Full wwPDB EM Validation Report

Mar 27, 2026 – 05:30 AM UTC

PDB ID	:	6NE3 / pdb_00006ne3
EMDB ID	:	EMD-9356
Title	:	Cryo-EM structure of singly-bound SNF2h-nucleosome complex with SNF2h bound at SHL-2
Authors	:	Armache, J.-P.; Gamarra, N.; Johnson, S.L.; Leonard, J.D.; Wu, S.; Narlikar, G.N.; Cheng, Y.
Deposited on	:	2018-12-16
Resolution	:	3.90 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

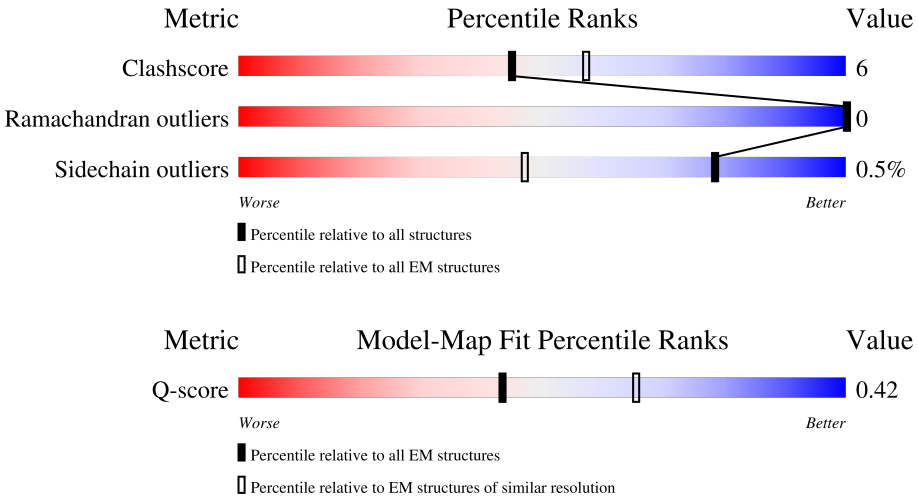
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	136	61% 12% 27%
1	E	136	54% 18% 27%
2	B	103	76% 10% 15%
2	F	103	69% 11% 19%

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Mol	Chain	Length	Quality of chain
3	C	130	78% 9% 12%
3	G	130	68% 15% 16%
4	D	99	87% 13%
5	H	93	83% 17%
6	J	156	85% 15%
7	I	156	85% 15%
8	W	467	8% 69% 29%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16336 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	99	Total	C	N	O	S	0	0
			806	509	154	140	3		
1	E	99	Total	C	N	O	S	0	0
			813	512	157	141	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	engineered mutation	UNP P84233
E	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	88	Total	C	N	O	S	0	0
			704	442	142	119	1		
2	F	83	Total	C	N	O	S	0	0
			652	412	125	114	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	114	Total	C	N	O	0	0
			867	545	169	153		
3	G	109	Total	C	N	O	0	0
			831	522	164	145		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	engineered mutation	UNP P06897
G	99	ARG	GLY	engineered mutation	UNP P06897

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	99	Total	C	N	O	S	0	0
			780	490	145	143	2		

- Molecule 5 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

- Molecule 6 is a DNA chain called DNA (156-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	156	Total	C	N	O	P	0	0
			3178	1512	573	938	155		

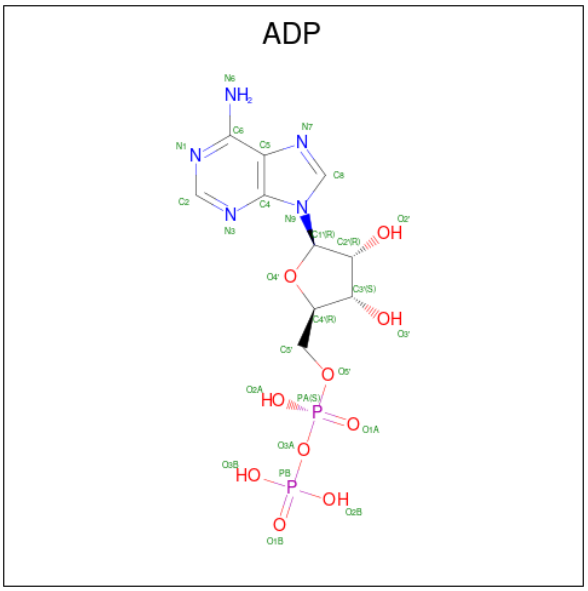
- Molecule 7 is a DNA chain called DNA (156-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	156	Total	C	N	O	P	0	0
			3215	1522	605	932	156		

- Molecule 8 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A member 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	461	Total	C	N	O	S	0	0
			3737	2388	655	670	24		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
9	W	1	Total	C	N	O	P	0
			27	10	5	10	2	

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 H3.2

Chain A:





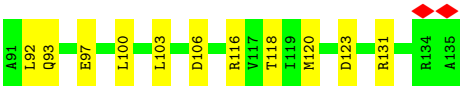


• Molecule 1: Histone H3.2

Chain E:



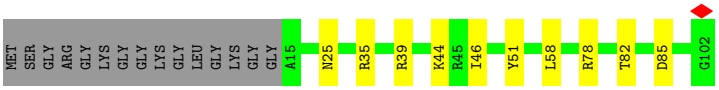




• Molecule 2: Histone H4

Chain B:

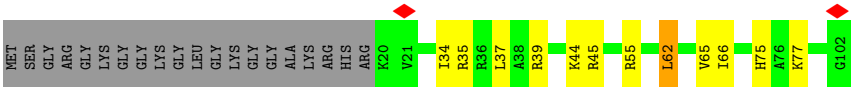




• Molecule 2: Histone H4

Chain F:

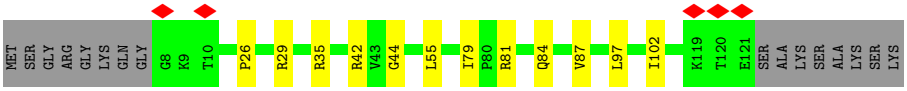




• Molecule 3: Histone H2A type 1

Chain C:

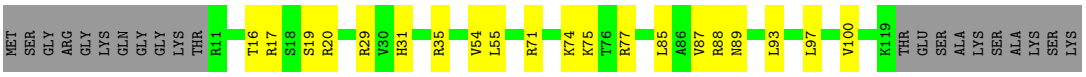




• Molecule 3: Histone H2A type 1

Chain G:

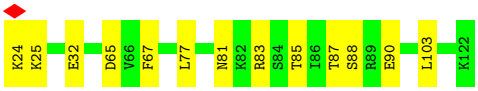




• Molecule 4: Histone H2B

Chain D:

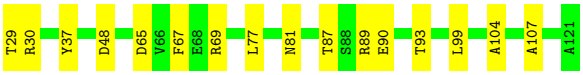




• Molecule 5: Histone H2B

Chain H:

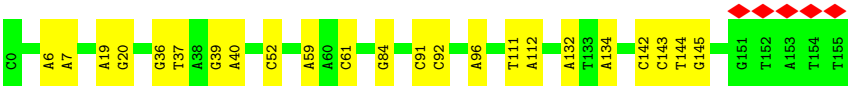




• Molecule 6: DNA (156-MER)

Chain J:

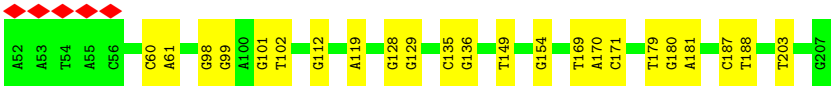




• Molecule 7: DNA (156-MER)

Chain I:

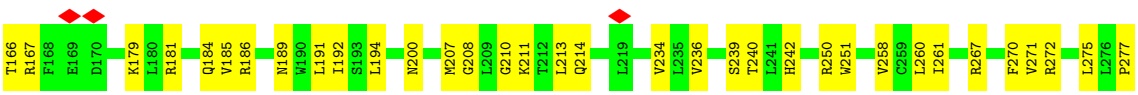


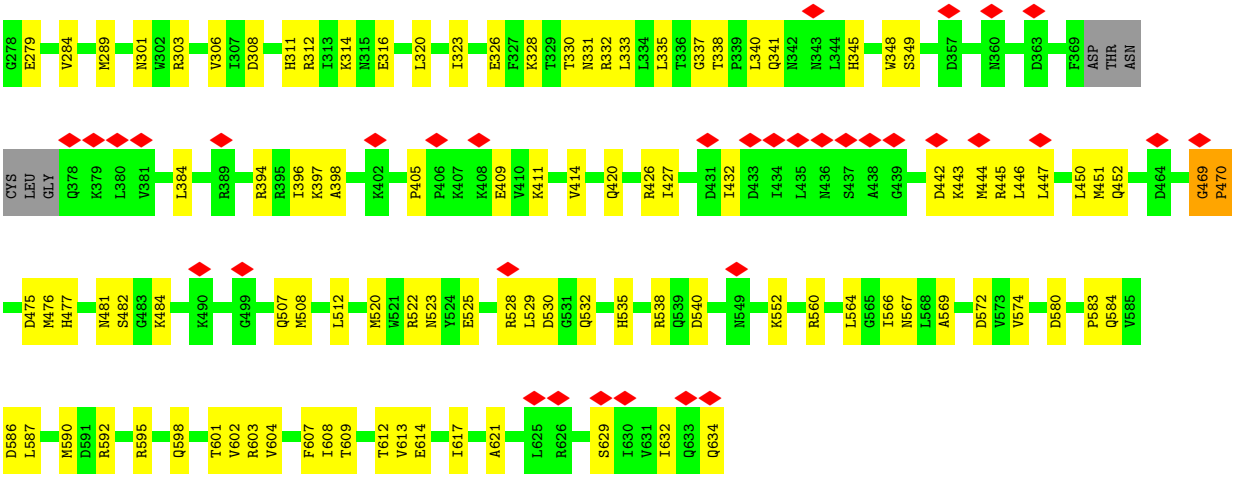


• Molecule 8: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A member 5

Chain W:






G278 E279 V284 M289 N301 W302 R303 V306 I307 D308 H311 R312 I313 K314 N315 E316 L320 I323 E326 F327 K328 T329 T330 N331 R332 L333 L334 L335 T336 G337 T338 P339 L340 Q341 N342 N343 L344 H345 W348 S349 D357 N360 D363 F369 ASP THR ASN
CYS LEU GLY Q378 K379 L380 V381 L384 R389 R394 R395 T396 K397 A398 K402 P405 P406 K407 K408 E409 V410 K411 V414 Q420 R426 I427 D431 I432 D433 I434 L435 N436 S437 A438 G439 D442 K443 M444 R445 L446 L447 L450 M451 Q452 D464 G469 P470
D475 M476 H477 N481 S482 G483 K484 K490 G499 Q507 M508 L512 M520 W521 R522 N523 Y524 E525 R528 L529 D530 G531 Q532 H535 R538 Q539 D540 N549 K552 R560 L564 G565 I566 N567 L568 A569 D572 V573 V574 D580 P583 Q584 V585
D586 L587 M590 D591 R592 R595 Q598 T601 V602 R603 V604 F607 I608 T609 T612 V613 E614 I617 A621 L625 R626 S629 I630 V631 I632 Q633 Q634

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.053	Depositor
Minimum map value	-1.175	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.245	Depositor
Map size (Å)	364.68, 364.68, 364.68	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.37	0/818	0.62	0/1100
1	E	0.40	0/825	0.61	2/1107 (0.2%)
2	B	0.39	0/712	0.62	0/951
2	F	0.42	0/659	0.62	0/883
3	C	0.37	0/877	0.54	0/1183
3	G	0.37	0/841	0.51	0/1137
4	D	0.35	0/791	0.56	0/1061
5	H	0.35	0/737	0.49	0/993
6	J	0.42	0/3560	0.59	0/5489
7	I	0.41	0/3611	0.52	0/5575
8	W	0.25	0/3818	0.55	1/5162 (0.0%)
All	All	0.37	0/17249	0.56	3/24641 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	W	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	602	VAL	N-CA-C	5.55	112.15	106.21
1	E	85	GLN	CA-C-N	5.06	131.21	121.54
1	E	85	GLN	C-N-CA	5.06	131.21	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	W	469	GLY	Peptide
8	W	470	PRO	Peptide

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	A	806	0	833	15	0
1	E	813	0	847	19	0
2	B	704	0	749	7	0
2	F	652	0	687	9	0
3	C	867	0	917	9	0
3	G	831	0	875	13	0
4	D	780	0	814	9	0
5	H	726	0	747	11	0
6	J	3178	0	1755	16	0
7	I	3215	0	1750	19	0
8	W	3737	0	3736	89	0
9	W	27	0	10	3	0
All	All	16336	0	13720	184	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 6.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:O	1:A:131:ARG:HB2	1.87	0.74
3:G:85:LEU:O	3:G:89:ASN:HB2	1.90	0.72
8:W:426:ARG:HB3	8:W:432:ILE:HD13	1.80	0.64
8:W:207:MET:O	8:W:397:LYS:NZ	2.32	0.62
8:W:260:LEU:HD11	8:W:267:ARG:HG2	1.80	0.62
1:E:116:ARG:NH1	1:E:120:MET:SD	2.73	0.62
1:E:40:ARG:NH2	6:J:84:DG:N3	2.48	0.61
1:A:69:ARG:HB3	2:B:25:ASN:HD21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:OG1	2:F:45:ARG:NH1	2.34	0.60
8:W:528:ARG:HE	8:W:530:ASP:HB3	1.66	0.60
3:C:87:VAL:HG21	3:C:97:LEU:HD22	1.84	0.60
8:W:341:GLN:HA	8:W:584:GLN:HE22	1.67	0.60
3:C:55:LEU:HD21	4:D:67:PHE:HB2	1.83	0.59
8:W:409:GLU:HA	8:W:604:VAL:HB	1.85	0.59
8:W:529:LEU:HD11	8:W:538:ARG:HG3	1.85	0.59
8:W:442:ASP:HB3	8:W:444:MET:HE3	1.84	0.58
1:A:116:ARG:NH2	1:A:123:ASP:OD2	2.36	0.58
1:E:62:ILE:HG23	1:E:93:GLN:HE21	1.68	0.58
8:W:427:ILE:HG13	8:W:445:ARG:HE	1.69	0.58
8:W:525:GLU:HB2	8:W:552:LYS:HA	1.87	0.57
8:W:301:ASN:OD1	8:W:328:LYS:NZ	2.38	0.57
1:A:85:GLN:HE21	2:B:82:THR:HA	1.70	0.57
1:A:63:ARG:HH21	6:J:61:DC:H4’	1.70	0.57
8:W:507:GLN:NE2	8:W:580:ASP:OD2	2.37	0.57
1:A:83:ARG:HG2	8:W:447:LEU:HD21	1.87	0.57
3:G:75:LYS:NZ	6:J:134:DA:OP2	2.38	0.56
5:H:65:ASP:OD2	5:H:69:ARG:NH2	2.38	0.56
7:I:154:DG:H3’	8:W:314:LYS:HE2	1.87	0.56
1:E:116:ARG:HH12	1:E:120:MET:HB2	1.70	0.56
2:F:39:ARG:NH1	2:F:44:LYS:O	2.39	0.56
2:F:62:LEU:HA	2:F:65:VAL:HG12	1.88	0.56
4:D:77:LEU:O	4:D:81:ASN:ND2	2.39	0.55
5:H:77:LEU:O	5:H:81:ASN:ND2	2.38	0.55
1:E:42:ARG:NH2	7:I:203:DT:OP2	2.39	0.55
8:W:330:THR:OG1	8:W:331:ASN:ND2	2.39	0.55
5:H:29:THR:OG1	5:H:30:ARG:N	2.40	0.55
1:E:79:LYS:NZ	1:E:80:THR:O	2.39	0.54
1:E:66:PRO:HA	1:E:69:ARG:HE	1.72	0.54
8:W:384:LEU:HD21	8:W:634:GLN:HB3	1.90	0.54
3:C:26:PRO:HB2	3:C:29:ARG:HB3	1.89	0.54
8:W:207:MET:HE3	8:W:595:ARG:HH11	1.71	0.54
8:W:540:ASP:N	8:W:540:ASP:OD1	2.41	0.54
3:G:87:VAL:HG21	3:G:97:LEU:HD12	1.89	0.53
8:W:612:THR:HG23	8:W:614:GLU:H	1.74	0.53
8:W:629:SER:HA	8:W:632:ILE:HG22	1.89	0.53
8:W:560:ARG:O	8:W:564:LEU:HB2	2.08	0.53
8:W:566:ILE:O	8:W:592:ARG:NH1	2.41	0.53
8:W:345:HIS:HA	8:W:348:TRP:HB3	1.90	0.53
5:H:87:THR:N	5:H:90:GLU:OE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:NH1	7:I:149:DT:O3'	2.43	0.52
8:W:239:SER:OG	8:W:538:ARG:NH1	2.42	0.52
8:W:211:LYS:HB3	8:W:335:LEU:HD11	1.92	0.52
3:G:71:ARG:O	3:G:74:LYS:NZ	2.43	0.52
3:G:88:ARG:NH2	3:G:100:VAL:O	2.41	0.52
6:J:59:DA:OP1	8:W:267:ARG:NH2	2.40	0.52
8:W:242:HIS:HE1	8:W:535:HIS:HB2	1.75	0.51
8:W:530:ASP:OD2	8:W:532:GLN:NE2	2.43	0.51
2:B:35:ARG:NH2	2:B:51:TYR:OH	2.43	0.51
2:F:35:ARG:HH21	2:F:39:ARG:HH21	1.58	0.51
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.43	0.51
8:W:185:VAL:O	8:W:189:ASN:ND2	2.44	0.51
8:W:191:LEU:HA	8:W:194:LEU:HD12	1.92	0.51
8:W:340:LEU:O	8:W:584:GLN:NE2	2.43	0.51
1:E:103:LEU:HA	1:E:131:ARG:HH22	1.75	0.51
8:W:572:ASP:OD2	8:W:603:ARG:NH2	2.44	0.51
3:C:35:ARG:NH2	7:I:171:DC:OP2	2.39	0.51
8:W:444:MET:O	8:W:452:GLN:NE2	2.44	0.50
3:C:84:GLN:HB2	3:C:102:ILE:HD11	1.93	0.50
6:J:6:DA:H2"	6:J:7:DA:H2'	1.92	0.50
8:W:186:ARG:HA	8:W:189:ASN:HD22	1.75	0.50
8:W:512:LEU:HD21	8:W:528:ARG:HG3	1.94	0.50
3:G:29:ARG:NH2	5:H:37:TYR:OH	2.45	0.49
8:W:411:LYS:HE2	8:W:608:ILE:HG21	1.93	0.49
2:F:34:ILE:HD11	2:F:55:ARG:HE	1.76	0.49
8:W:271:VAL:HG23	8:W:275:LEU:HB2	1.93	0.49
1:A:119:ILE:HD11	2:B:46:ILE:HG23	1.94	0.49
4:D:32:GLU:HA	7:I:181:DA:H5"	1.95	0.49
1:A:96:SER:HB2	2:B:58:LEU:HD11	1.94	0.49
3:C:44:GLY:HA2	7:I:170:DA:H5"	1.96	0.48
8:W:210:GLY:O	8:W:214:GLN:N	2.47	0.48
8:W:405:PRO:HG2	8:W:601:THR:HA	1.95	0.48
8:W:477:HIS:O	8:W:481:ASN:ND2	2.46	0.48
5:H:48:ASP:N	5:H:48:ASP:OD1	2.45	0.48
8:W:396:ILE:HG23	8:W:398:ALA:H	1.77	0.48
8:W:614:GLU:HA	8:W:617:ILE:HD12	1.95	0.48
3:C:29:ARG:NH2	7:I:181:DA:OP1	2.47	0.48
3:C:79:ILE:HG13	3:C:81:ARG:H	1.78	0.48
8:W:277:PRO:HG2	8:W:279:GLU:HB2	1.95	0.48
8:W:476:MET:SD	8:W:522:ARG:NH2	2.73	0.48
8:W:569:ALA:O	8:W:598:GLN:NE2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:NH1	7:I:119:DA:OP1	2.47	0.47
6:J:144:DT:H1'	6:J:145:DG:H5'	1.96	0.47
8:W:306:VAL:HG22	8:W:333:LEU:HB2	1.95	0.47
8:W:312:ARG:HG2	8:W:320:LEU:HD13	1.95	0.47
3:G:77:ARG:HH21	6:J:132:DA:H4'	1.79	0.47
8:W:181:ARG:N	8:W:184:GLN:OE1	2.46	0.47
8:W:267:ARG:NH1	8:W:289:MET:SD	2.85	0.47
8:W:522:ARG:HA	8:W:522:ARG:HD3	1.68	0.47
3:C:42:ARG:HG3	4:D:85:THR:HG23	1.97	0.47
8:W:311:HIS:NE2	8:W:338:THR:O	2.49	0.46
6:J:39:DG:N2	7:I:169:DT:O2	2.48	0.46
3:G:55:LEU:HD11	5:H:67:PHE:HB2	1.96	0.46
8:W:167:ARG:HD2	8:W:192:ILE:HG21	1.96	0.46
8:W:213:LEU:HD11	8:W:251:TRP:CD2	2.51	0.46
3:G:87:VAL:HG23	3:G:93:LEU:HB3	1.98	0.46
8:W:520:MET:O	8:W:523:ASN:ND2	2.48	0.46
7:I:179:DT:H2"	7:I:180:DG:C8	2.51	0.46
8:W:450:LEU:HB2	8:W:613:VAL:HG11	1.98	0.46
2:B:39:ARG:NH1	2:B:44:LYS:O	2.46	0.45
8:W:451:MET:HE2	8:W:451:MET:HB2	1.86	0.45
1:E:97:GLU:HG2	2:F:37:LEU:HD21	1.97	0.45
1:E:64:LYS:HD2	1:E:90:MET:HE1	1.97	0.45
2:F:75:HIS:HB2	5:H:93:THR:HG21	1.98	0.45
8:W:414:VAL:HG11	8:W:484:LYS:HA	1.98	0.45
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.50	0.45
1:E:120:MET:N	1:E:123:ASP:OD2	2.49	0.45
2:F:77:LYS:HG3	5:H:89:ARG:HH22	1.82	0.45
6:J:36:DG:H2"	6:J:37:DT:H5"	1.99	0.45
2:F:66:ILE:HD13	2:F:66:ILE:HA	1.85	0.45
1:E:116:ARG:NH2	1:E:123:ASP:OD1	2.50	0.45
8:W:420:GLN:HE21	8:W:482:SER:HB3	1.81	0.45
8:W:583:PRO:HB3	8:W:621:ALA:HB1	1.99	0.45
3:G:17:ARG:HG2	3:G:20:ARG:HH21	1.82	0.44
3:G:54:VAL:HG13	5:H:107:ALA:HB1	2.00	0.44
1:A:68:GLN:HE21	1:A:72:ARG:HH21	1.66	0.44
8:W:303:ARG:O	8:W:330:THR:OG1	2.31	0.44
8:W:595:ARG:NH1	9:W:801:ADP:O2A	2.49	0.44
4:D:87:THR:N	4:D:90:GLU:OE1	2.39	0.43
3:G:16:THR:O	3:G:19:SER:OG	2.30	0.43
8:W:484:LYS:HE3	8:W:609:THR:HG23	1.99	0.43
8:W:567:ASN:OD1	8:W:567:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:99:LEU:HB2	5:H:104:ALA:HB2	2.00	0.43
6:J:39:DG:H1'	6:J:40:DA:C5	2.53	0.43
8:W:250:ARG:HD2	8:W:250:ARG:HA	1.88	0.43
8:W:338:THR:O	8:W:338:THR:OG1	2.31	0.43
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.87	0.43
8:W:584:GLN:HA	8:W:587:LEU:HD12	2.00	0.43
8:W:179:LYS:H	8:W:251:TRP:HZ3	1.65	0.43
8:W:469:GLY:HA2	8:W:470:PRO:HD3	1.86	0.43
3:G:31:HIS:CD2	3:G:35:ARG:HE	2.36	0.42
6:J:96:DA:N6	7:I:112:DG:O6	2.52	0.42
7:I:187:DC:H2"	7:I:188:DT:C5	2.55	0.42
1:A:89:VAL:HA	1:A:92:LEU:HD23	2.01	0.42
1:A:127:ALA:O	1:A:131:ARG:CB	2.61	0.42
6:J:111:DT:H2"	6:J:112:DA:C8	2.54	0.42
7:I:60:DC:H2"	7:I:61:DA:C8	2.55	0.42
8:W:337:GLY:O	8:W:394:ARG:NH1	2.53	0.42
8:W:166:THR:OG1	8:W:167:ARG:N	2.52	0.42
8:W:234:VAL:HB	8:W:284:VAL:HG12	2.02	0.42
6:J:91:DC:H1'	6:J:92:DC:C5	2.55	0.42
8:W:272:ARG:HD3	8:W:272:ARG:HA	1.78	0.42
8:W:316:GLU:HB3	8:W:349:SER:HB2	2.02	0.42
8:W:443:LYS:HG2	8:W:446:LEU:HD22	2.00	0.42
8:W:475:ASP:OD1	8:W:475:ASP:N	2.53	0.42
8:W:586:ASP:O	8:W:590:MET:HB2	2.20	0.42
6:J:142:DC:H2"	6:J:143:DC:H5"	2.02	0.42
8:W:211:LYS:N	9:W:801:ADP:O1A	2.52	0.42
8:W:508:MET:HE3	8:W:508:MET:HB3	1.87	0.42
8:W:427:ILE:HD11	8:W:452:GLN:HB3	2.01	0.42
7:I:98:DG:H2"	7:I:99:DG:H8	1.85	0.41
7:I:169:DT:H2'	7:I:170:DA:C8	2.54	0.41
1:E:61:LEU:N	1:E:97:GLU:OE2	2.51	0.41
6:J:52:DC:H4'	8:W:447:LEU:HB2	2.02	0.41
8:W:208:GLY:HA2	9:W:801:ADP:H5'2	2.02	0.41
1:A:72:ARG:HD3	8:W:443:LYS:HE3	2.02	0.41
8:W:236:VAL:HG12	8:W:308:ASP:HB3	2.02	0.41
6:J:19:DA:H1'	6:J:20:DG:C5	2.54	0.41
7:I:135:DC:H2"	7:I:136:DG:C8	2.56	0.41
4:D:24:LYS:HB3	4:D:25:LYS:H	1.53	0.41
8:W:320:LEU:HA	8:W:323:ILE:HG22	2.03	0.41
4:D:87:THR:OG1	4:D:88:SER:N	2.50	0.41
8:W:258:VAL:HB	8:W:270:PHE:HZ	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.87	0.41
7:I:128:DG:H2"	7:I:129:DG:C8	2.56	0.41
8:W:200:ASN:OD1	8:W:332:ARG:N	2.48	0.41
8:W:207:MET:HE3	8:W:207:MET:HB2	1.96	0.41
8:W:484:LYS:HG2	8:W:607:PHE:HB3	2.02	0.41
1:A:63:ARG:HD3	7:I:149:DT:H4'	2.02	0.41
4:D:103:LEU:HD12	4:D:103:LEU:HA	1.95	0.41
8:W:261:ILE:HD12	8:W:261:ILE:HA	1.91	0.40
1:A:80:THR:OG1	1:A:81:ASP:N	2.55	0.40
4:D:83:ARG:NH1	4:D:90:GLU:OE2	2.45	0.40
1:E:41:TYR:HE1	1:E:49:ARG:HH22	1.70	0.40
7:I:101:DG:H1'	7:I:102:DT:H5'	2.03	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	97/136 (71%)	92 (95%)	5 (5%)	0	100	100
1	E	97/136 (71%)	91 (94%)	6 (6%)	0	100	100
2	B	86/103 (84%)	80 (93%)	6 (7%)	0	100	100
2	F	81/103 (79%)	77 (95%)	4 (5%)	0	100	100
3	C	112/130 (86%)	106 (95%)	6 (5%)	0	100	100
3	G	107/130 (82%)	103 (96%)	4 (4%)	0	100	100
4	D	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
5	H	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
8	W	457/467 (98%)	413 (90%)	44 (10%)	0	100	100
All	All	1225/1397 (88%)	1140 (93%)	85 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	84/111 (76%)	84 (100%)	0	100 100
1	E	85/111 (77%)	85 (100%)	0	100 100
2	B	71/79 (90%)	71 (100%)	0	100 100
2	F	66/79 (84%)	65 (98%)	1 (2%)	57 70
3	C	87/101 (86%)	87 (100%)	0	100 100
3	G	83/101 (82%)	83 (100%)	0	100 100
4	D	84/85 (99%)	83 (99%)	1 (1%)	63 72
5	H	79/79 (100%)	79 (100%)	0	100 100
8	W	408/429 (95%)	405 (99%)	3 (1%)	76 78
All	All	1047/1175 (89%)	1042 (100%)	5 (0%)	78 82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	65	ASP
2	F	62	LEU
8	W	240	THR
8	W	326	GLU
8	W	574	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	68	GLN
1	A	85	GLN
1	A	108	ASN
2	B	25	ASN

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Mol	Chain	Res	Type
3	C	31	HIS
3	C	104	GLN
4	D	46	HIS
4	D	60	ASN
1	E	85	GLN
1	E	93	GLN
1	E	108	ASN
3	G	24	GLN
3	G	31	HIS
5	H	60	ASN
8	W	189	ASN
8	W	242	HIS
8	W	243	ASN
8	W	331	ASN
8	W	481	ASN
8	W	523	ASN
8	W	543	ASN
8	W	584	GLN
8	W	611	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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ADP	W	801	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	W	801	-	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	801	ADP	C5-C4	4.74	1.47	1.39
9	W	801	ADP	C5-C6	2.75	1.48	1.41
9	W	801	ADP	C5-N7	-2.39	1.34	1.39
9	W	801	ADP	C8-N7	2.32	1.36	1.31

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	801	ADP	C5-C4-N3	-5.82	118.70	126.72
9	W	801	ADP	N3-C4-N9	4.48	134.79	127.17
9	W	801	ADP	C4-C5-N7	-3.71	106.34	110.58
9	W	801	ADP	C2-N3-C4	3.64	120.72	111.83
9	W	801	ADP	N3-C2-N1	-3.21	123.72	128.58
9	W	801	ADP	C5-N7-C8	2.62	107.57	103.45
9	W	801	ADP	C3'-C2'-C1'	2.47	106.13	101.46
9	W	801	ADP	C4-N9-C8	2.43	108.29	105.74
9	W	801	ADP	C2'-C1'-N9	-2.31	107.57	113.30
9	W	801	ADP	C6-C5-N7	2.07	136.09	132.09
9	W	801	ADP	C2-N1-C6	2.05	122.10	118.73

There are no chirality outliers.

There are no torsion outliers.

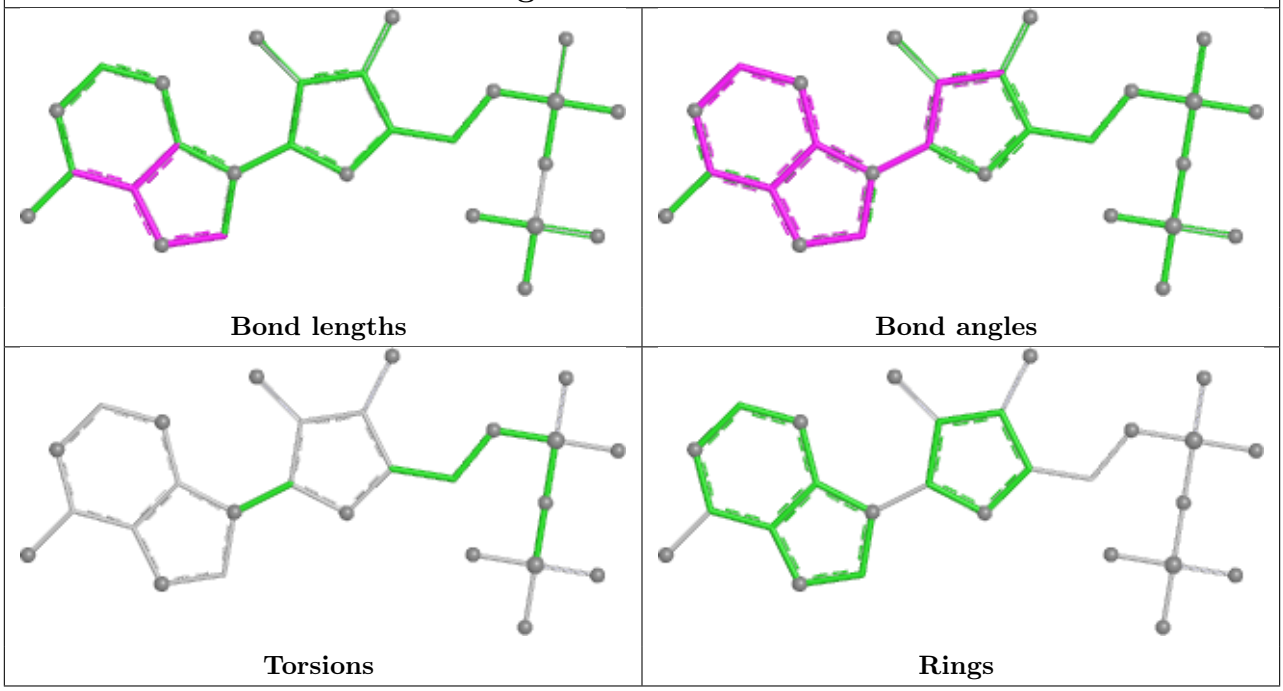
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	801	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP W 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

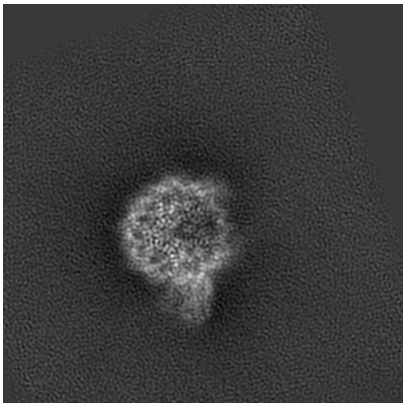
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9356. These allow visual inspection of the internal detail of the map and identification of artifacts.

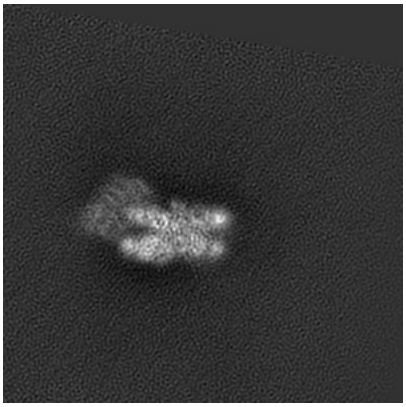
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

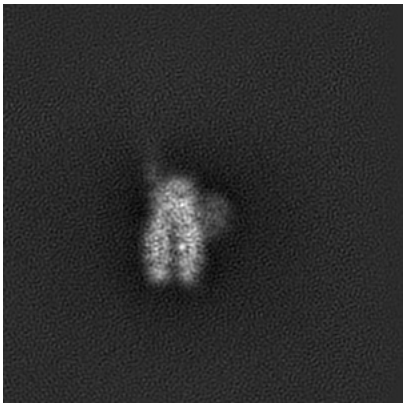
6.1.1 Primary map



X



Y

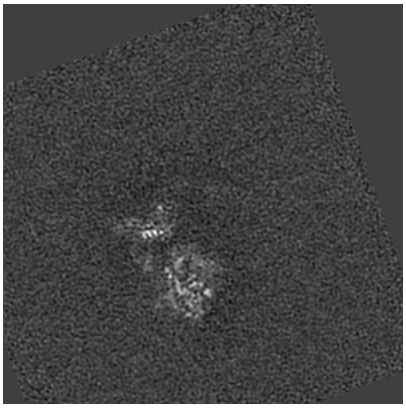


Z

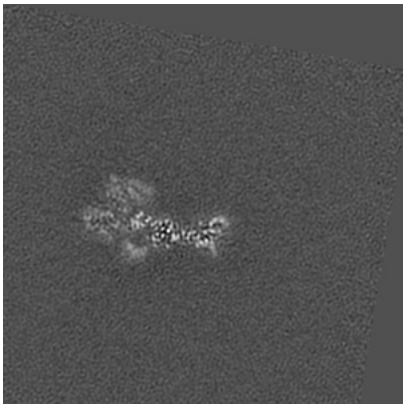
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 150



Y Index: 150

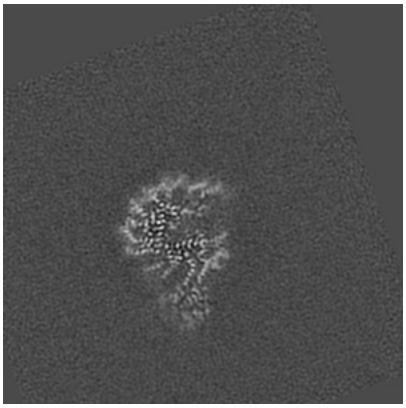


Z Index: 150

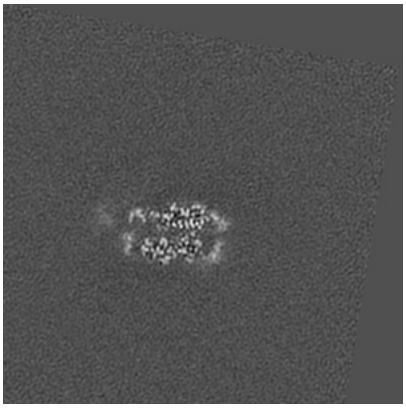
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

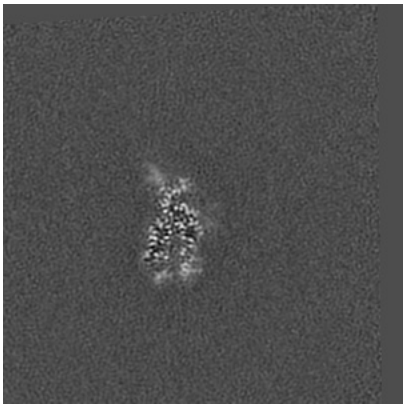
6.3.1 Primary map



X Index: 136



Y Index: 119

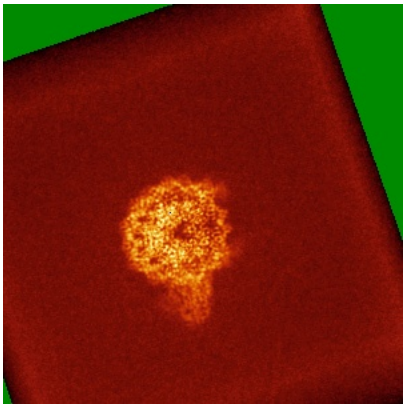


Z Index: 113

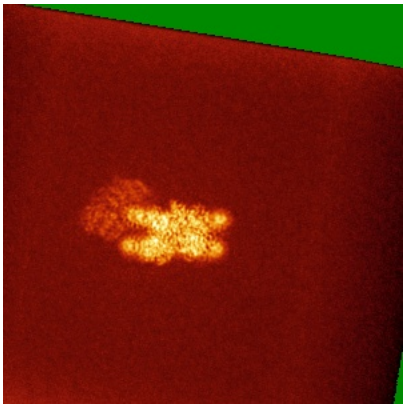
The images above show the largest variance slices of the map in three orthogonal directions.

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

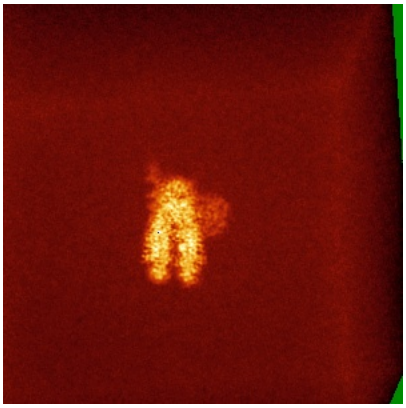
6.4.1 Primary map



X



Y

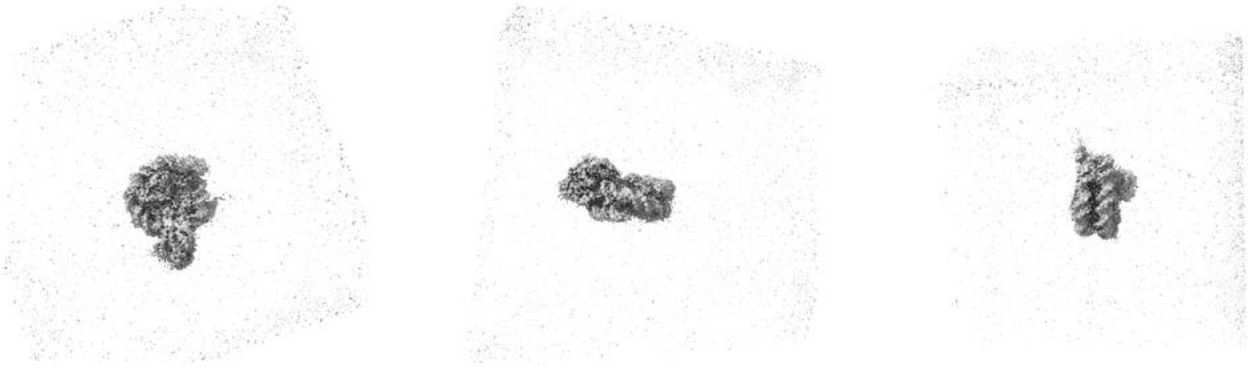


Z

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 0.245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

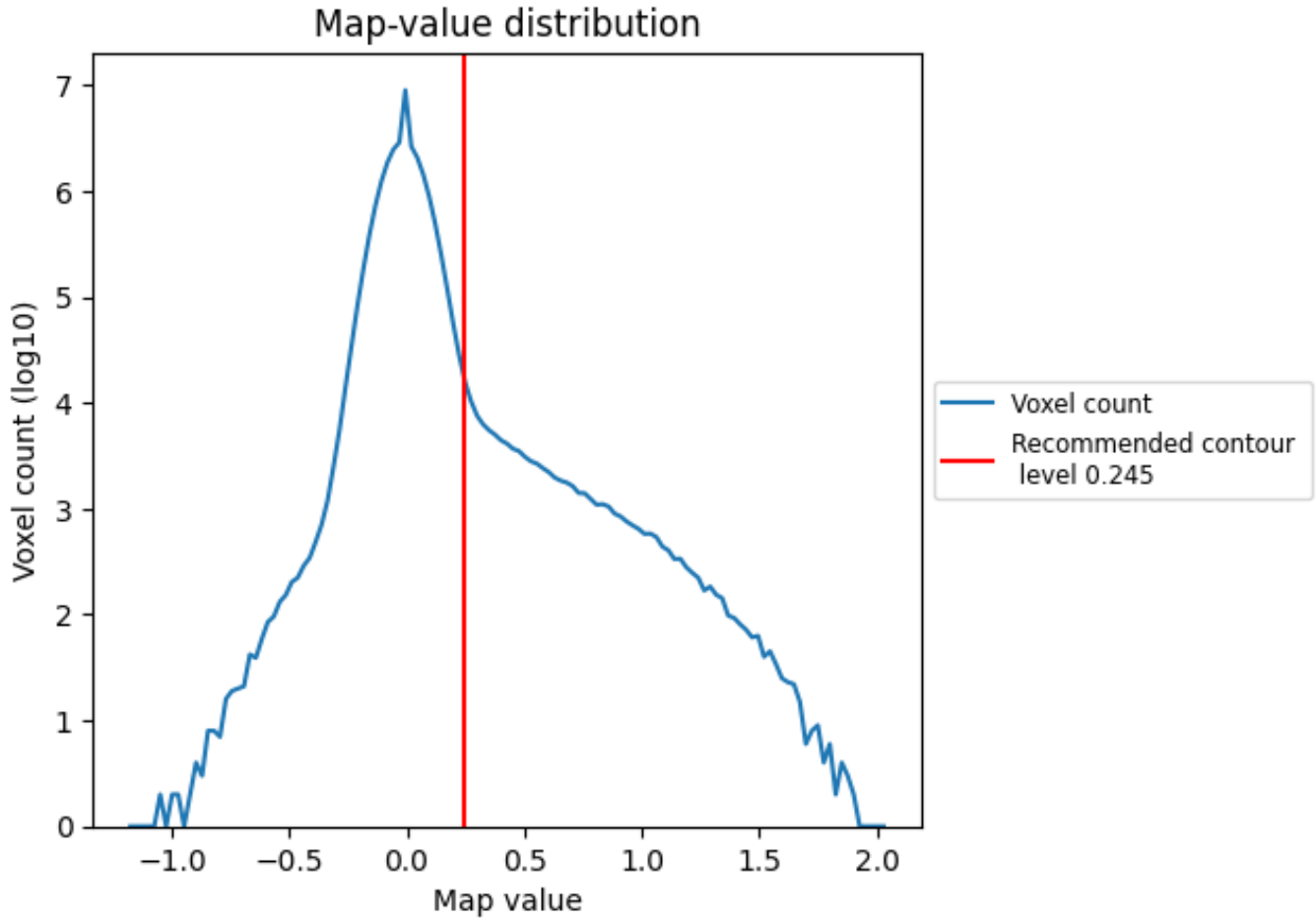
6.6 Mask visualisation (i)

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

7 Map analysis

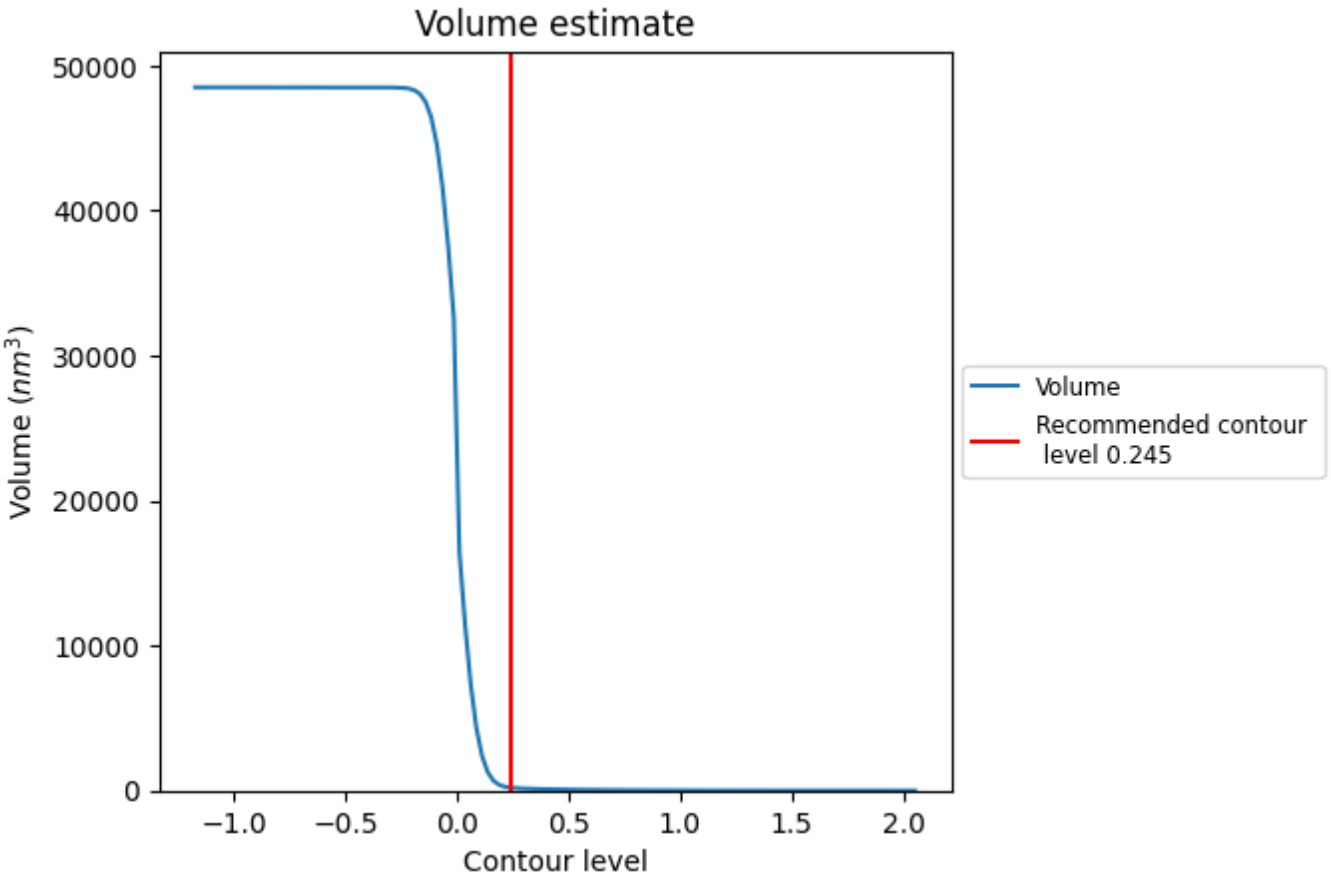
This section contains the results of statistical analysis of the map.

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.

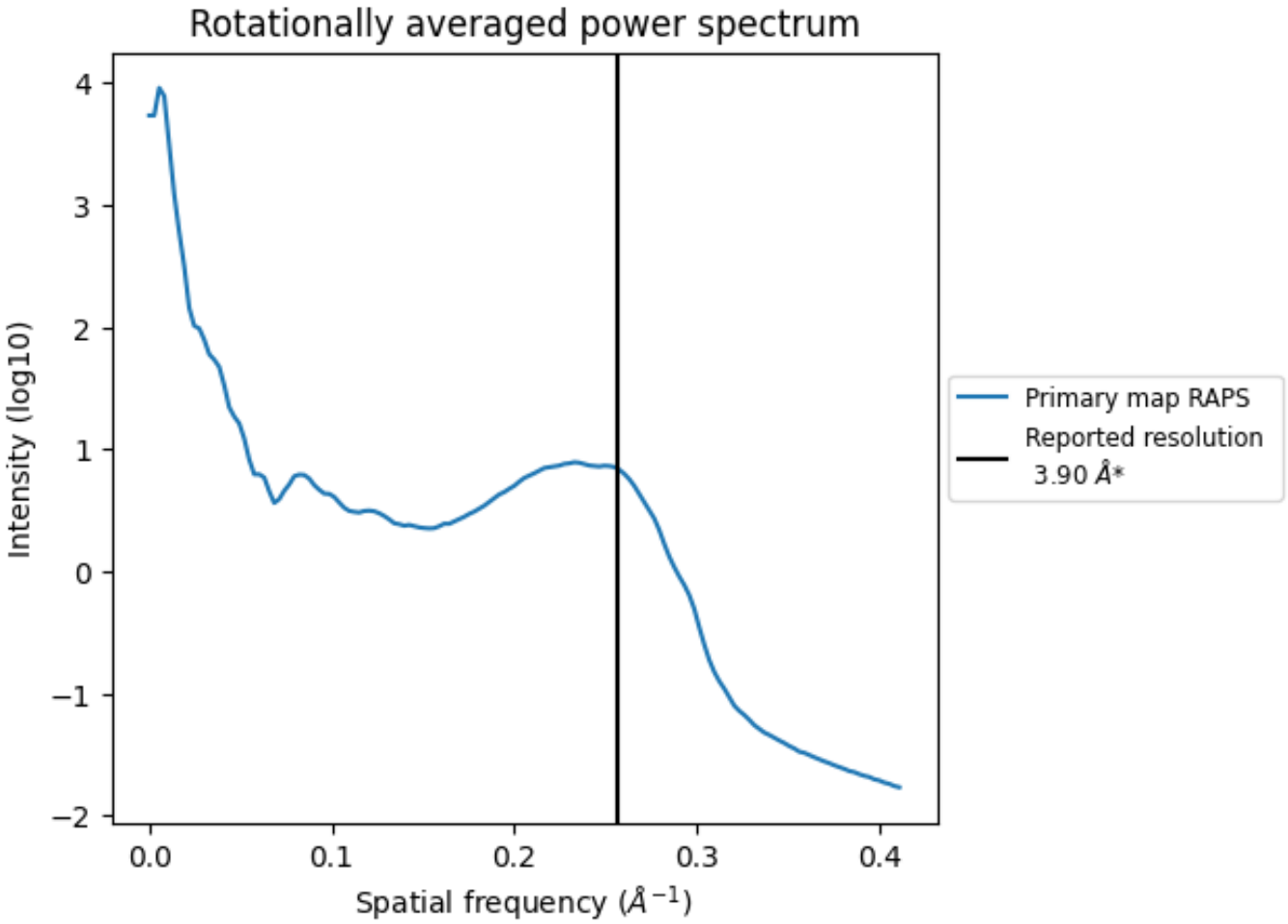
7.2 Volume estimate



The volume at the recommended contour level is 192 nm^3; this corresponds to an approximate mass of 174 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 0.256 $Å^{-1}$

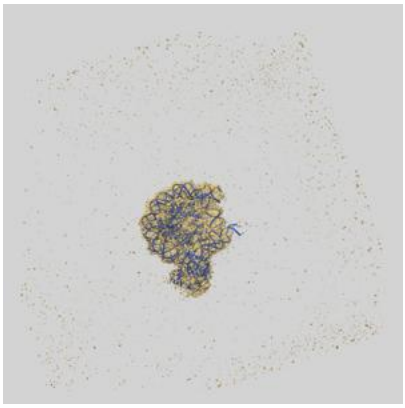
8 Fourier-Shell correlation (i)

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

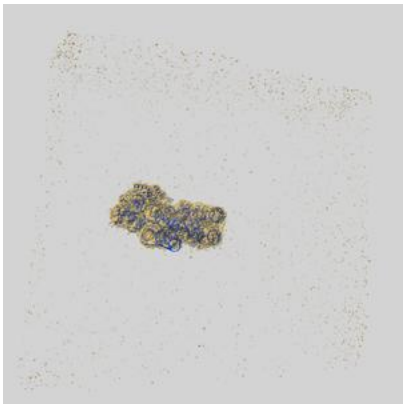
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9356 and PDB model 6NE3. Per-residue inclusion information can be found in section 3 on page 7.

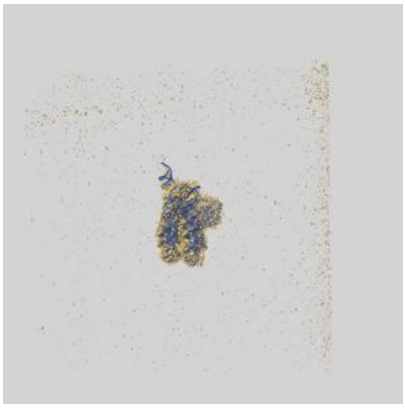
9.1 Map-model overlay



X



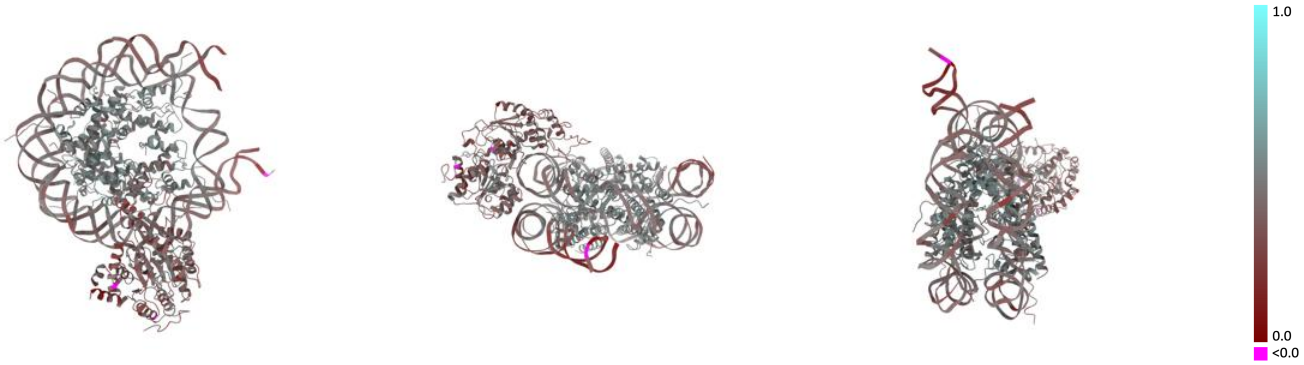
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.245 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.

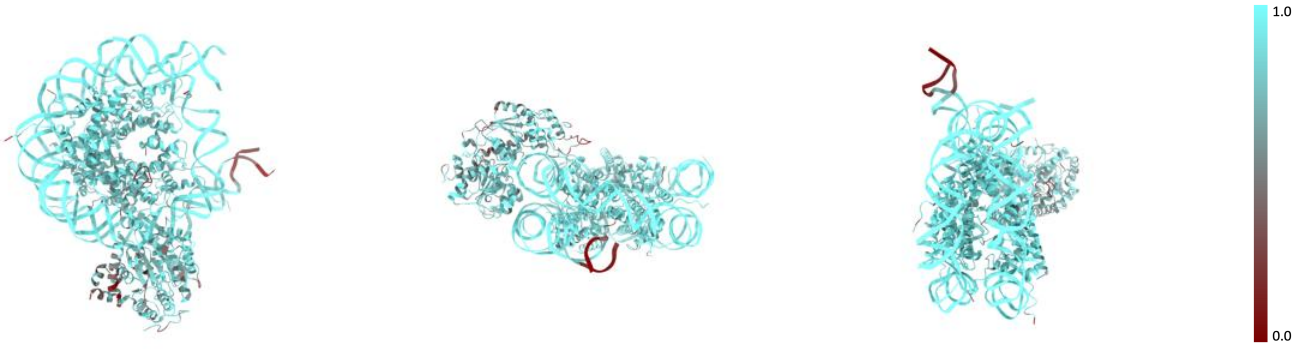
9.2 Q-score mapped to coordinate model



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.

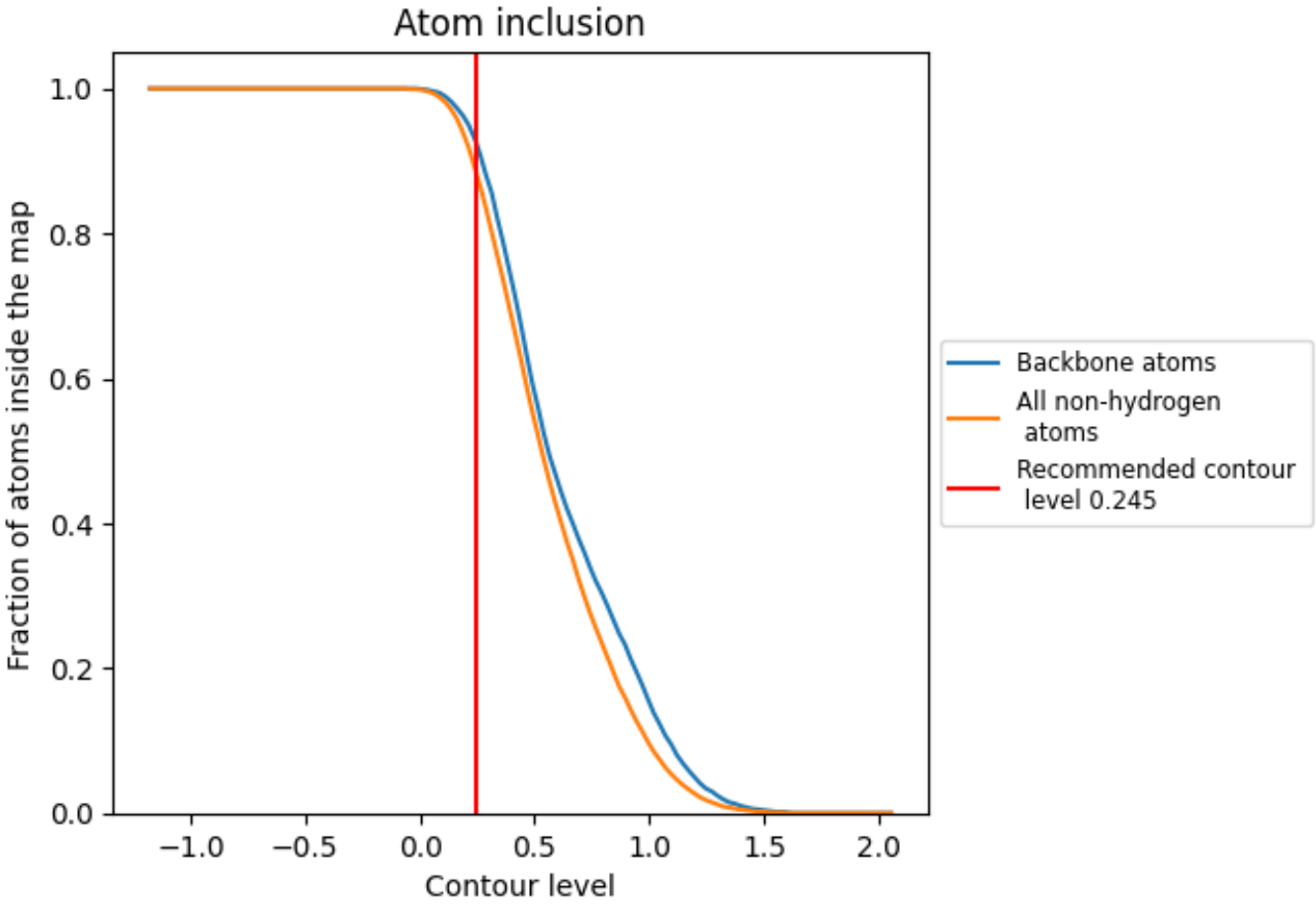
9.3 Atom inclusion mapped to coordinate model



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 (0.245).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8850	0.4200
A	0.9340	0.5030
B	0.9010	0.4900
C	0.8930	0.4940
D	0.9080	0.4800
E	0.9160	0.4990
F	0.9380	0.5070
G	0.9230	0.4960
H	0.9290	0.4890
I	0.9430	0.3810
J	0.9380	0.3870
W	0.7350	0.3580

