
2:C:729:LYS:HB3	2:C:730:PRO:HD3	1.90	0.53
5:E:300:GLY:C	5:E:302:GLY:H	2.13	0.53
2:C:932:ILE:O	2:C:936:VAL:HG23	2.07	0.53
4:A:438:LEU:HD22	4:A:776:GLN:HB3	1.90	0.53
4:A:474:ILE:HG22	4:A:476:VAL:HG23	1.90	0.53
2:C:565:ASP:O	2:C:568:ARG:HG3	2.08	0.53
4:A:187:MET:HE1	4:A:231:HIS:CE1	2.44	0.53
4:A:555:VAL:HG13	4:A:565:TYR:HA	1.89	0.53
4:A:955:PHE:CD1	4:A:995:THR:HG21	2.43	0.53
5:E:132:LYS:HG3	5:E:132:LYS:O	2.08	0.53
1:B:47:PHE:CZ	4:A:35:GLY:HA3	2.44	0.53
4:A:200:ALA:O	4:A:204:THR:OG1	2.22	0.52
4:A:436:ARG:HH11	4:A:776:GLN:HE22	1.56	0.52
5:E:145:LYS:HB2	5:E:145:LYS:HZ3	1.73	0.52
4:A:443:GLU:CD	4:A:443:GLU:H	2.17	0.52
2:C:1199:VAL:HG11	2:C:1204:CYS:SG	2.49	0.52
2:C:971:MET:HA	2:C:974:LEU:HG	1.91	0.52
4:A:539:PRO:O	4:A:542:LYS:NZ	2.42	0.52
4:A:550:ASN:HB2	4:A:592:LEU:HD11	1.92	0.52
2:C:1179:ASP:O	2:C:1185:ARG:NH1	2.41	0.51
4:A:899:THR:OG1	4:A:900:GLY:N	2.43	0.51
2:C:883:ASP:OD1	2:C:883:ASP:N	2.43	0.51
4:A:1176:GLY:HA2	4:A:1179:CYS:HB2	1.92	0.50
4:A:636:GLN:HG2	4:A:670:GLN:HG2	1.94	0.50
2:C:770:MET:O	2:C:774:ILE:HG12	2.11	0.50
2:C:826:ASP:OD1	2:C:827:ARG:N	2.44	0.50
2:C:746:PHE:O	2:C:750:ILE:HG12	2.12	0.50
2:C:513:LYS:CE	5:E:158:GLU:HG3	2.42	0.50
4:A:553:GLN:HE21	4:A:601:ARG:HD2	1.76	0.49
1:B:58:ASN:O	4:A:856:LYS:NZ	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:812:PRO:HB2	2:C:813:PRO:HD3	1.94	0.49
2:C:1180:ARG:NH1	5:E:442:ARG:HA	2.28	0.49
4:A:512:GLY:H	4:A:515:ALA:HB3	1.77	0.49
2:C:662:HIS:CE1	2:C:700:LYS:CD	2.82	0.49
5:E:133:ARG:C	5:E:133:ARG:CD	2.85	0.49
2:C:741:LYS:HE2	5:E:79:GLU:HB2	1.84	0.49
2:C:1084:ILE:O	2:C:1088:ILE:HG12	2.12	0.49
2:C:700:LYS:HG3	5:E:80:GLU:HG3	1.94	0.49
2:C:903:GLN:NE2	2:C:906:GLU:HA	2.27	0.49
4:A:525:ARG:HG2	4:A:527:ILE:HD11	1.94	0.49
4:A:673:VAL:HA	4:A:690:ARG:HA	1.95	0.49
2:C:622:GLU:OE1	5:E:77:GLU:OE2	2.30	0.49
2:C:661:ARG:NH1	2:C:696:ASP:OD2	2.46	0.48
4:A:404:LEU:HD11	4:A:438:LEU:HD11	1.95	0.48
4:A:849:GLU:HG2	4:A:854:ALA:HA	1.94	0.48
4:A:608:GLY:HA2	4:A:614:VAL:HA	1.96	0.48
4:A:864:SER:HB3	4:A:882:LEU:HD12	1.94	0.48
4:A:550:ASN:ND2	4:A:595:VAL:HG13	2.29	0.48
4:A:716:SER:OG	4:A:717:SER:N	2.46	0.48
2:C:1071:LYS:O	2:C:1075:ARG:HG2	2.14	0.48
4:A:471:ASP:O	4:A:487:ILE:HG21	2.13	0.48
4:A:807:TYR:CE2	4:A:857:ALA:HB3	2.48	0.48
2:C:732:TRP:CZ2	2:C:765:TYR:HB3	2.48	0.48
2:C:810:ILE:O	2:C:813:PRO:HD2	2.14	0.48
4:A:606:ALA:HB3	4:A:642:ILE:HD11	1.95	0.48
4:A:665:LEU:HD21	4:A:667:ILE:HD11	1.96	0.48
4:A:994:GLN:HG2	4:A:1038:LEU:HG	1.96	0.48
2:C:591:VAL:O	2:C:595:GLU:HG3	2.13	0.47
2:C:605:GLY:O	2:C:609:MET:HG2	2.14	0.47
4:A:500:LEU:HB2	4:A:525:ARG:HH22	1.79	0.47
2:C:935:THR:O	2:C:939:ARG:HG2	2.14	0.47
4:A:1201:PRO:HB2	4:A:1202:PRO:HD3	1.96	0.47
5:E:114:ASP:N	5:E:115:PRO:HD2	2.29	0.47
2:C:945:ALA:HA	2:C:948:ARG:HB2	1.95	0.47
4:A:822:GLU:HA	4:A:825:GLU:HG2	1.95	0.47
2:C:648:LEU:HA	2:C:651:VAL:HG12	1.96	0.47
4:A:515:ALA:HA	4:A:528:ARG:HA	1.95	0.47
4:A:642:ILE:HG13	4:A:665:LEU:HD12	1.95	0.47
3:D:26:CYS:HB3	3:D:29:LYS:HE2	1.95	0.47
4:A:137:LYS:O	4:A:137:LYS:HG2	2.15	0.47
4:A:697:ARG:HB2	4:A:717:SER:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:946:LYS:HB3	2:C:946:LYS:HE3	1.68	0.46
2:C:886:HIS:C	2:C:888:LEU:H	2.23	0.46
4:A:48:GLY:HA3	4:A:398:VAL:HG11	1.97	0.46
2:C:495:ARG:O	2:C:495:ARG:NH2	2.43	0.46
2:C:1007:HIS:ND1	2:C:1049:TYR:OH	2.46	0.46
2:C:1187:THR:O	2:C:1191:VAL:HG23	2.14	0.46
2:C:1275:GLY:O	2:C:1276:SER:OG	2.31	0.46
4:A:336:ALA:HA	4:A:351:SER:HA	1.97	0.46
4:A:221:VAL:CG1	5:E:146:GLY:C	2.86	0.46
2:C:908:SER:OG	2:C:912:ASN:ND2	2.49	0.46
2:C:786:LYS:HE2	2:C:828:ARG:HH12	1.81	0.46
5:E:590:GLY:O	5:E:594:GLU:HA	2.16	0.46
2:C:630:ARG:NH2	5:E:68:ASN:CB	2.67	0.46
4:A:581:LYS:HD2	4:A:625:LEU:HD12	1.98	0.46
2:C:575:LEU:O	2:C:579:GLU:HB2	2.16	0.46
2:C:663:THR:O	2:C:667:ILE:HG13	2.16	0.46
4:A:530:ASP:OD2	4:A:530:ASP:N	2.49	0.46
2:C:636:ALA:HB2	2:C:644:LEU:HD22	1.97	0.45
2:C:763:ASN:O	2:C:767:ARG:HG2	2.16	0.45
2:C:735:ILE:HD12	2:C:772:ILE:HD13	1.97	0.45
2:C:1140:GLU:O	2:C:1144:GLN:HG3	2.16	0.45
4:A:477:SER:HA	4:A:482:THR:HA	1.99	0.45
4:A:550:ASN:OD1	4:A:551:GLN:N	2.41	0.45
2:C:911:LEU:HD21	2:C:953:ASP:HB2	1.97	0.45
2:C:925:VAL:HG23	2:C:928:TYR:HB2	1.99	0.45
4:A:579:GLU:OE1	4:A:625:LEU:HG	2.16	0.45
4:A:873:GLN:HG3	4:A:875:ASN:HD22	1.82	0.45
4:A:556:ILE:HG22	4:A:557:ALA:H	1.80	0.45
3:D:29:LYS:HG2	3:D:36:TYR:CZ	2.52	0.45
2:C:1092:ASP:OD2	2:C:1092:ASP:N	2.49	0.45
2:C:1136:TYR:HB2	2:C:1147:VAL:HG11	1.97	0.45
4:A:465:HIS:CE1	4:A:467:GLU:H	2.35	0.45
4:A:587:VAL:HG21	4:A:590:MET:HE3	1.99	0.44
4:A:1009:PHE:HZ	4:A:1046:GLY:HA3	1.81	0.44
2:C:925:VAL:HG23	2:C:928:TYR:HD2	1.81	0.44
2:C:1256:HIS:HD2	2:C:1258:ALA:H	1.65	0.44
2:C:766:THR:O	2:C:770:MET:HB2	2.17	0.44
5:E:133:ARG:CZ	5:E:134:LEU:HB2	2.47	0.44
2:C:630:ARG:CZ	5:E:68:ASN:HB2	2.44	0.44
2:C:783:GLU:HG3	5:E:75:TYR:HD2	1.78	0.44
2:C:855:ASP:OD1	2:C:891:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:663:LEU:HD23	4:A:679:LEU:HB3	1.99	0.44
4:A:318:ASP:O	4:A:319:GLU:C	2.61	0.44
4:A:643:VAL:HG12	4:A:703:ARG:HD3	2.00	0.44
2:C:568:ARG:HH12	5:E:130:ASP:CG	2.25	0.44
2:C:866:LYS:HG3	2:C:909:VAL:HG11	1.99	0.44
4:A:538:THR:HG21	4:A:558:LEU:HD13	1.98	0.44
4:A:620:ASP:OD1	4:A:621:PRO:HD2	2.16	0.44
4:A:1165:SER:OG	4:A:1170:VAL:HG23	2.18	0.44
5:E:145:LYS:O	5:E:145:LYS:HG2	2.17	0.44
4:A:219:HIS:CD2	5:E:148:ARG:HD3	2.52	0.44
4:A:509:SER:HB2	4:A:549:VAL:HG11	2.00	0.44
5:E:70:ASP:HB2	5:E:73:ASN:CG	2.43	0.44
5:E:299:THR:HA	5:E:300:GLY:HA2	1.71	0.44
2:C:1053:ARG:HH22	2:C:1057:ARG:HD2	1.83	0.44
2:C:876:MET:HE2	2:C:876:MET:HB3	1.74	0.43
2:C:721:ILE:HD13	2:C:756:LEU:HB3	2.01	0.43
2:C:804:ASN:O	2:C:808:THR:HG22	2.17	0.43
2:C:623:TYR:O	2:C:627:THR:HG23	2.18	0.43
4:A:745:PHE:HD2	4:A:750:CYS:HB2	1.84	0.43
4:A:1114:SER:HB2	4:A:1215:TYR:CE1	2.53	0.43
2:C:886:HIS:O	2:C:887:LYS:HB3	2.18	0.43
4:A:537:LYS:HE3	4:A:537:LYS:HB2	1.56	0.43
4:A:1104:LEU:HD23	4:A:1119:TYR:HB3	2.01	0.43
2:C:1125:PRO:HG2	2:C:1165:TYR:CE2	2.53	0.43
2:C:904:THR:OG1	2:C:905:THR:N	2.52	0.43
2:C:655:LYS:HZ1	5:E:115:PRO:HD3	1.83	0.43
4:A:618:SER:OG	4:A:628:LEU:HD21	2.19	0.43
4:A:873:GLN:HG3	4:A:875:ASN:ND2	2.33	0.43
2:C:819:TRP:C	2:C:820:GLN:HG2	2.44	0.42
4:A:230:GLU:OE1	4:A:268:ARG:NH2	2.52	0.42
4:A:947:GLU:HG2	4:A:964:GLY:HA3	2.02	0.42
2:C:869:MET:HE1	2:C:896:ILE:HG22	2.01	0.42
4:A:697:ARG:HH11	4:A:717:SER:HA	1.84	0.42
4:A:710:GLU:OE2	4:A:710:GLU:HA	2.19	0.42
2:C:873:GLU:OE1	2:C:912:ASN:HB3	2.20	0.42
5:E:133:ARG:C	5:E:133:ARG:HD2	2.45	0.42
4:A:758:SER:HB2	4:A:763:ARG:HE	1.84	0.42
4:A:980:LYS:HD2	4:A:980:LYS:HA	1.75	0.42
1:B:7:ILE:HG13	3:D:8:LEU:O	2.19	0.42
2:C:806:ILE:HG12	2:C:810:ILE:HD12	2.00	0.42
2:C:1025:LYS:HA	2:C:1025:LYS:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:32:VAL:HG22	4:A:39:GLU:HB3	2.00	0.42
2:C:1053:ARG:CZ	2:C:1053:ARG:HB3	2.49	0.42
4:A:1035:THR:HG22	4:A:1047:ALA:HB3	2.00	0.42
4:A:370:GLU:OE2	4:A:390:ARG:HD3	2.18	0.42
2:C:641:ILE:HD11	2:C:675:MET:SD	2.60	0.42
2:C:1260:LYS:HA	2:C:1260:LYS:HD3	1.84	0.42
2:C:568:ARG:NH2	5:E:130:ASP:OD1	2.53	0.42
2:C:774:ILE:O	2:C:777:PHE:HB2	2.19	0.42
2:C:1009:MET:HG2	2:C:1011:PRO:HD2	2.02	0.42
2:C:1289:ASN:HD21	2:C:1296:ILE:H	1.68	0.42
4:A:267:ILE:HD13	4:A:322:VAL:HG12	2.01	0.42
4:A:1214:ARG:HG2	4:A:1215:TYR:CE2	2.55	0.42
4:A:743:SER:OG	4:A:744:GLY:O	2.38	0.41
2:C:732:TRP:O	2:C:735:ILE:HG13	2.19	0.41
2:C:811:LEU:HD22	2:C:815:PHE:HE2	1.84	0.41
2:C:929:LEU:N	2:C:930:PRO:HD2	2.35	0.41
2:C:1110:VAL:O	2:C:1114:VAL:HG23	2.19	0.41
4:A:629:SER:OG	4:A:681:PRO:O	2.38	0.41
4:A:821:GLU:O	4:A:824:VAL:HG12	2.19	0.41
4:A:858:GLY:HA3	4:A:861:GLN:HG3	2.03	0.41
1:B:32:LEU:HD11	2:C:1287:ILE:HG21	2.02	0.41
2:C:631:ALA:O	2:C:635:VAL:HG12	2.20	0.41
2:C:814:PHE:O	2:C:818:PHE:HB2	2.20	0.41
2:C:1070:LYS:NZ	2:C:1070:LYS:HB3	2.36	0.41
4:A:947:GLU:HG3	4:A:948:VAL:N	2.33	0.41
4:A:1018:GLU:N	4:A:1018:GLU:OE2	2.52	0.41
4:A:638:GLU:HG3	4:A:670:GLN:HB3	2.02	0.41
2:C:1180:ARG:NH2	5:E:442:ARG:HA	2.35	0.41
2:C:1250:CYS:SG	2:C:1269:TYR:HB2	2.60	0.41
4:A:172:GLY:O	4:A:237:THR:OG1	2.30	0.41
4:A:472:ALA:O	4:A:487:ILE:HG22	2.20	0.41
2:C:551:LEU:O	2:C:555:VAL:HG23	2.20	0.41
4:A:895:ARG:HG2	4:A:902:ASP:O	2.21	0.41
1:B:57:GLU:O	1:B:59:GLU:N	2.53	0.41
2:C:641:ILE:N	2:C:642:PRO:HD2	2.35	0.41
2:C:745:ALA:HB2	5:E:76:PHE:CE1	2.55	0.41
2:C:776:GLU:O	2:C:779:SER:HB3	2.21	0.41
2:C:1014:LYS:H	2:C:1014:LYS:HE2	1.84	0.41
2:C:1141:LEU:C	2:C:1143:VAL:H	2.29	0.41
4:A:451:GLU:HG3	4:A:760:ASN:O	2.21	0.41
5:E:134:LEU:HD12	5:E:134:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1193:GLN:HB2	2:C:1233:ALA:HA	2.02	0.41
4:A:761:THR:HG22	4:A:762:LEU:H	1.85	0.41
3:D:22:LEU:HG	3:D:69:ALA:HB2	2.03	0.41
4:A:168:TYR:HB2	4:A:185:LEU:HB2	2.03	0.41
3:D:59:VAL:HG13	3:D:87:LYS:HA	2.02	0.41
4:A:423:LEU:HB2	4:A:438:LEU:HB2	2.03	0.40
2:C:856:ASP:HB3	2:C:864:TYR:CE2	2.57	0.40
2:C:925:VAL:HG23	2:C:928:TYR:CD2	2.56	0.40
2:C:943:LYS:HB3	2:C:947:VAL:HG21	2.02	0.40
2:C:955:ILE:HD13	2:C:974:LEU:HD13	2.03	0.40
4:A:521:PRO:HA	4:A:544:ILE:HB	2.02	0.40
2:C:514:ALA:O	2:C:518:GLN:HG3	2.21	0.40
2:C:583:ILE:HD13	2:C:627:THR:HG22	2.02	0.40
2:C:772:ILE:HG23	2:C:775:ARG:HH21	1.86	0.40
2:C:849:ILE:O	2:C:853:ILE:HG12	2.21	0.40
2:C:1055:TRP:CE3	2:C:1055:TRP:HA	2.56	0.40
3:D:49:CYS:HB3	3:D:87:LYS:HD3	2.02	0.40
4:A:618:SER:CB	4:A:628:LEU:HD21	2.51	0.40
2:C:766:THR:HA	2:C:769:VAL:HG12	2.03	0.40
2:C:783:GLU:OE2	2:C:786:LYS:HE3	2.21	0.40
4:A:34:ARG:H	4:A:34:ARG:HG2	1.75	0.40
4:A:492:GLU:N	4:A:492:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	76/86 (88%)	75 (99%)	1 (1%)	0	100	100
2	C	813/872 (93%)	784 (96%)	29 (4%)	0	100	100
3	D	91/110 (83%)	86 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	1165/1250 (93%)	1088 (93%)	76 (6%)	1 (0%)	48 71
5	E	474/958 (50%)	459 (97%)	12 (2%)	3 (1%)	22 43
All	All	2619/3276 (80%)	2492 (95%)	123 (5%)	4 (0%)	45 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	301	SER
5	E	595	LYS
5	E	275	GLN
4	A	234	PHE

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	B	69/77 (90%)	65 (94%)	4 (6%)	17 36
2	C	701/753 (93%)	666 (95%)	35 (5%)	20 43
3	D	80/95 (84%)	77 (96%)	3 (4%)	28 54
4	A	1020/1071 (95%)	940 (92%)	80 (8%)	10 22
5	E	51/787 (6%)	39 (76%)	12 (24%)	0 1
All	All	1921/2783 (69%)	1787 (93%)	134 (7%)	15 27

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	ILE
1	B	21	THR
1	B	32	LEU
1	B	50	LEU
2	C	500	LEU
2	C	560	LEU
2	C	576	VAL

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Mol	Chain	Res	Type
2	C	582	LEU
2	C	617	ILE
2	C	618	ASP
2	C	621	ASP
2	C	635	VAL
2	C	654	SER
2	C	655	LYS
2	C	683	LEU
2	C	700	LYS
2	C	722	GLU
2	C	754	ILE
2	C	756	LEU
2	C	760	GLU
2	C	779	SER
2	C	792	VAL
2	C	828	ARG
2	C	857	LEU
2	C	870	GLU
2	C	902	GLU
2	C	905	THR
2	C	906	GLU
2	C	931	GLN
2	C	949	GLN
2	C	956	SER
2	C	993	ILE
2	C	1048	GLU
2	C	1070	LYS
2	C	1092	ASP
2	C	1100	ASN
2	C	1101	LEU
2	C	1123	CYS
2	C	1271	SER
3	D	26	CYS
3	D	35	SER
3	D	97	ASP
4	A	8	LEU
4	A	12	THR
4	A	64	SER
4	A	152	LEU
4	A	156	SER
4	A	171	VAL
4	A	229	GLU

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Mol	Chain	Res	Type
4	A	252	SER
4	A	278	LEU
4	A	295	THR
4	A	296	LYS
4	A	297	SER
4	A	326	ARG
4	A	351	SER
4	A	364	LEU
4	A	367	ASP
4	A	374	SER
4	A	390	ARG
4	A	435	LEU
4	A	450	SER
4	A	452	LEU
4	A	465	HIS
4	A	469	GLU
4	A	477	SER
4	A	491	VAL
4	A	503	THR
4	A	516	LEU
4	A	520	TYR
4	A	530	ASP
4	A	538	THR
4	A	541	LYS
4	A	543	THR
4	A	546	LYS
4	A	547	CYS
4	A	576	GLU
4	A	578	THR
4	A	587	VAL
4	A	588	VAL
4	A	591	SER
4	A	592	LEU
4	A	599	GLU
4	A	618	SER
4	A	640	LEU
4	A	641	CYS
4	A	665	LEU
4	A	677	THR
4	A	685	ASP
4	A	689	THR
4	A	713	LEU

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Mol	Chain	Res	Type
4	A	734	LEU
4	A	743	SER
4	A	750	CYS
4	A	761	THR
4	A	767	LEU
4	A	770	LEU
4	A	775	ASN
4	A	776	GLN
4	A	805	ASN
4	A	824	VAL
4	A	864	SER
4	A	865	VAL
4	A	873	GLN
4	A	890	SER
4	A	897	SER
4	A	899	THR
4	A	920	VAL
4	A	959	VAL
4	A	984	LYS
4	A	986	ILE
4	A	994	GLN
4	A	995	THR
4	A	1020	GLN
4	A	1066	VAL
4	A	1103	SER
4	A	1133	THR
4	A	1137	ASP
4	A	1151	GLU
4	A	1170	VAL
4	A	1184	SER
4	A	1217	PHE
5	E	68	ASN
5	E	70	ASP
5	E	79	GLU
5	E	116	LEU
5	E	120	MET
5	E	126	GLN
5	E	133	ARG
5	E	145	LYS
5	E	148	ARG
5	E	149	ASP
5	E	155	ASP

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Mol	Chain	Res	Type
5	E	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	B	35	GLN
2	C	599	ASN
2	C	662	HIS
2	C	737	GLN
2	C	738	HIS
2	C	794	GLN
2	C	829	ASN
2	C	863	GLN
2	C	891	GLN
2	C	903	GLN
2	C	941	ASN
2	C	1002	ASN
2	C	1028	HIS
2	C	1104	GLN
2	C	1108	ASN
2	C	1134	ASN
2	C	1184	HIS
2	C	1228	GLN
2	C	1256	HIS
2	C	1289	ASN
2	C	1293	ASN
3	D	78	GLN
4	A	138	GLN
4	A	218	ASN
4	A	219	HIS
4	A	254	ASN
4	A	264	GLN
4	A	307	GLN
4	A	417	ASN
4	A	465	HIS
4	A	551	GLN
4	A	553	GLN
4	A	749	GLN
4	A	776	GLN
4	A	796	ASN
4	A	804	HIS

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Mol	Chain	Res	Type
4	A	805	ASN
4	A	870	ASN
4	A	873	GLN
4	A	875	ASN
4	A	916	ASN
4	A	1017	ASN
4	A	1052	ASN
4	A	1094	ASN
4	A	1181	GLN
5	E	68	ASN
5	E	167	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

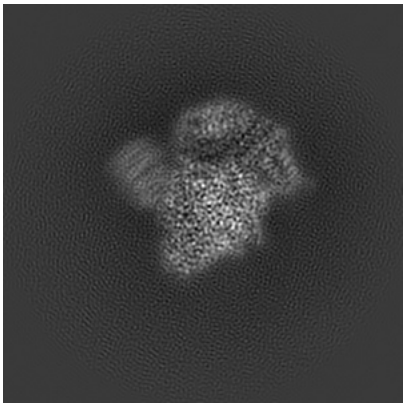
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31330. These allow visual inspection of the internal detail of the map and identification of artifacts.

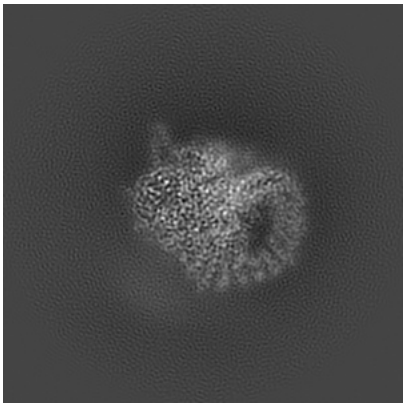
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

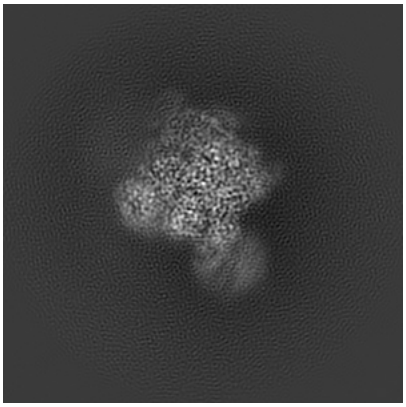
6.1.1 Primary map



X



Y

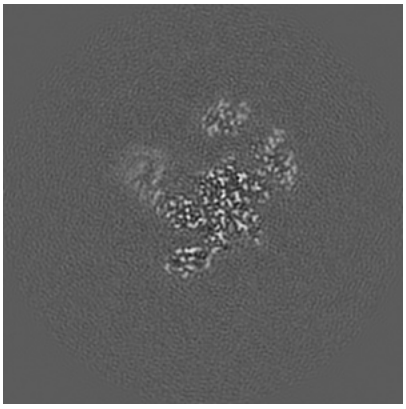


Z

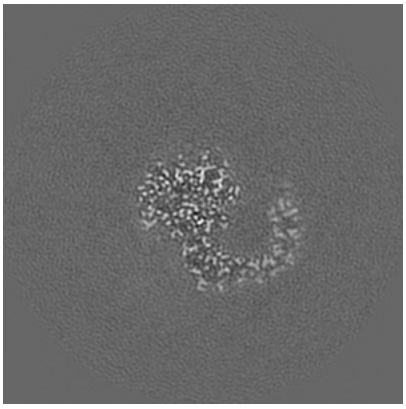
The images above show the map projected in three orthogonal directions.

6.2 Central slices

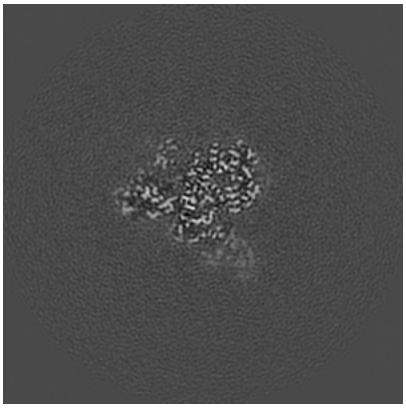
6.2.1 Primary map



X Index: 120



Y Index: 120

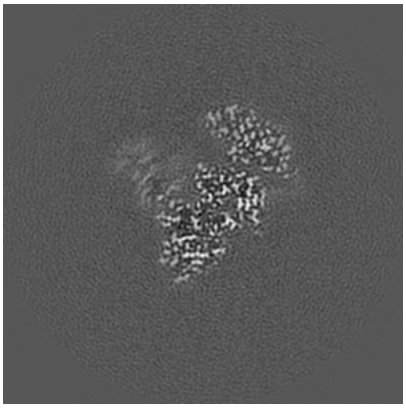


Z Index: 120

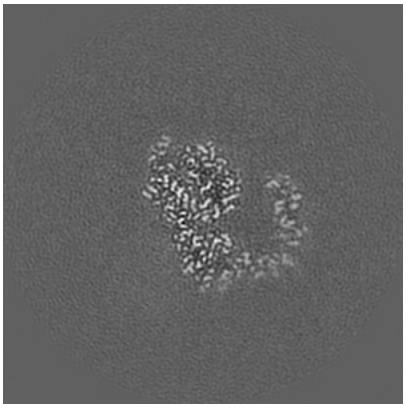
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

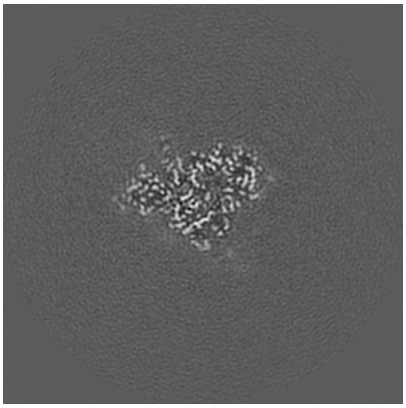
6.3.1 Primary map



X Index: 127



Y Index: 127

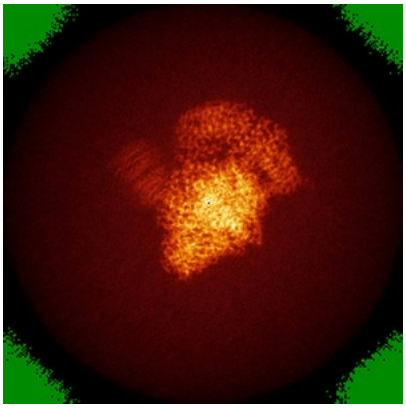


Z Index: 116

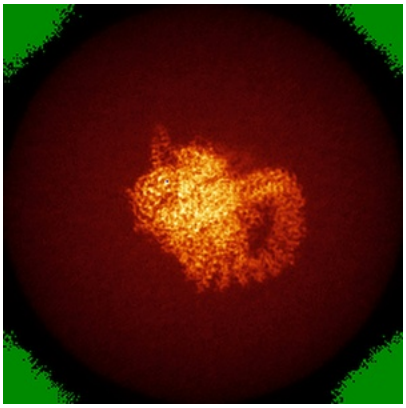
The images above show the largest variance slices of the map in three orthogonal directions.

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

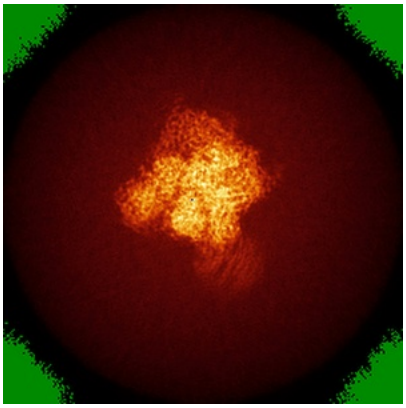
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

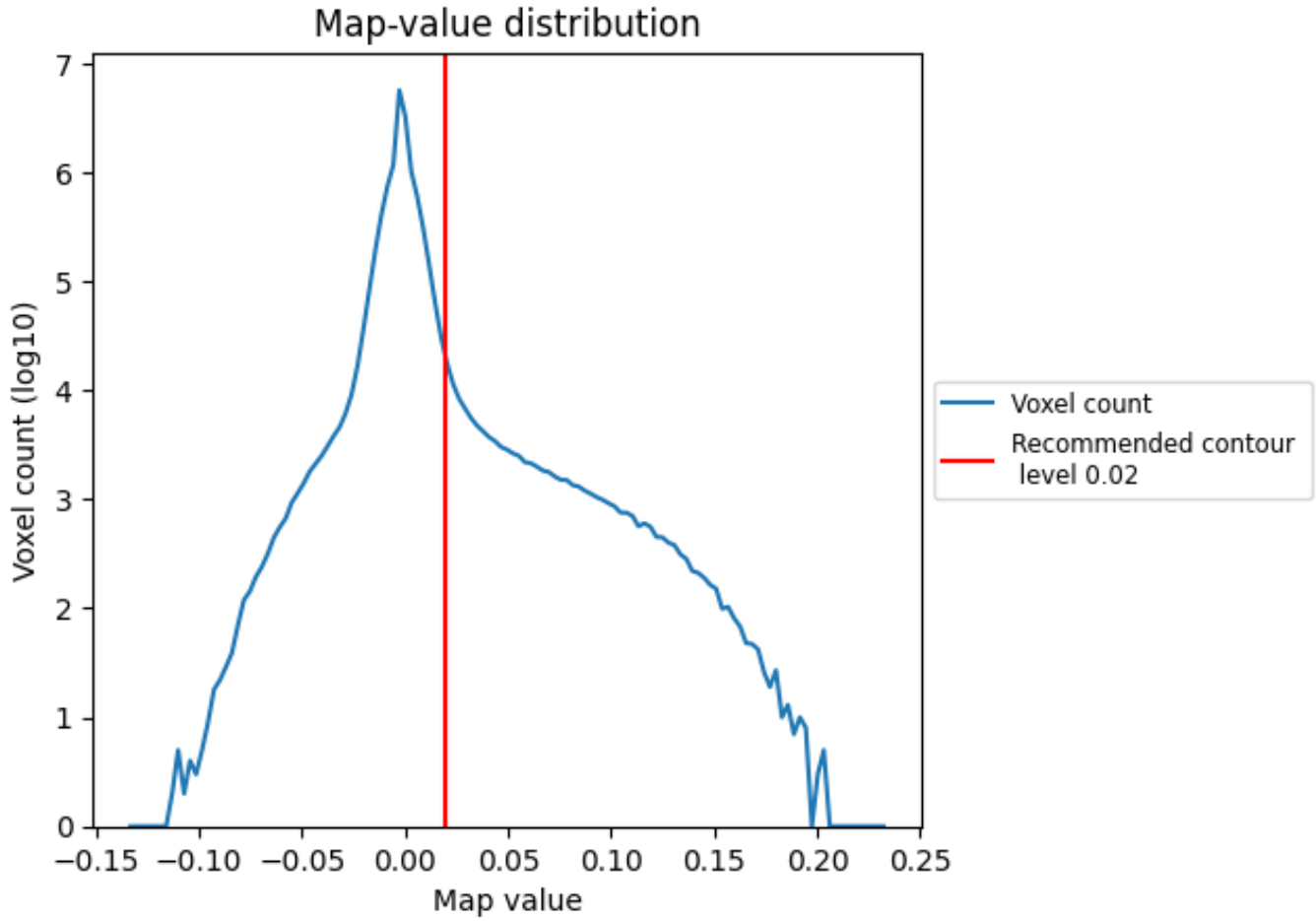
6.6 Mask visualisation (i)

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

7 Map analysis

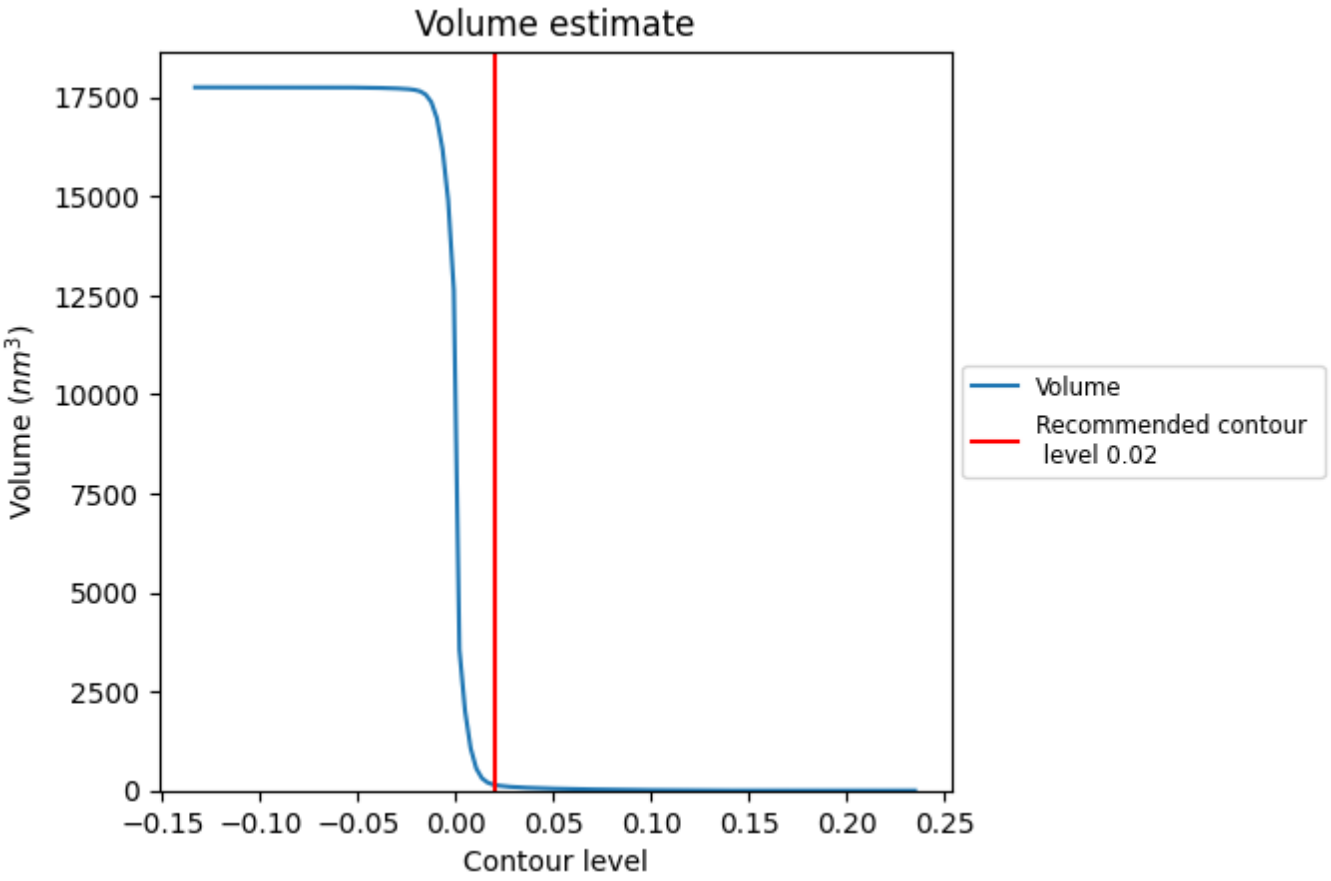
This section contains the results of statistical analysis of the map.

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.

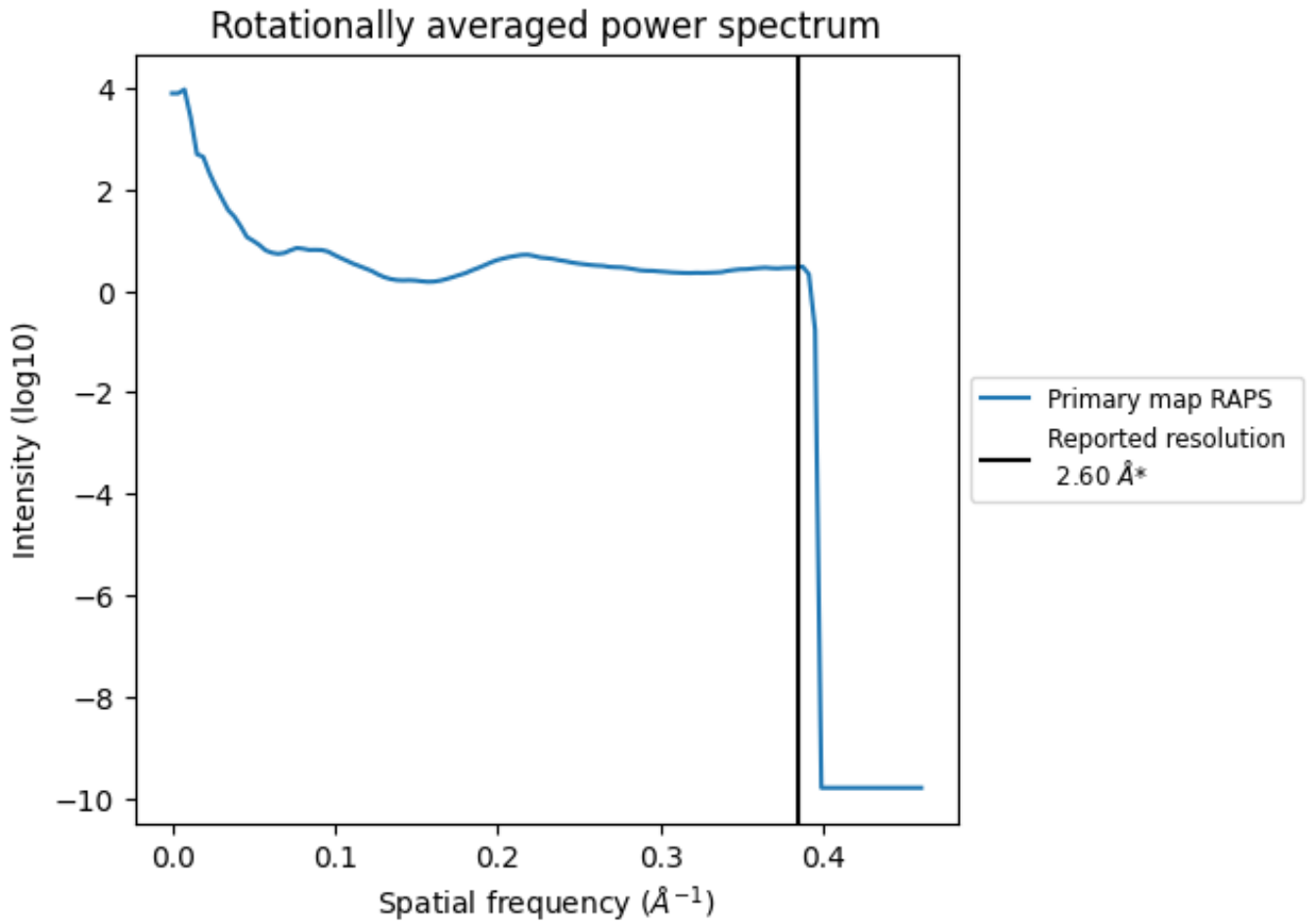
7.2 Volume estimate



The volume at the recommended contour level is 145 nm^3; this corresponds to an approximate mass of 131 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 0.385 Å^{-1}

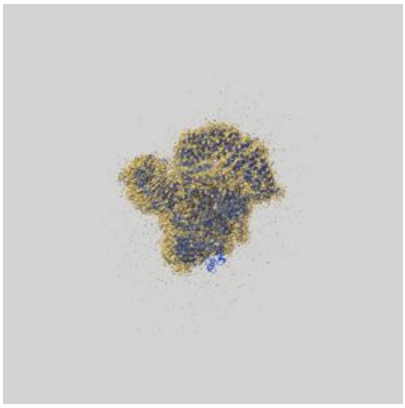
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

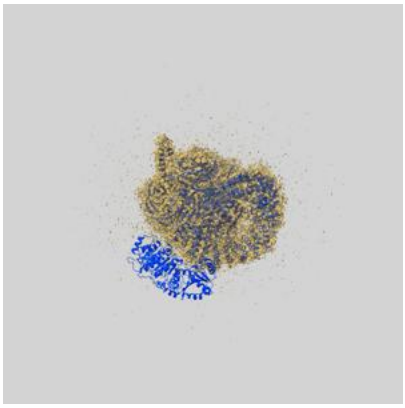
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31330 and PDB model 7EVN. Per-residue inclusion information can be found in section 3 on page 6.

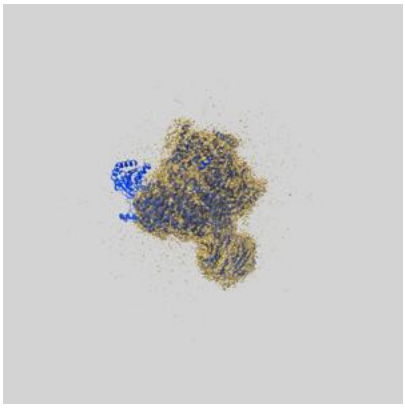
9.1 Map-model overlay



X



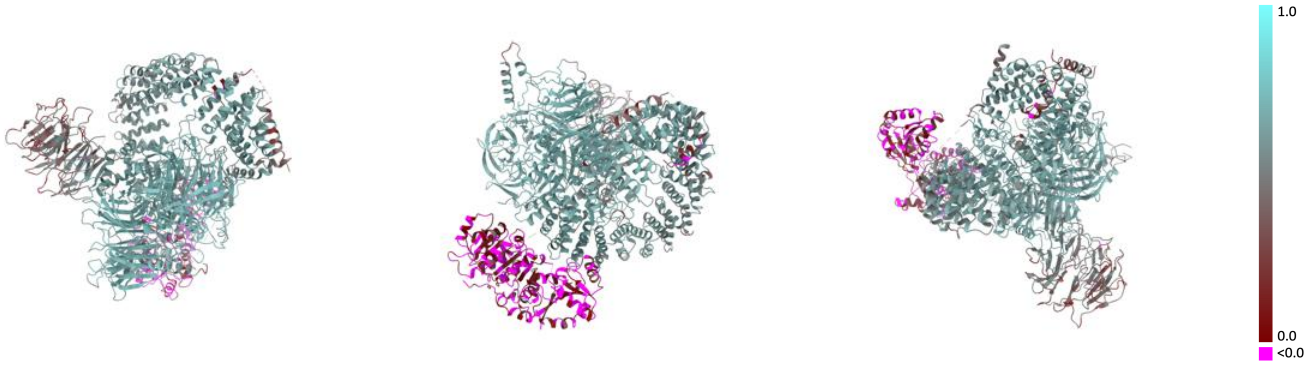
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

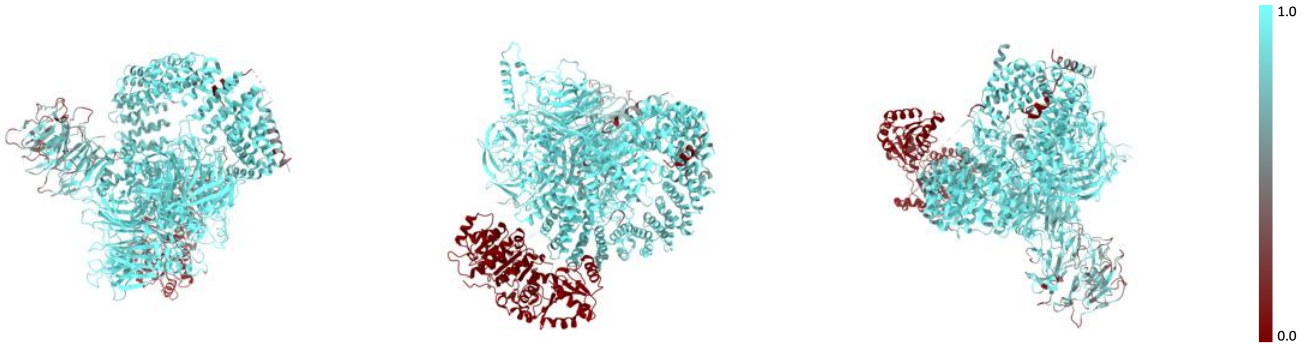
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

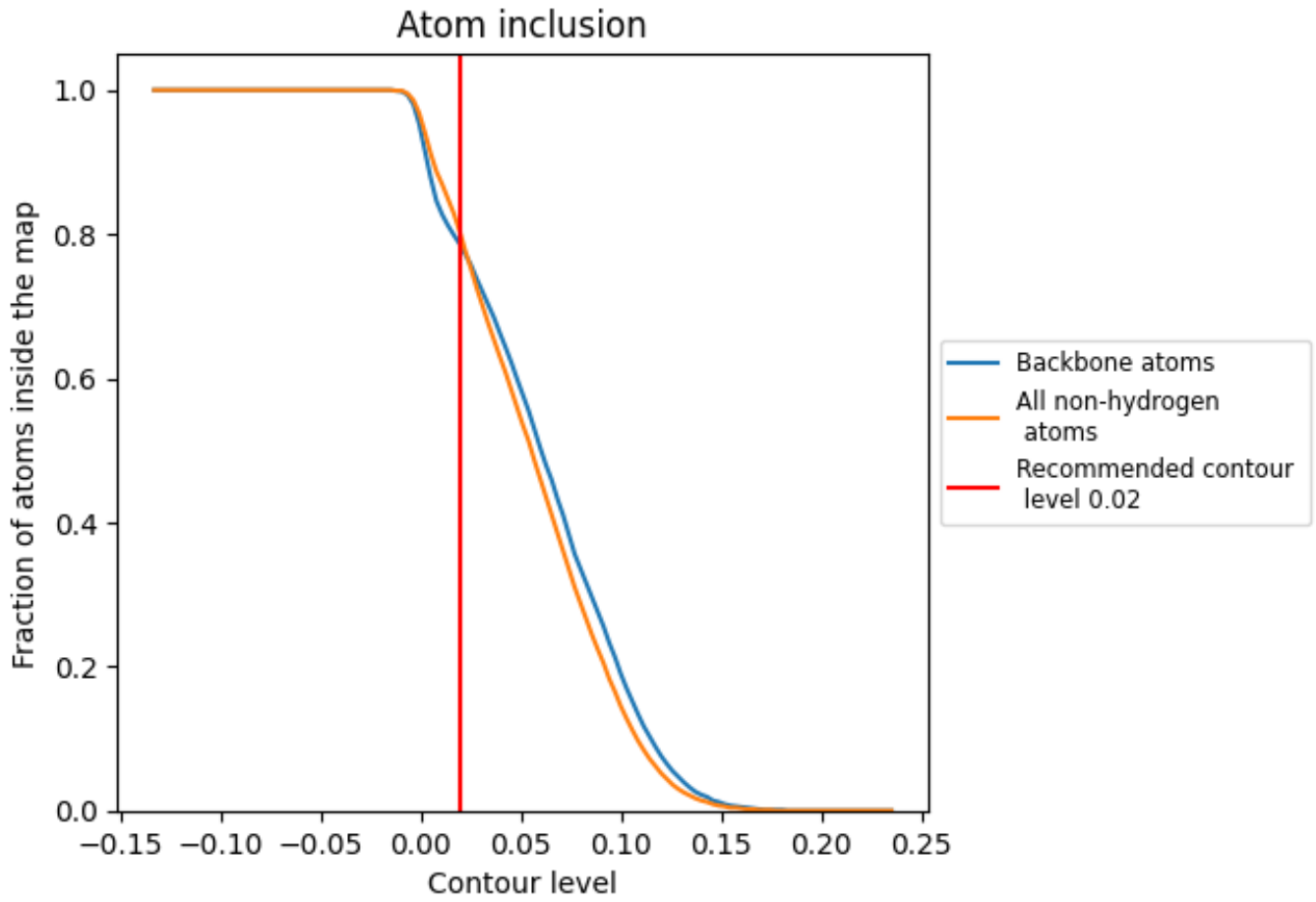
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 80% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.5400
A	0.8870	0.6040
B	0.9840	0.6760
C	0.9300	0.6110
D	0.9240	0.6470
E	0.0950	0.0770