



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:43 AM UTC

PDB ID : 9JT2 / pdb_00009jt2
EMDB ID : EMD-61790
Title : substrate-bound NbaSPARDA complexes
Authors : Zhuang, L.
Deposited on : 2024-10-01
Resolution : 3.19 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:

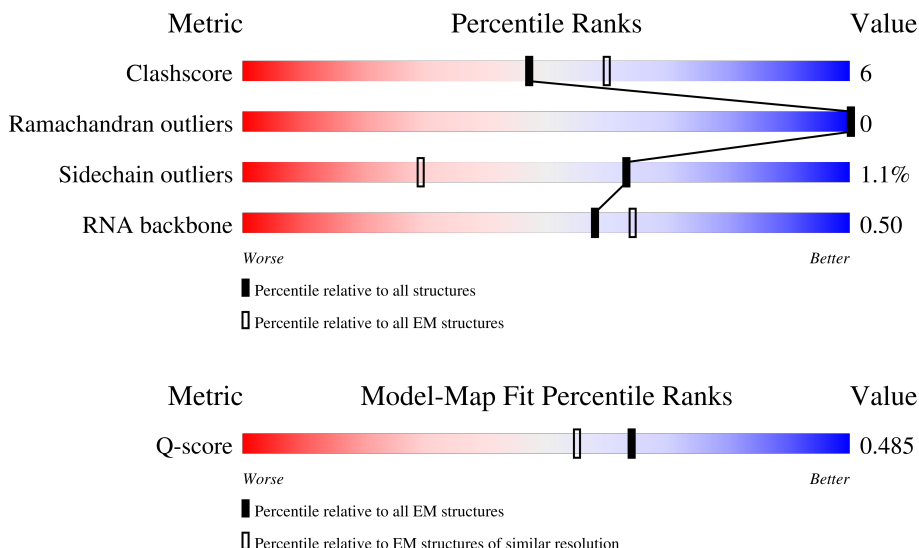
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.19 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	14455 (2.69 - 3.69)

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 $\leq 5\%$. 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	485	
1	E	485	
1	I	485	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	485	 84% 12%
2	B	442	 74% 18% 7%
2	F	442	 78% 14% 7%
2	J	442	 73% 14% 12%
2	N	442	 5% 66% 21% 12%
3	C	20	 50% 40% 5% 5%
3	G	20	 40% 55% 5%
3	K	20	 40% 50% 10%
3	O	20	 30% 50% 15% 5%
4	D	21	 81% 5% 14%
4	H	21	 5% 62% 29% 10%
4	L	21	 62% 24% 14%
4	P	21	 81% 5% 14%
5	Q	8	 75% 25%
5	R	8	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 31178 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 Ago.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	468	Total	C	N	O	S	0	0
			3715	2356	655	690	14		
1	E	468	Total	C	N	O	S	0	0
			3715	2356	655	690	14		
1	I	465	Total	C	N	O	S	0	0
			3696	2344	651	687	14		
1	M	465	Total	C	N	O	S	0	0
			3696	2344	651	687	14		

- Molecule 2 is a protein called DREN-APAZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	410	Total	C	N	O	S	0	0
			3304	2106	575	614	9		
2	F	409	Total	C	N	O	S	0	0
			3297	2101	574	613	9		
2	J	389	Total	C	N	O	S	0	0
			3149	2001	551	588	9		
2	N	389	Total	C	N	O	S	0	0
			3149	2001	551	588	9		

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*CP*GP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	19	Total	C	N	O	P	0	0
			405	181	73	132	19		
3	G	20	Total	C	N	O	P	0	0
			427	191	78	138	20		
3	K	18	Total	C	N	O	P	0	0
			385	172	71	124	18		
3	O	19	Total	C	N	O	P	0	0
			405	181	73	132	19		

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	18	Total	C	N	O	P	0	0
			370	176	67	109	18		
4	H	19	Total	C	N	O	P	0	0
			391	186	69	117	19		
4	L	18	Total	C	N	O	P	0	0
			370	176	67	109	18		
4	P	18	Total	C	N	O	P	0	0
			370	176	67	109	18		

- Molecule 5 is a DNA chain called DNA (5'-D(P*GP*AP*TP*AP*CP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	8	Total	C	N	O	P	0	0
			164	78	30	48	8		
5	R	8	Total	C	N	O	P	0	0
			164	78	30	48	8		

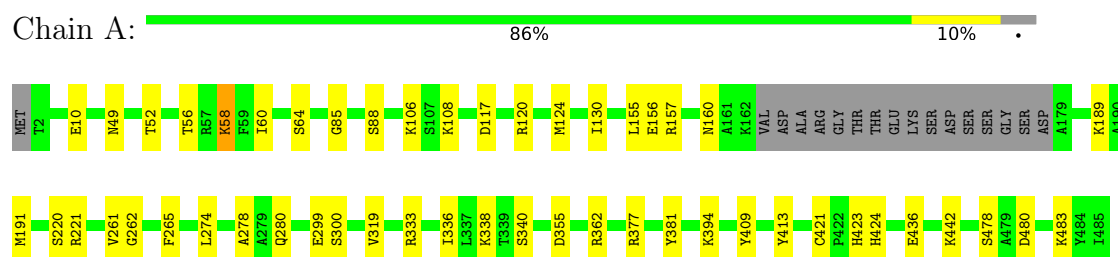
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	
6	I	1	Total	Mg	0
			1	1	
6	M	1	Total	Mg	0
			1	1	

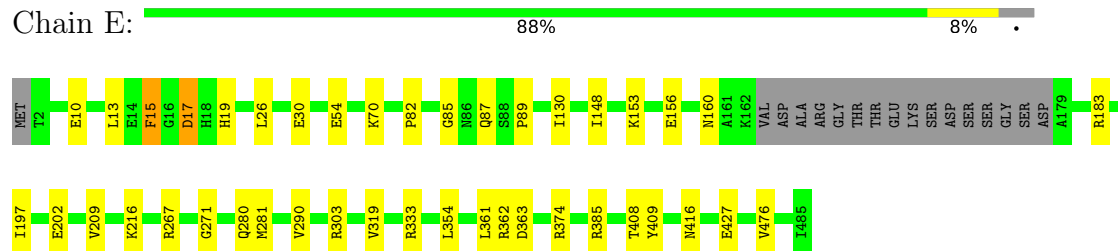
3 Residue-property plots

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.

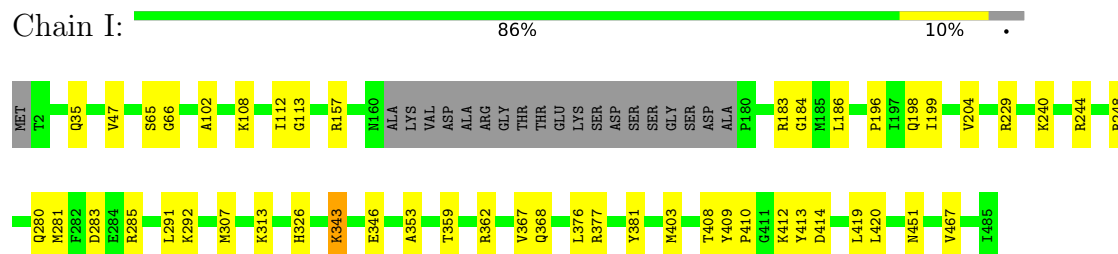
• Molecule 1: Ago



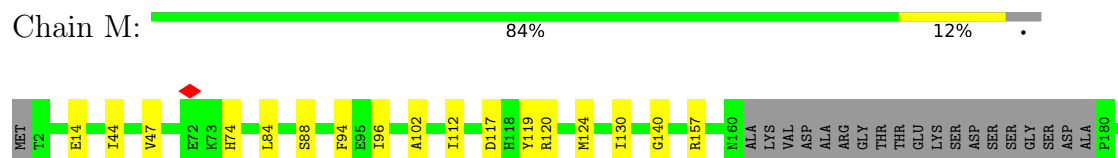
• Molecule 1: Ago

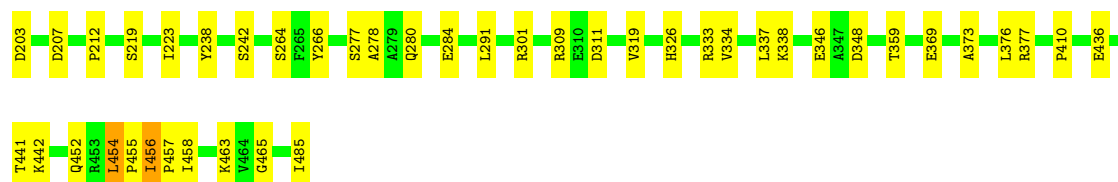


• Molecule 1: Ago



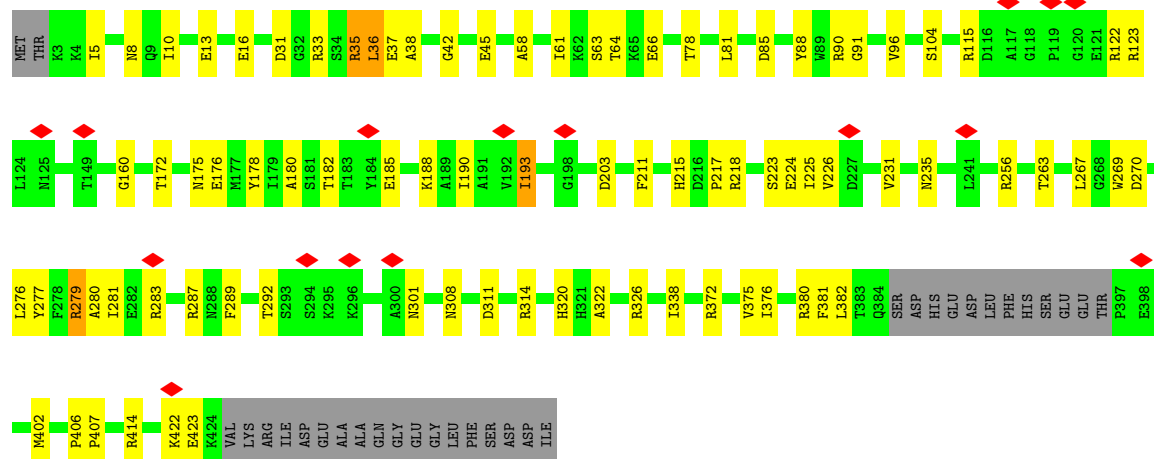
• Molecule 1: Ago





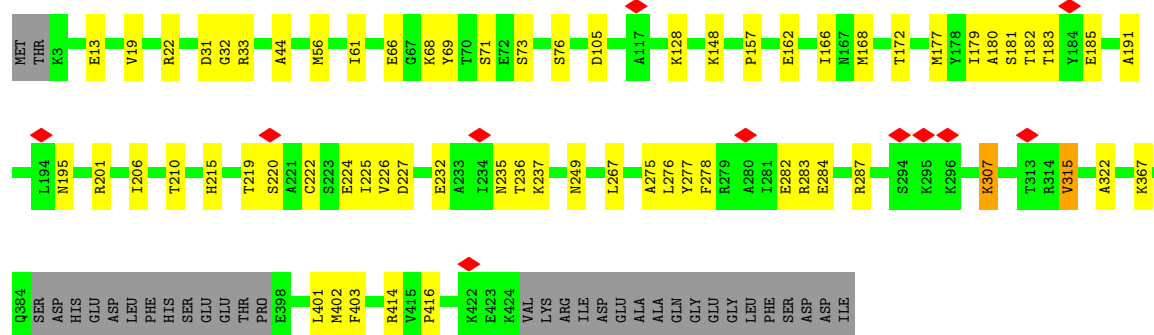
• Molecule 2: DREN-APAZ

Chain B: 74% 18% 7%



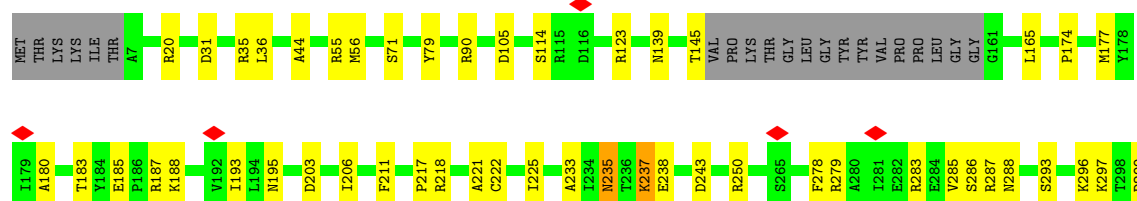
• Molecule 2: DREN-APAZ

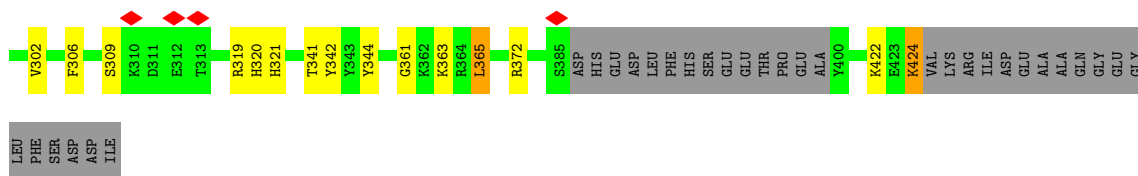
Chain F: 78% 14% 7%



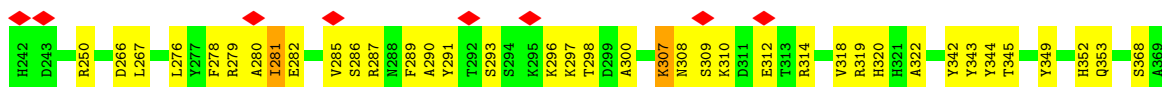
• Molecule 2: DREN-APAZ

Chain J: 73% 14% 12%





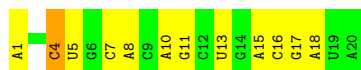
• Molecule 2: DREN-APAZ



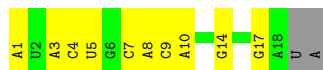
• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C P*GP*AP*UP*A)-3')



• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C P*GP*AP*UP*A)-3')

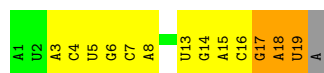


• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C P*GP*AP*UP*A)-3')




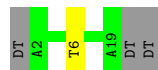
• Molecule 3: RNA (5'-R(P*AP*UP*AP*CP*UP*GP*CP*AP*CP*AP*GP*CP*UP*GP*AP*C P*GP*AP*UP*A)-3')

Chain O: 



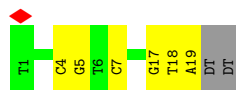
- Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3')

Chain D: 



- Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3')

Chain H: 




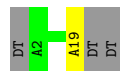
- Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3')

Chain L: 




- Molecule 4: DNA (5'-D(*TP*AP*TP*CP*GP*TP*CP*AP*GP*CP*TP*GP*TP*GP*CP*AP*GP*TP*AP*TP*T)-3')

Chain P: 



- Molecule 5: DNA (5'-D(P*GP*AP*TP*AP*CP*TP*AP*C)-3')

Chain Q: 



- Molecule 5: DNA (5'-D(P*GP*AP*TP*AP*CP*TP*AP*C)-3')

Chain R: 

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.277	Depositor
Minimum map value	-1.316	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.193	Depositor
Map size (\AA)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.15	0/3800	0.38	0/5131
1	E	0.14	0/3800	0.35	0/5131
1	I	0.14	0/3781	0.36	0/5105
1	M	0.14	0/3781	0.35	0/5105
2	B	0.16	0/3386	0.41	0/4588
2	F	0.18	0/3378	0.48	0/4577
2	J	0.18	0/3224	0.47	0/4365
2	N	0.19	0/3224	0.50	0/4365
3	C	0.15	0/452	0.33	0/700
3	G	0.11	0/477	0.25	0/739
3	K	0.12	0/430	0.30	0/666
3	O	0.15	0/452	0.37	0/700
4	D	0.22	0/414	0.45	0/637
4	H	0.18	0/437	0.42	0/671
4	L	0.21	0/414	0.41	0/637
4	P	0.20	0/414	0.41	0/637
5	Q	0.20	0/183	0.48	0/278
5	R	0.20	0/183	0.45	0/278
All	All	0.16	0/32230	0.41	0/44310

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3715	0	3695	30	0
1	E	3715	0	3695	25	0
1	I	3696	0	3673	31	0
1	M	3696	0	3673	39	0
2	B	3304	0	3243	59	0
2	F	3297	0	3235	44	0
2	J	3149	0	3073	45	0
2	N	3149	0	3073	74	0
3	C	405	0	206	6	0
3	G	427	0	217	6	0
3	K	385	0	196	6	0
3	O	405	0	206	9	0
4	D	370	0	204	1	0
4	H	391	0	216	5	0
4	L	370	0	204	8	0
4	P	370	0	204	1	0
5	Q	164	0	91	2	0
5	R	164	0	91	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	M	1	0	0	0	0
All	All	31178	0	29195	362	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 (362) 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:N:308:ASN:HB3	2:N:314:ARG:HG2	1.47	0.94
3:C:13:U:H2'	3:C:14:G:H8	1.38	0.89
2:N:79:TYR:O	2:N:123:ARG:HA	1.75	0.86
3:C:13:U:H2'	3:C:14:G:C8	2.11	0.85
2:N:161:GLY:HA3	2:N:411:LEU:O	1.79	0.82
2:B:280:ALA:HA	2:B:287:ARG:HE	1.45	0.80
1:M:291:LEU:HD21	1:M:456:ILE:HD11	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:456:ILE:HG23	1:M:457:PRO:HD3	1.68	0.76
1:M:455:PRO:HB2	1:M:457:PRO:HD2	1.73	0.70
2:F:166:ILE:HG23	2:F:168:MET:H	1.58	0.68
2:N:307:LYS:HE2	2:N:309:SER:HA	1.76	0.66
1:M:280:GLN:HG2	1:M:319:VAL:HG22	1.78	0.65
2:N:308:ASN:CB	2:N:314:ARG:HG2	2.25	0.64
2:N:180:ALA:HB3	2:N:211:PHE:HB3	1.78	0.63
2:J:187:ARG:HH21	3:K:17:G:H21	1.46	0.63
2:J:221:ALA:O	2:J:225:ILE:N	2.32	0.63
2:N:29:GLN:HB2	2:N:45:GLU:HB3	1.80	0.62
2:N:169:LEU:HD12	2:N:403:PHE:HB3	1.80	0.62
1:I:47:VAL:HG22	1:I:102:ALA:HB3	1.81	0.62
2:F:201:ARG:NH2	2:F:220:SER:OG	2.33	0.62
2:J:293:SER:HB3	2:J:296:LYS:HB2	1.82	0.60
2:F:249:ASN:HB2	4:H:7:DC:H4'	1.82	0.60
2:B:280:ALA:HB2	2:B:287:ARG:HG2	1.83	0.60
2:B:36:LEU:HD13	2:N:29:GLN:HG2	1.83	0.60
1:E:156:GLU:HA	1:E:160:ASN:HB2	1.84	0.60
2:B:31:ASP:O	2:B:42:GLY:HA3	2.02	0.59
2:B:33:ARG:NH2	2:N:45:GLU:OE1	2.35	0.59
1:E:374:ARG:NH2	1:E:416:ASN:OD1	2.36	0.59
2:F:162:GLU:HG2	2:F:414:ARG:HG3	1.84	0.59
2:J:235:ASN:CG	2:J:237:LYS:H	2.10	0.59
1:A:130:ILE:HG13	1:A:189:LYS:HB3	1.85	0.59
1:E:280:GLN:HG2	1:E:319:VAL:HG22	1.85	0.59
2:F:185:GLU:H	2:F:206:ILE:HG21	1.67	0.59
2:B:292:THR:O	2:B:380:ARG:NH1	2.34	0.59
2:N:90:ARG:HH21	2:N:120:GLY:HA2	1.67	0.59
2:B:91:GLY:O	2:N:55:ARG:NH1	2.36	0.59
2:F:179:ILE:HG23	2:F:232:GLU:HB2	1.86	0.58
1:I:368:GLN:HE21	1:I:419:LEU:HD23	1.69	0.58
2:J:55:ARG:HD3	2:J:145:THR:HB	1.86	0.58
4:L:17:DG:H2"	4:L:18:DT:C6	2.38	0.58
1:M:377:ARG:NH1	2:N:417:GLU:OE2	2.35	0.57
2:F:267:LEU:HB3	2:F:276:LEU:HB3	1.86	0.57
1:M:338:LYS:NZ	1:M:346:GLU:OE2	2.37	0.57
2:B:203:ASP:OD1	2:B:203:ASP:N	2.38	0.57
2:F:73:SER:O	2:F:128:LYS:NZ	2.37	0.57
2:N:319:ARG:HH21	2:N:342:TYR:HB3	1.69	0.57
1:A:333:ARG:NH2	1:A:436:GLU:OE1	2.37	0.57
2:N:307:LYS:HE3	2:N:312:GLU:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:NH2	3:C:2:U:OP1	2.39	0.56
1:E:267:ARG:NH1	1:E:271:GLY:O	2.38	0.56
1:E:333:ARG:HB3	1:E:361:LEU:HB2	1.87	0.56
2:F:224:GLU:CD	2:F:224:GLU:H	2.12	0.56
1:I:65:SER:OG	1:I:66:GLY:N	2.39	0.56
2:J:44:ALA:O	2:J:56:MET:HA	2.06	0.56
2:B:276:LEU:H	2:B:322:ALA:HB1	1.70	0.56
2:B:311:ASP:OD2	2:B:311:ASP:N	2.37	0.55
4:H:4:DC:N4	4:H:5:DG:O6	2.39	0.55
1:A:117:ASP:O	1:A:157:ARG:NH2	2.39	0.55
2:N:278:PHE:HE2	2:N:287:ARG:HG2	1.70	0.55
2:F:191:ALA:O	2:F:195:ASN:ND2	2.39	0.55
2:N:320:HIS:HB2	2:N:343:TYR:O	2.06	0.55
1:M:74:HIS:O	1:M:74:HIS:ND1	2.34	0.55
2:N:289:PHE:H	2:N:300:ALA:HB3	1.72	0.55
1:I:367:VAL:HG12	1:I:420:LEU:HD23	1.89	0.55
2:B:185:GLU:HG2	2:B:225:ILE:HD12	1.89	0.55
2:N:73:SER:OG	2:N:74:ASP:N	2.39	0.55
1:M:207:ASP:OD1	1:M:207:ASP:N	2.38	0.55
2:B:270:ASP:OD1	2:B:270:ASP:N	2.38	0.54
2:N:55:ARG:HB3	2:N:145:THR:HG21	1.89	0.54
2:N:375:VAL:O	2:N:379:HIS:ND1	2.40	0.54
2:B:281:ILE:HG13	2:B:283:ARG:H	1.71	0.54
2:F:105:ASP:OD1	2:F:105:ASP:N	2.40	0.54
2:N:31:ASP:O	2:N:42:GLY:HA2	2.07	0.54
2:N:280:ALA:HB2	2:N:287:ARG:HB2	1.90	0.54
2:J:183:THR:HG23	2:J:185:GLU:H	1.72	0.54
1:E:10:GLU:OE2	1:E:385:ARG:NH1	2.39	0.54
2:F:180:ALA:H	2:F:210:THR:HG23	1.72	0.54
2:N:178:TYR:HA	2:N:233:ALA:HA	1.90	0.54
2:N:290:ALA:HA	2:N:298:THR:HB	1.90	0.54
2:J:279:ARG:O	2:J:287:ARG:NH2	2.39	0.54
2:N:344:TYR:HD1	2:N:353:GLN:HE21	1.55	0.54
2:B:160:GLY:HA2	2:B:414:ARG:HB2	1.89	0.54
2:F:181:SER:OG	2:F:182:THR:N	2.41	0.54
1:I:204:VAL:HG13	1:I:229:ARG:HD2	1.90	0.53
2:N:204:TRP:HZ2	2:N:207:ASN:HB2	1.72	0.53
2:J:319:ARG:NH1	2:J:344:TYR:OH	2.36	0.53
2:F:284:GLU:OE2	2:F:287:ARG:NH1	2.41	0.53
1:M:47:VAL:HG22	1:M:102:ALA:HB3	1.89	0.53
2:N:169:LEU:HD21	2:N:379:HIS:CD2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:SER:HA	2:B:226:VAL:HB	1.90	0.53
2:J:90:ARG:NH1	2:J:114:SER:O	2.42	0.53
1:E:183:ARG:NH1	3:G:1:A:OP3	2.41	0.53
1:A:85:GLY:N	1:A:88:SER:OG	2.42	0.53
2:J:180:ALA:HB3	2:J:233:ALA:HB2	1.90	0.52
2:B:263:THR:O	2:B:267:LEU:N	2.41	0.52
1:E:281:MET:HA	1:E:290:VAL:O	2.10	0.52
2:F:68:LYS:NZ	2:F:69:TYR:O	2.43	0.52
2:F:235:ASN:OD1	2:F:235:ASN:N	2.43	0.52
2:J:283:ARG:HG3	2:J:285:VAL:HG22	1.92	0.52
2:B:256:ARG:HG2	2:B:269:TRP:HH2	1.75	0.51
1:I:183:ARG:NH1	3:K:1:A:OP1	2.43	0.51
1:I:186:LEU:HD23	1:I:199:ILE:HD11	1.93	0.51
2:N:307:LYS:HB2	2:N:314:ARG:HB3	1.92	0.51
2:B:308:ASN:HD22	2:B:314:ARG:HB2	1.76	0.51
1:M:333:ARG:NH2	1:M:436:GLU:OE1	2.43	0.51
1:I:313:LYS:HG3	1:I:353:ALA:HB2	1.92	0.51
1:I:198:GLN:OE1	1:I:240:LYS:NZ	2.44	0.51
4:L:19:DA:H2'	4:L:19:DA:N3	2.24	0.51
2:F:33:ARG:NH1	2:J:31:ASP:OD2	2.44	0.51
1:I:281:MET:HE2	1:I:291:LEU:HD13	1.93	0.51
1:I:307:MET:HB2	1:I:346:GLU:HG2	1.92	0.51
2:N:291:TYR:HD1	2:N:293:SER:H	1.59	0.51
1:A:156:GLU:OE1	1:A:160:ASN:ND2	2.43	0.50
1:E:408:THR:OG1	1:E:409:TYR:N	2.43	0.50
1:I:408:THR:OG1	1:I:409:TYR:N	2.44	0.50
2:B:90:ARG:NE	2:B:115:ARG:O	2.44	0.50
1:E:333:ARG:NH2	1:E:363:ASP:OD2	2.44	0.50
1:M:410:PRO:HA	4:P:19:DA:H5'	1.93	0.50
2:N:185:GLU:OE2	2:N:188:LYS:HB2	2.11	0.50
1:E:82:PRO:HG2	1:E:89:PRO:HD3	1.93	0.50
2:N:222:CYS:SG	2:N:227:ASP:N	2.84	0.50
1:E:148:ILE:HD11	1:E:197:ILE:HB	1.94	0.50
2:J:35:ARG:NH1	2:N:37:GLU:OE1	2.45	0.50
1:E:202:GLU:HG2	1:E:209:VAL:HG11	1.94	0.49
2:F:183:THR:HG21	2:F:226:VAL:HB	1.94	0.49
1:M:157:ARG:O	1:M:157:ARG:NH1	2.44	0.49
2:B:289:PHE:H	2:B:301:ASN:HD21	1.59	0.49
1:I:403:MET:HE1	1:I:451:ASN:HB3	1.93	0.49
2:B:280:ALA:HA	2:B:287:ARG:NE	2.21	0.49
2:B:287:ARG:HD2	2:B:289:PHE:HE2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:SER:O	2:F:76:SER:OG	2.31	0.49
2:N:167:ASN:OD1	2:N:167:ASN:N	2.42	0.49
2:N:376:ILE:HA	2:N:379:HIS:CE1	2.48	0.49
1:I:377:ARG:NH1	1:I:381:TYR:O	2.45	0.49
3:O:13:U:H2'	3:O:14:G:C8	2.48	0.49
2:B:66:GLU:HB3	2:B:104:SER:HB3	1.94	0.48
1:I:184:GLY:HA2	1:I:467:VAL:HG23	1.94	0.48
4:L:17:DG:H2''	4:L:18:DT:H6	1.78	0.48
4:L:18:DT:H3'	4:L:19:DA:C8	2.48	0.48
1:M:463:LYS:HD3	1:M:485:ILE:HG22	1.96	0.48
2:B:277:TYR:HB2	2:B:320:HIS:HB2	1.96	0.48
2:F:201:ARG:NH2	2:F:222:CYS:SG	2.83	0.48
2:F:401:LEU:HD22	2:F:403:PHE:HE1	1.78	0.48
2:N:194:LEU:HD23	2:N:200:LYS:HZ1	1.79	0.48
1:A:262:GLY:O	1:A:278:ALA:HA	2.13	0.48
2:F:283:ARG:H	2:F:283:ARG:HD3	1.79	0.48
1:I:248:ARG:NH1	1:I:283:ASP:OD1	2.45	0.48
2:N:41:ASP:OD1	2:N:41:ASP:N	2.46	0.48
1:M:120:ARG:O	1:M:124:MET:HG3	2.13	0.48
2:N:279:ARG:NH2	2:N:349:TYR:OH	2.45	0.48
2:B:36:LEU:H	2:B:36:LEU:HG	1.53	0.48
1:I:244:ARG:NH1	1:M:140:GLY:O	2.47	0.48
2:N:345:THR:HA	2:N:353:GLN:NE2	2.28	0.48
2:B:81:LEU:O	2:B:122:ARG:NH1	2.40	0.48
3:C:9:C:H2'	3:C:10:A:H8	1.79	0.47
2:F:249:ASN:HD22	4:H:7:DC:H1'	1.79	0.47
2:J:361:GLY:O	2:J:365:LEU:HG	2.14	0.47
2:B:256:ARG:HH12	4:D:6:DT:H5''	1.78	0.47
1:I:113:GLY:HA2	1:I:157:ARG:HG2	1.95	0.47
1:M:238:TYR:O	1:M:242:SER:HB3	2.14	0.47
2:N:173:LEU:HB2	2:N:237:LYS:HG2	1.96	0.47
1:M:44:ILE:HB	1:M:96:ILE:HD13	1.95	0.47
3:O:14:G:H2'	3:O:15:A:C8	2.49	0.47
1:M:309:ARG:NH1	1:M:348:ASP:OD2	2.44	0.47
1:E:70:LYS:HE3	4:H:19:DA:H61	1.80	0.47
1:I:410:PRO:HA	4:L:19:DA:P	2.54	0.47
1:I:413:TYR:HD1	1:I:414:ASP:HB2	1.80	0.47
2:J:278:PHE:O	2:J:320:HIS:ND1	2.41	0.47
1:M:454:LEU:HD13	1:M:455:PRO:HD2	1.96	0.47
1:A:409:TYR:OH	1:A:413:TYR:O	2.29	0.47
2:B:78:THR:HG21	2:B:123:ARG:HH21	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:C:H2'	3:C:10:A:C8	2.49	0.47
2:J:309:SER:O	2:J:309:SER:OG	2.24	0.47
1:M:334:VAL:HG23	1:M:359:THR:HG21	1.97	0.47
2:J:71:SER:O	2:J:71:SER:OG	2.32	0.47
1:M:456:ILE:O	1:M:457:PRO:C	2.57	0.47
2:N:267:LEU:HD23	2:N:278:PHE:HB3	1.97	0.47
2:B:178:TYR:HD1	2:B:231:VAL:HG13	1.80	0.46
2:F:236:THR:OG1	2:F:237:LYS:NZ	2.48	0.46
2:J:286:SER:OG	2:J:288:ASN:OD1	2.32	0.46
1:A:299:GLU:HG3	1:A:300:SER:H	1.80	0.46
2:F:148:LYS:HD2	2:F:148:LYS:HA	1.75	0.46
2:J:105:ASP:OD1	2:J:105:ASP:N	2.46	0.46
1:M:84:LEU:HA	1:M:88:SER:HB3	1.97	0.46
1:E:26:LEU:O	1:E:30:GLU:HB2	2.14	0.46
1:M:264:SER:H	1:M:277:SER:HB3	1.81	0.46
3:O:4:C:H2'	3:O:5:U:C6	2.50	0.46
2:N:266:ASP:OD1	2:N:266:ASP:N	2.49	0.46
2:N:318:VAL:HB	2:N:345:THR:HG23	1.97	0.46
1:A:261:VAL:HB	1:A:336:ILE:HD13	1.98	0.46
1:I:359:THR:O	1:I:362:ARG:NH2	2.48	0.46
2:B:182:THR:OG1	2:B:185:GLU:OE1	2.34	0.46
2:J:174:PRO:O	2:J:237:LYS:HG3	2.15	0.46
2:N:280:ALA:HA	2:N:287:ARG:HD3	1.98	0.46
2:B:45:GLU:OE1	2:N:33:ARG:NH2	2.47	0.46
1:A:280:GLN:HG2	1:A:319:VAL:HG22	1.97	0.46
2:B:58:ALA:HB3	2:B:96:VAL:HG12	1.97	0.46
1:E:216:LYS:HB2	1:E:216:LYS:HE3	1.67	0.46
2:B:279:ARG:HE	2:B:280:ALA:H	1.63	0.45
1:I:376:LEU:HD13	2:J:372:ARG:HA	1.98	0.45
2:J:177:MET:HE3	2:J:235:ASN:OD1	2.16	0.45
3:K:9:C:H2'	3:K:10:A:C8	2.50	0.45
2:N:217:PRO:HD2	2:N:218:ARG:NH1	2.31	0.45
2:B:175:ASN:OD1	2:B:235:ASN:ND2	2.49	0.45
2:B:176:GLU:OE1	2:B:215:HIS:ND1	2.48	0.45
2:B:326:ARG:HA	2:B:326:ARG:HD2	1.75	0.45
1:A:355:ASP:OD1	1:A:362:ARG:NH2	2.49	0.45
2:J:218:ARG:H	2:J:218:ARG:HG2	1.64	0.45
2:B:37:GLU:HA	2:N:29:GLN:HE22	1.82	0.45
2:J:422:LYS:HD3	2:J:422:LYS:HA	1.75	0.45
1:A:377:ARG:NH1	1:A:381:TYR:O	2.45	0.45
2:J:306:PHE:HE2	2:J:319:ARG:HE	1.62	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:HB2	1:E:15:PHE:CE1	2.51	0.45
2:F:367:LYS:H	2:F:367:LYS:HG2	1.48	0.45
1:I:413:TYR:HE2	2:J:363:LYS:HD2	1.81	0.45
2:J:203:ASP:HA	2:J:211:PHE:HE2	1.82	0.45
2:J:235:ASN:OD1	2:J:237:LYS:HD2	2.17	0.45
2:N:67:GLY:O	2:N:102:ARG:NH1	2.50	0.45
2:N:188:LYS:HB3	2:N:188:LYS:HE2	1.62	0.45
2:N:368:SER:O	2:N:370:ALA:N	2.50	0.45
3:O:3:A:H2'	3:O:4:C:C6	2.52	0.45
2:B:338:ILE:HD11	2:B:375:VAL:HG13	1.99	0.45
1:E:354:LEU:HD13	1:E:362:ARG:HG2	1.99	0.45
1:I:280:GLN:HE21	1:I:292:LYS:HD3	1.81	0.45
1:M:377:ARG:NH2	2:N:162:GLU:OE1	2.42	0.44
2:N:186:PRO:O	2:N:187:ARG:HB2	2.16	0.44
2:F:227:ASP:N	2:F:227:ASP:OD2	2.47	0.44
2:F:19:VAL:HG11	2:F:61:ILE:HG12	1.99	0.44
2:N:352:HIS:N	2:N:353:GLN:OE1	2.50	0.44
1:I:108:LYS:O	1:I:112:ILE:HG12	2.17	0.44
4:L:18:DT:H5'	4:L:19:DA:C4	2.53	0.44
2:J:206:ILE:HG12	2:J:250:ARG:HG2	1.99	0.44
2:N:402:MET:SD	2:N:402:MET:N	2.90	0.44
2:B:172:THR:OG1	2:B:402:MET:O	2.34	0.44
3:C:4:C:H2'	3:C:5:U:C6	2.53	0.44
1:A:106:LYS:HE2	1:A:106:LYS:HB2	1.83	0.44
2:B:35:ARG:NH2	2:B:36:LEU:HD23	2.33	0.44
2:B:381:PHE:HD1	2:B:382:LEU:HD22	1.83	0.44
3:G:7:C:H2'	3:G:8:A:C8	2.53	0.44
2:N:267:LEU:HD22	2:N:276:LEU:HB3	1.99	0.44
2:F:267:LEU:HD23	2:F:278:PHE:H	1.82	0.44
2:N:180:ALA:HA	2:N:231:VAL:HG11	2.00	0.44
2:N:296:LYS:HE3	2:N:297:LYS:H	1.83	0.44
3:O:5:U:H2'	3:O:6:G:C8	2.52	0.44
3:O:18:A:H2'	3:O:19:U:C6	2.53	0.44
1:A:191:MET:HE1	1:A:478:SER:H	1.83	0.43
2:F:215:HIS:NE2	2:F:222:CYS:SG	2.89	0.43
1:M:337:LEU:HB3	1:M:458:ILE:HD11	1.98	0.43
1:I:285:ARG:H	1:I:326:HIS:HE1	1.66	0.43
2:J:177:MET:O	2:J:235:ASN:HB3	2.18	0.43
1:M:266:TYR:CE1	1:M:465:GLY:HA3	2.53	0.43
2:N:279:ARG:HH12	2:N:281:ILE:C	2.26	0.43
3:G:16:C:H2'	3:G:17:G:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:343:LYS:HE2	1:I:343:LYS:HB3	1.71	0.43
1:M:301:ARG:NH2	1:M:311:ASP:OD1	2.52	0.43
2:N:222:CYS:HB2	2:N:228:ILE:HG22	2.00	0.43
1:E:153:LYS:HD2	1:E:153:LYS:HA	1.83	0.43
2:F:307:LYS:HZ2	2:F:315:VAL:HA	1.84	0.43
1:M:130:ILE:HD13	1:M:130:ILE:HA	1.90	0.43
2:N:237:LYS:HD2	2:N:237:LYS:HA	1.79	0.43
2:N:307:LYS:HE3	2:N:312:GLU:CA	2.49	0.43
1:A:108:LYS:HE2	1:A:108:LYS:HB2	1.85	0.43
1:M:284:GLU:OE1	1:M:326:HIS:NE2	2.51	0.43
2:N:206:ILE:HD12	2:N:206:ILE:HA	1.93	0.43
1:A:220:SER:OG	1:A:221:ARG:N	2.51	0.43
2:B:13:GLU:OE1	2:J:20:ARG:NH2	2.52	0.43
1:E:85:GLY:O	1:E:87:GLN:N	2.52	0.43
2:F:157:PRO:HB3	2:F:416:PRO:HD3	1.99	0.43
2:J:341:THR:OG1	2:J:342:TYR:N	2.51	0.43
1:M:44:ILE:HD11	1:M:94:PHE:HD2	1.84	0.43
1:M:117:ASP:O	1:M:119:TYR:N	2.52	0.43
1:E:130:ILE:HD13	1:E:130:ILE:HA	1.90	0.43
2:F:73:SER:OG	2:F:76:SER:OG	2.33	0.43
3:G:4:C:H2'	3:G:5:U:C6	2.53	0.43
1:I:204:VAL:O	1:I:229:ARG:NH1	2.52	0.43
1:I:412:LYS:HA	1:I:412:LYS:HD3	1.77	0.43
1:M:291:LEU:HD21	1:M:456:ILE:CD1	2.43	0.43
1:M:373:ALA:HB1	2:N:166:ILE:HD11	2.01	0.43
2:B:422:LYS:HG3	2:B:423:GLU:HB2	2.00	0.42
2:J:177:MET:HE3	2:J:177:MET:HB3	1.76	0.42
1:M:277:SER:OG	1:M:278:ALA:N	2.51	0.42
2:N:406:PRO:HA	2:N:407:PRO:HD3	1.86	0.42
2:B:372:ARG:O	2:B:376:ILE:HG22	2.18	0.42
2:F:172:THR:HB	2:F:402:MET:HB3	2.01	0.42
3:K:4:C:H2'	3:K:5:U:C6	2.55	0.42
1:A:58:LYS:N	1:A:58:LYS:HD2	2.33	0.42
2:B:38:ALA:HB3	2:B:88:TYR:OH	2.19	0.42
2:F:275:ALA:HB1	2:F:322:ALA:HB1	2.00	0.42
1:I:196:PRO:HB2	1:I:240:LYS:HD3	2.01	0.42
3:O:7:C:H2'	3:O:8:A:C8	2.54	0.42
2:B:5:ILE:HD12	2:B:5:ILE:HA	1.86	0.42
1:M:441:THR:HG22	1:M:452:GLN:HB2	2.02	0.42
1:A:423:HIS:O	1:A:424:HIS:ND1	2.53	0.42
3:G:10:A:H2'	3:G:11:G:C8	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:165:LEU:HD21	2:J:372:ARG:HE	1.85	0.42
4:L:4:DC:H2'	4:L:5:DG:H8	1.85	0.42
1:A:60:ILE:O	1:A:64:SER:OG	2.31	0.42
2:J:36:LEU:HD23	2:N:13:GLU:HG3	2.01	0.42
1:E:303:ARG:NH1	3:G:13:U:OP1	2.52	0.42
2:J:188:LYS:HB3	2:J:188:LYS:HE3	1.64	0.42
2:N:172:THR:OG1	2:N:173:LEU:N	2.52	0.42
1:A:394:LYS:HD2	1:A:421:CYS:HB3	2.02	0.42
2:B:281:ILE:HG13	2:B:283:ARG:N	2.35	0.42
2:F:22:ARG:HA	2:F:22:ARG:HD3	1.88	0.42
2:F:219:THR:OG1	2:F:220:SER:N	2.52	0.42
2:F:177:MET:HG3	2:F:236:THR:HG22	2.02	0.41
1:A:10:GLU:OE2	1:A:442:LYS:NZ	2.47	0.41
1:A:56:THR:O	1:A:60:ILE:HG22	2.21	0.41
2:B:406:PRO:HA	2:B:407:PRO:HD3	1.84	0.41
1:E:15:PHE:CD2	1:E:15:PHE:N	2.87	0.41
2:J:79:TYR:O	2:J:123:ARG:HA	2.19	0.41
2:N:234:ILE:HG23	2:N:235:ASN:HB2	2.00	0.41
2:N:250:ARG:NH2	3:O:17:G:OP1	2.52	0.41
2:B:188:LYS:H	2:B:188:LYS:HG2	1.65	0.41
2:F:235:ASN:HB2	2:F:237:LYS:HG2	2.02	0.41
2:J:217:PRO:O	2:J:222:CYS:N	2.46	0.41
1:M:212:PRO:HA	1:M:219:SER:HA	2.02	0.41
1:A:49:ASN:O	1:A:52:THR:OG1	2.31	0.41
1:A:338:LYS:HG2	1:A:340:SER:H	1.85	0.41
1:E:54:GLU:CD	1:E:54:GLU:H	2.27	0.41
2:N:55:ARG:HD2	2:N:55:ARG:HA	1.93	0.41
1:A:157:ARG:HD2	1:A:157:ARG:HA	1.84	0.41
2:B:217:PRO:HG2	2:B:218:ARG:HD2	2.02	0.41
2:B:224:GLU:HG2	2:B:225:ILE:HG12	2.02	0.41
2:N:132:LEU:HB3	2:N:134:ASN:HD22	1.85	0.41
3:O:13:U:H2'	3:O:14:G:H8	1.84	0.41
1:A:480:ASP:HB3	1:A:483:LYS:HG3	2.02	0.41
1:E:17:ASP:C	1:E:19:HIS:H	2.28	0.41
2:F:31:ASP:OD1	2:F:32:GLY:N	2.54	0.41
2:J:193:ILE:HG22	2:J:195:ASN:H	1.85	0.41
1:M:442:LYS:HB2	1:M:442:LYS:HE2	1.85	0.41
2:B:63:SER:OG	2:B:64:THR:N	2.53	0.41
1:I:35:GLN:HB2	1:I:244:ARG:HB3	2.03	0.41
2:J:302:VAL:HG13	2:J:321:HIS:HB2	2.02	0.41
4:L:17:DG:C2	4:L:18:DT:C2	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:HB3	1:A:274:LEU:HD12	2.03	0.41
2:B:8:ASN:ND2	5:Q:6:DT:O2	2.54	0.41
2:B:190:ILE:HA	2:B:193:ILE:HG22	2.02	0.41
2:F:277:TYR:HA	2:F:322:ALA:HB2	2.03	0.41
2:F:282:GLU:OE1	2:F:284:GLU:HG2	2.21	0.41
4:H:17:DG:H2'	4:H:18:DT:H5'	2.03	0.41
2:J:139:ASN:OD1	2:J:139:ASN:N	2.53	0.41
2:J:177:MET:HE3	2:J:235:ASN:CG	2.46	0.41
2:J:424:LYS:HB3	2:J:424:LYS:HE3	1.73	0.41
3:K:7:C:H2'	3:K:8:A:C8	2.56	0.41
2:N:285:VAL:HG23	2:N:286:SER:H	1.86	0.41
5:Q:5:DC:H2'	5:Q:6:DT:C6	2.56	0.41
2:B:280:ALA:CB	2:B:287:ARG:HG2	2.49	0.41
2:F:44:ALA:O	2:F:56:MET:HA	2.21	0.41
1:M:203:ASP:HB3	1:M:223:ILE:HD13	2.03	0.41
2:N:276:LEU:O	2:N:322:ALA:HA	2.21	0.40
1:M:369:GLU:N	1:M:369:GLU:OE1	2.54	0.40
2:B:10:ILE:HD13	2:B:10:ILE:HA	1.96	0.40
2:B:35:ARG:HE	2:F:13:GLU:HB2	1.87	0.40
2:B:180:ALA:HB3	2:B:211:PHE:HB2	2.03	0.40
2:J:297:LYS:HZ1	2:J:299:ASP:HB3	1.87	0.40
2:N:279:ARG:NH1	2:N:282:GLU:O	2.54	0.40
1:A:58:LYS:NZ	1:A:58:LYS:HA	2.36	0.40
3:K:3:A:H2'	3:K:4:C:C6	2.57	0.40
1:A:120:ARG:O	1:A:124:MET:HG3	2.21	0.40
2:B:16:GLU:HG2	2:B:61:ILE:HD12	2.03	0.40
2:N:140:LYS:O	2:N:143:ALA:HB3	2.21	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	464/485 (96%)	439 (95%)	25 (5%)	0	100	100
1	E	464/485 (96%)	429 (92%)	35 (8%)	0	100	100
1	I	461/485 (95%)	428 (93%)	33 (7%)	0	100	100
1	M	461/485 (95%)	427 (93%)	34 (7%)	0	100	100
2	B	406/442 (92%)	360 (89%)	46 (11%)	0	100	100
2	F	405/442 (92%)	352 (87%)	53 (13%)	0	100	100
2	J	383/442 (87%)	340 (89%)	43 (11%)	0	100	100
2	N	383/442 (87%)	313 (82%)	70 (18%)	0	100	100
All	All	3427/3708 (92%)	3088 (90%)	339 (10%)	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	394/408 (97%)	392 (100%)	2 (0%)	81	85
1	E	394/408 (97%)	390 (99%)	4 (1%)	68	80
1	I	393/408 (96%)	392 (100%)	1 (0%)	86	88
1	M	393/408 (96%)	388 (99%)	5 (1%)	61	78
2	B	352/380 (93%)	347 (99%)	5 (1%)	59	77
2	F	351/380 (92%)	347 (99%)	4 (1%)	65	79
2	J	336/380 (88%)	330 (98%)	6 (2%)	51	74
2	N	336/380 (88%)	330 (98%)	6 (2%)	51	74
All	All	2949/3152 (94%)	2916 (99%)	33 (1%)	63	79

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	155	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	35	ARG
2	B	36	LEU
2	B	85	ASP
2	B	193	ILE
2	B	279	ARG
1	E	15	PHE
1	E	17	ASP
1	E	427	GLU
1	E	476	VAL
2	F	66	GLU
2	F	225	ILE
2	F	307	LYS
2	F	315	VAL
1	I	343	LYS
2	J	235	ASN
2	J	237	LYS
2	J	238	GLU
2	J	243	ASP
2	J	365	LEU
2	J	424	LYS
1	M	14	GLU
1	M	112	ILE
1	M	376	LEU
1	M	454	LEU
1	M	456	ILE
2	N	185	GLU
2	N	187	ARG
2	N	188	LYS
2	N	281	ILE
2	N	307	LYS
2	N	310	LYS

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

Mol	Chain	Res	Type
1	A	181	ASN
1	A	224	GLN
2	B	333	GLN
1	E	118	HIS
1	E	273	GLN
2	F	60	GLN
2	F	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	249	ASN
2	F	352	HIS
2	F	384	GLN
1	I	213	GLN
1	I	424	HIS
2	J	273	HIS
2	J	410	HIS
1	M	21	HIS
1	M	198	GLN
1	M	424	HIS
1	M	444	ASN
2	N	17	ASN
2	N	29	GLN
2	N	249	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	18/20 (90%)	3 (16%)	0
3	G	19/20 (95%)	3 (15%)	0
3	K	17/20 (85%)	1 (5%)	0
3	O	18/20 (90%)	3 (16%)	1 (5%)
All	All	72/80 (90%)	10 (13%)	1 (1%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	12	C
3	C	13	U
3	C	19	U
3	G	4	C
3	G	15	A
3	G	18	A
3	K	14	G
3	O	16	C
3	O	17	G
3	O	19	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	O	18	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

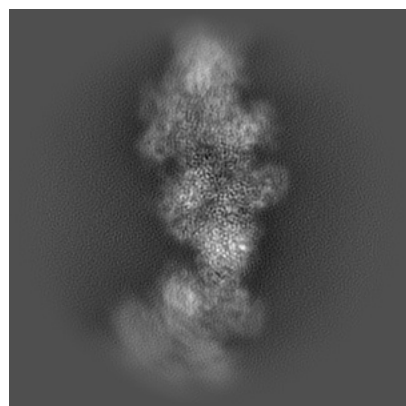
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61790. These allow visual inspection of the internal detail of the map and identification of artifacts.

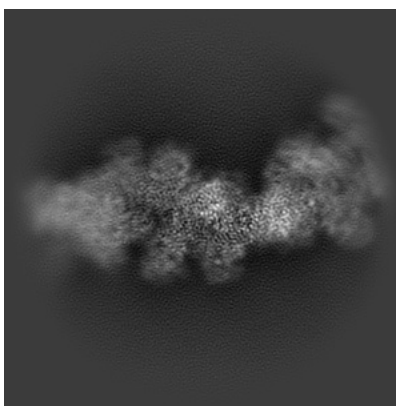
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

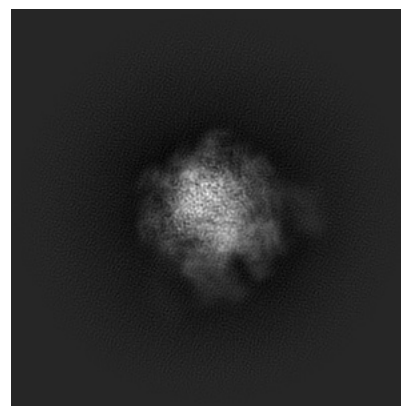
6.1.1 Primary map



X

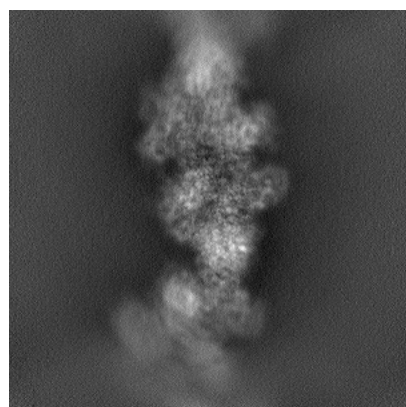


Y

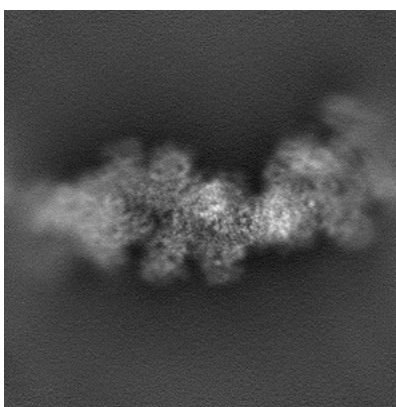


Z

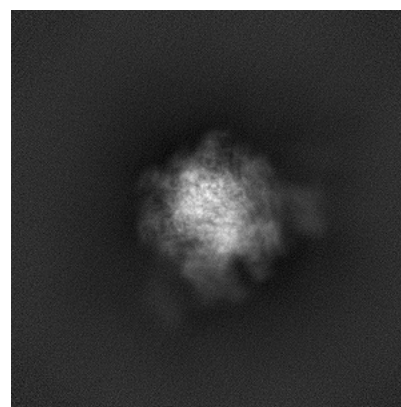
6.1.2 Raw map



X



Y

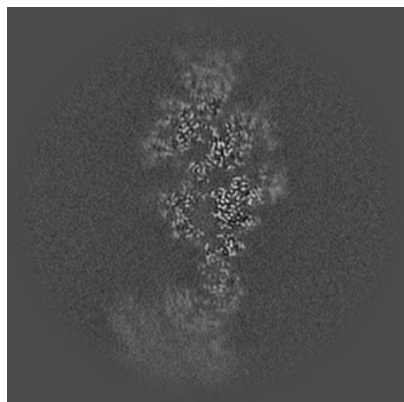


Z

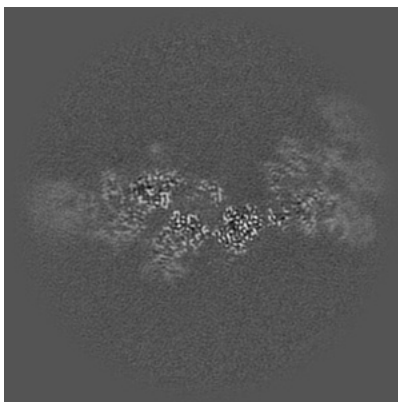
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

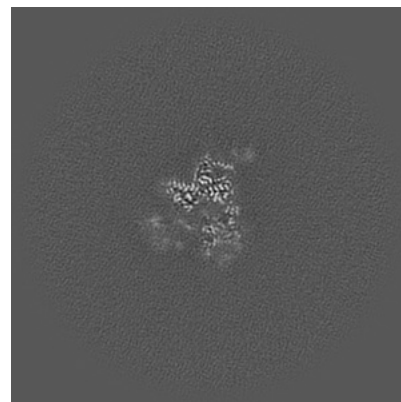
6.2.1 Primary map



X Index: 256

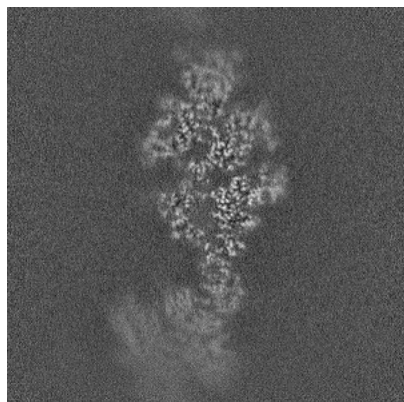


Y Index: 256

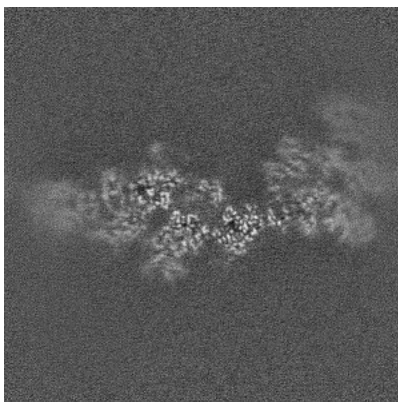


Z Index: 256

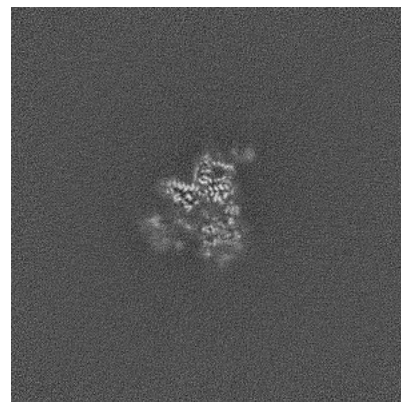
6.2.2 Raw map



X Index: 256



Y Index: 256

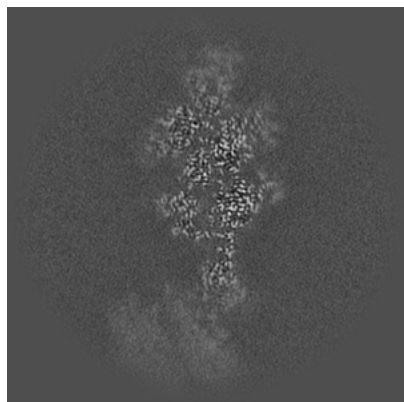


Z Index: 256

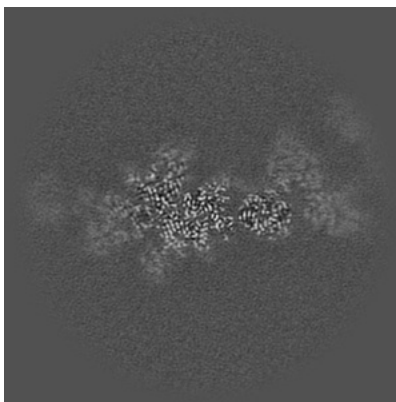
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

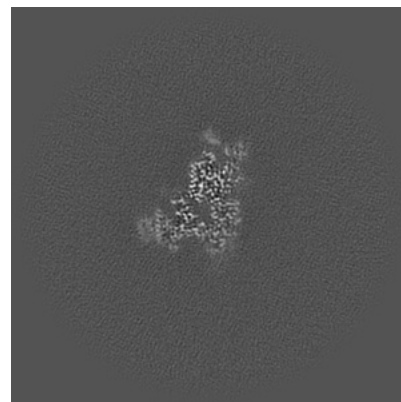
6.3.1 Primary map



X Index: 250

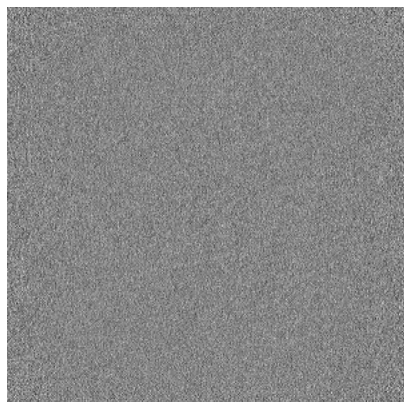


Y Index: 282

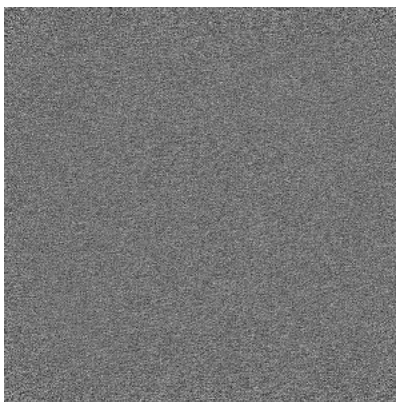


Z Index: 272

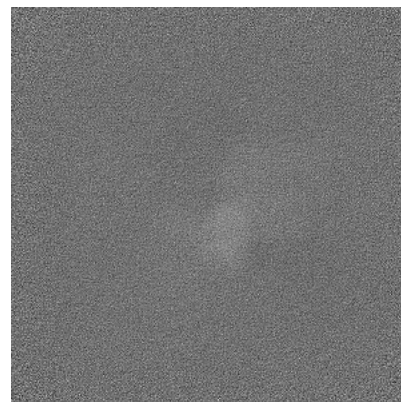
6.3.2 Raw map



X Index: 0



Y Index: 0

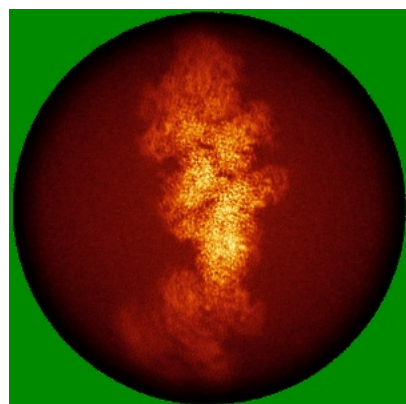


Z Index: 0

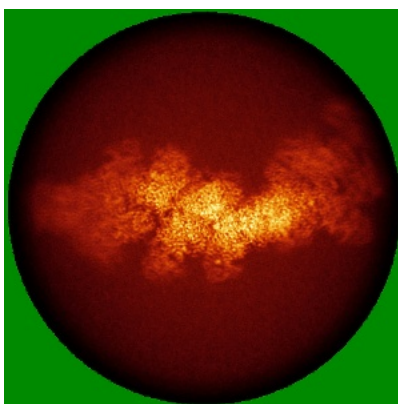
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

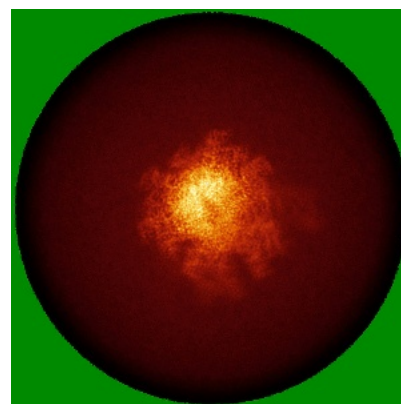
6.4.1 Primary map



X

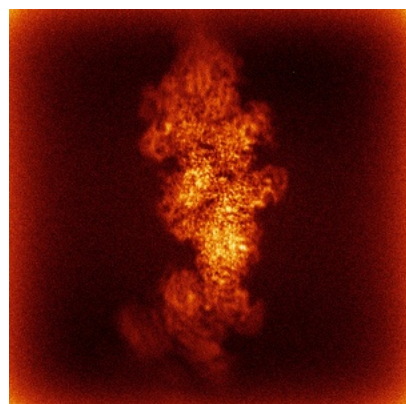


Y

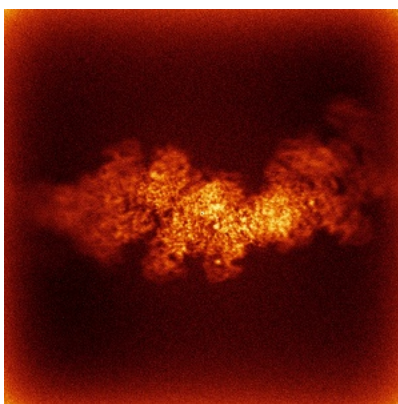


Z

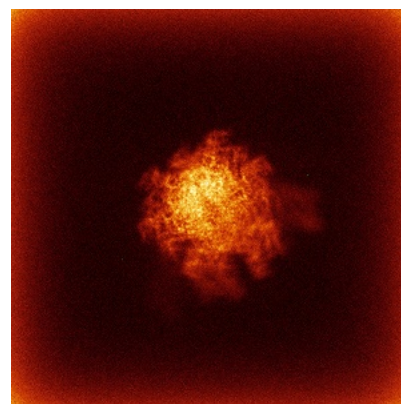
6.4.2 Raw map



X



Y

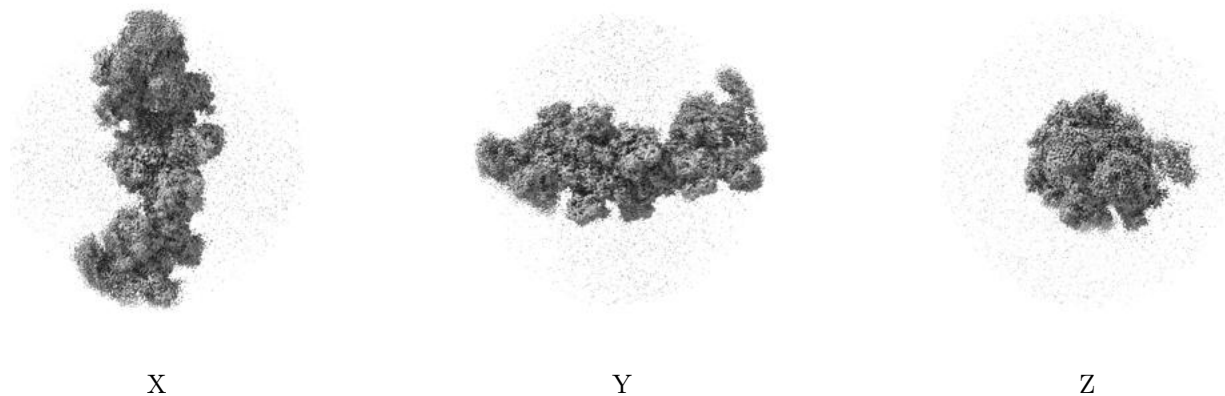


Z

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.

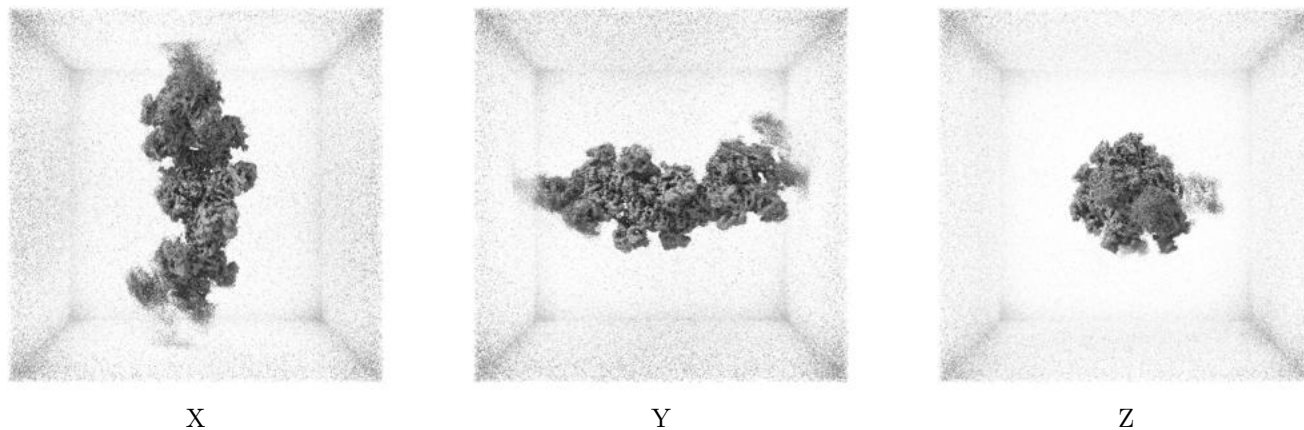
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.193. 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



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.

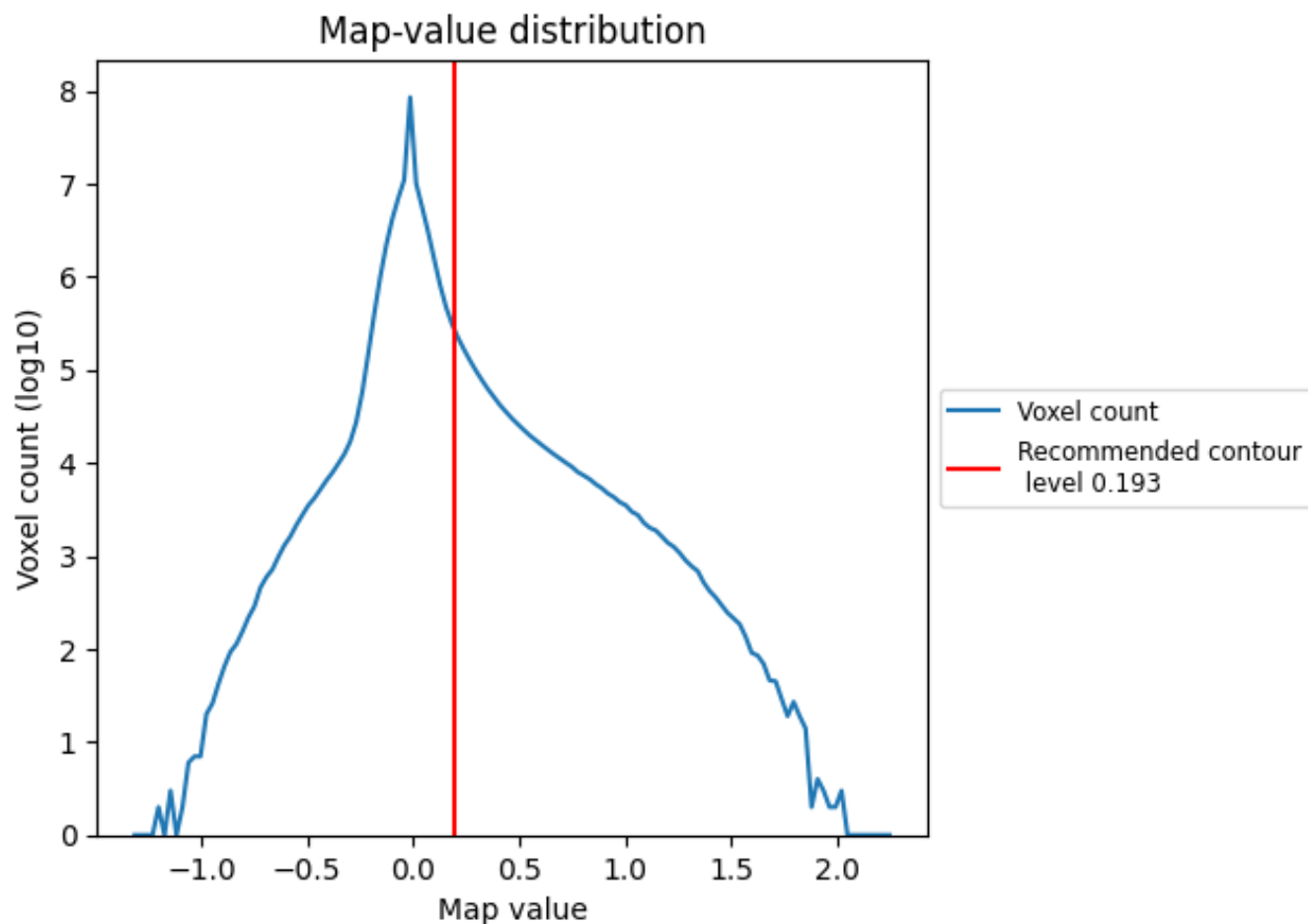
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

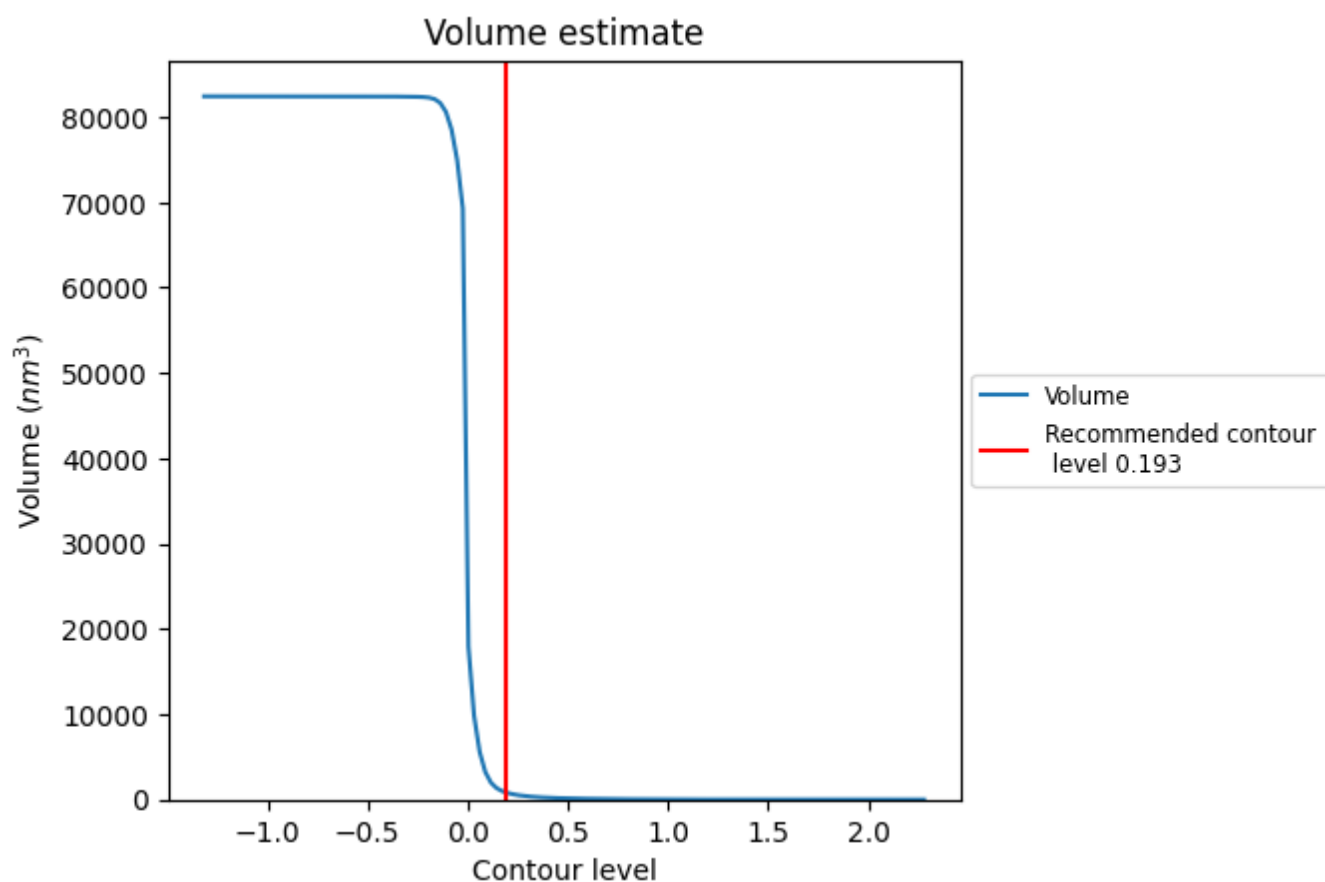
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

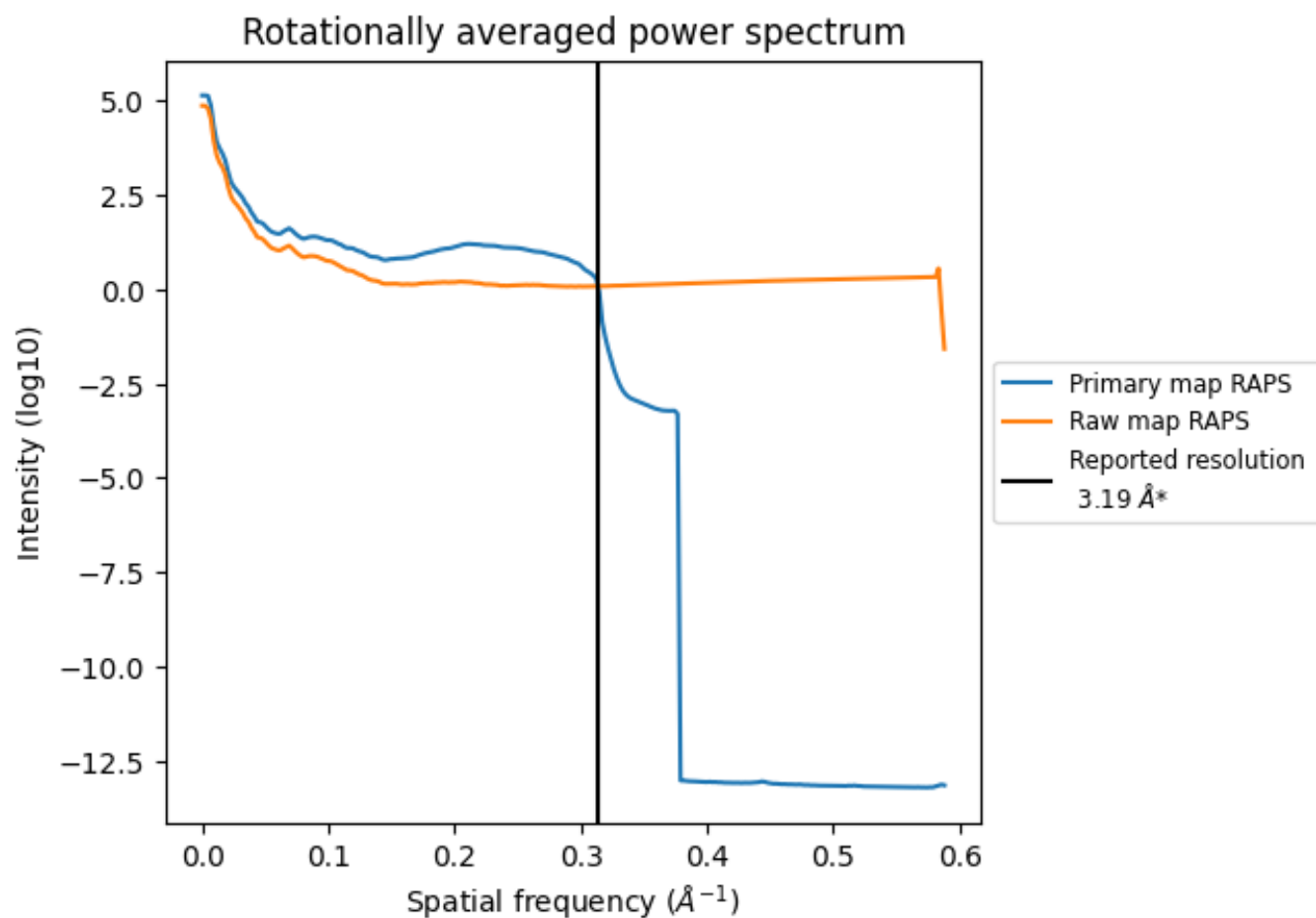
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm³; this corresponds to an approximate mass of 744 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 ⓘ

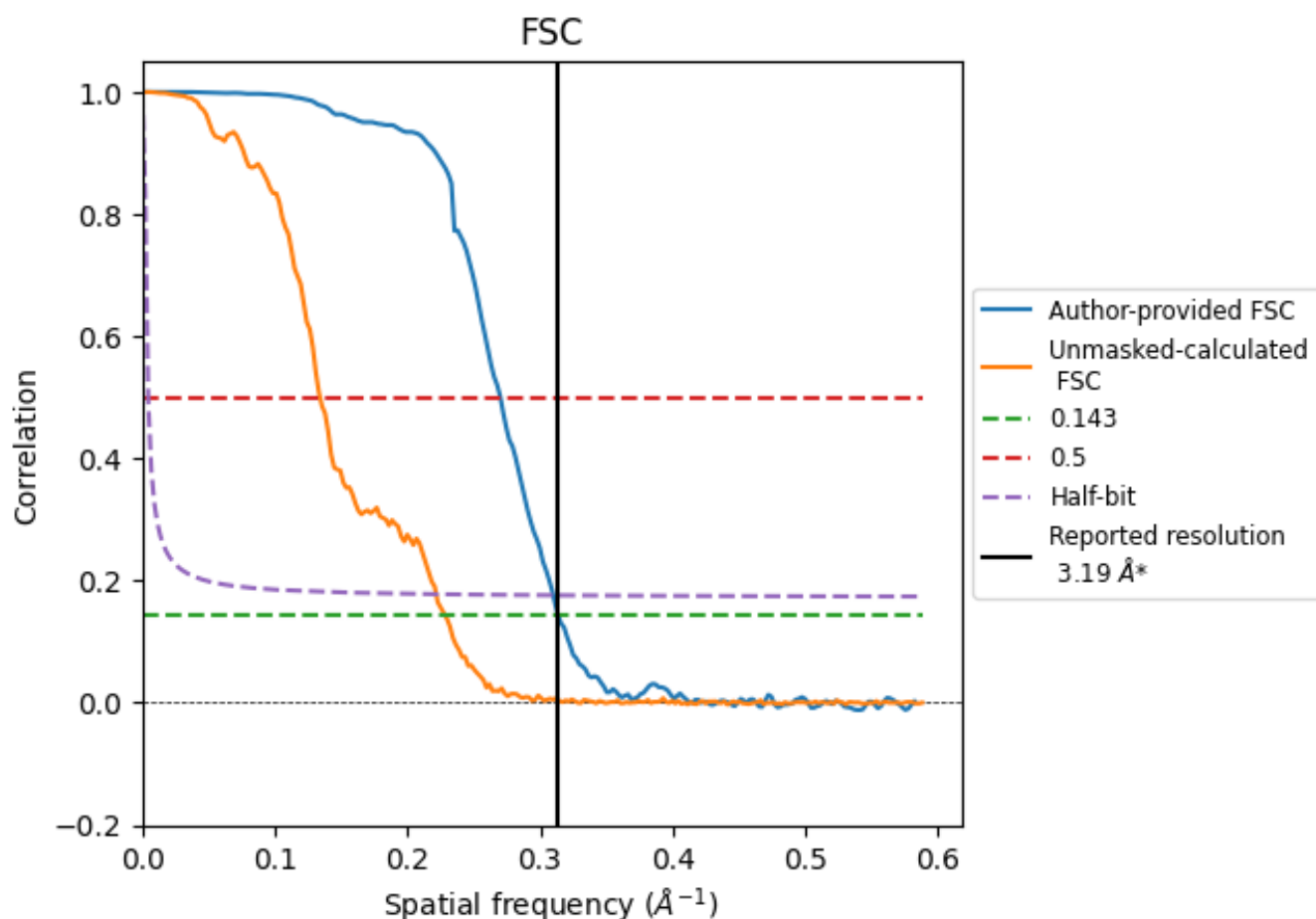


*Reported resolution corresponds to spatial frequency of 0.313 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.313 \AA^{-1}

8.2 Resolution estimates [i](#)

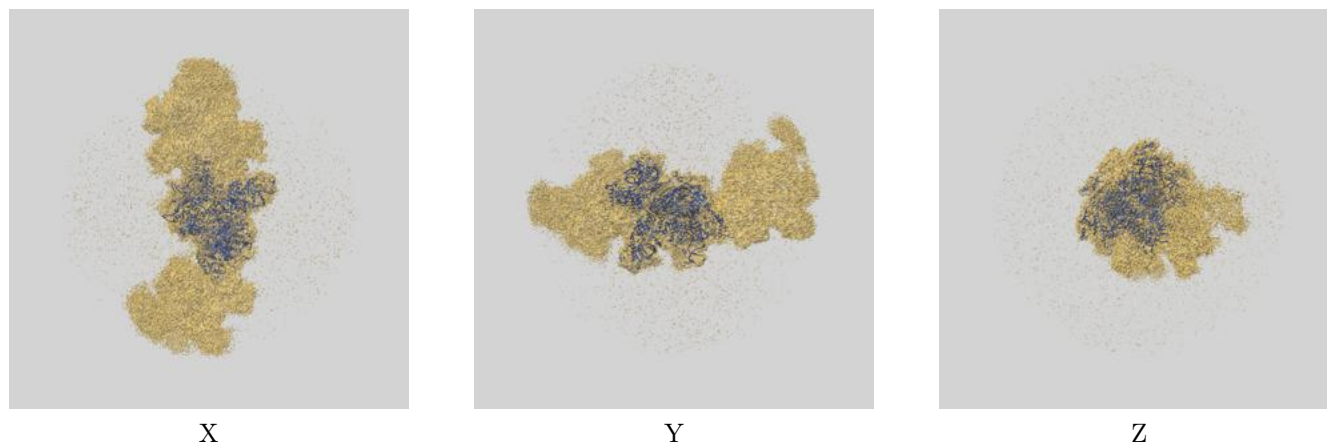
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.19	3.70	3.23
Unmasked-calculated*	4.38	7.46	4.51

*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 4.38 differs from the reported value 3.19 by more than 10 %

9 Map-model fit [i](#)

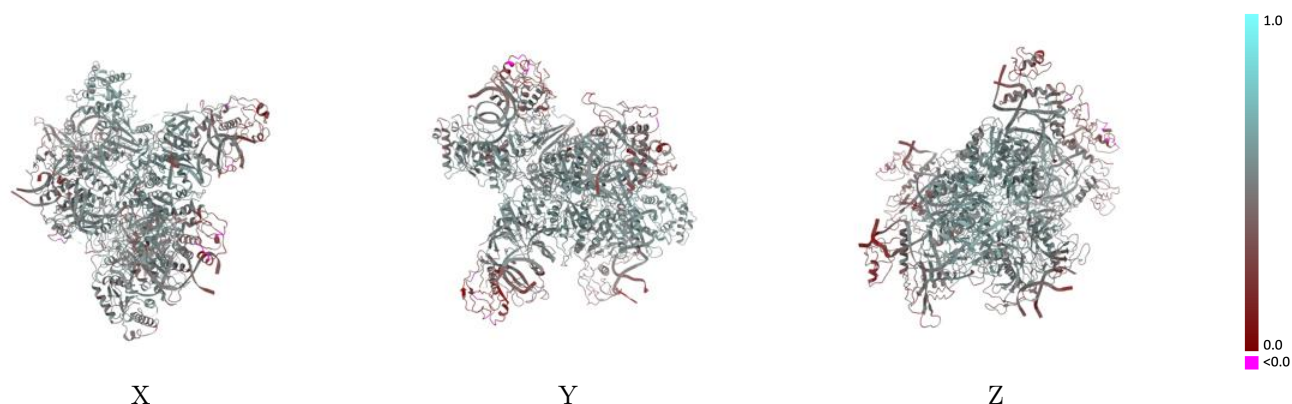
This section contains information regarding the fit between EMDB map EMD-61790 and PDB model 9JT2. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



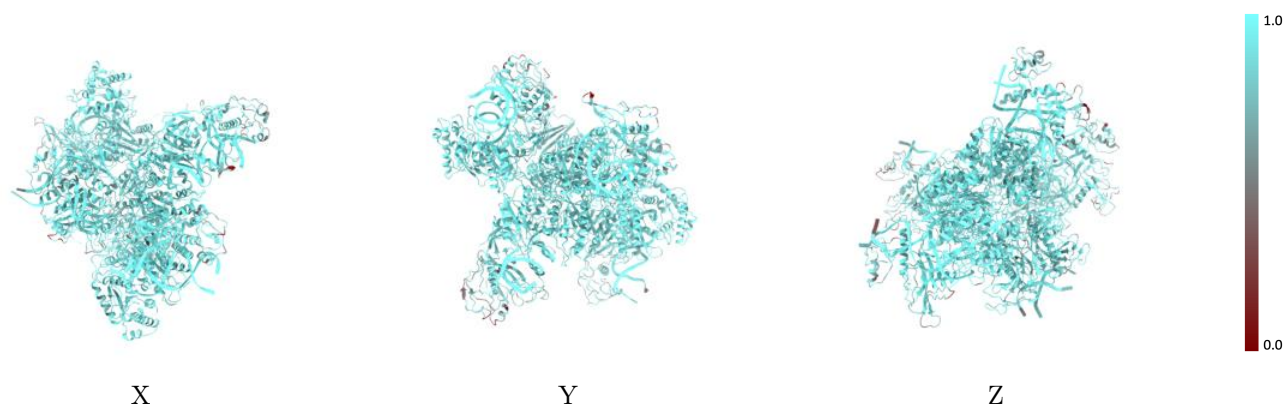
The images above show the 3D surface view of the map at the recommended contour level 0.193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



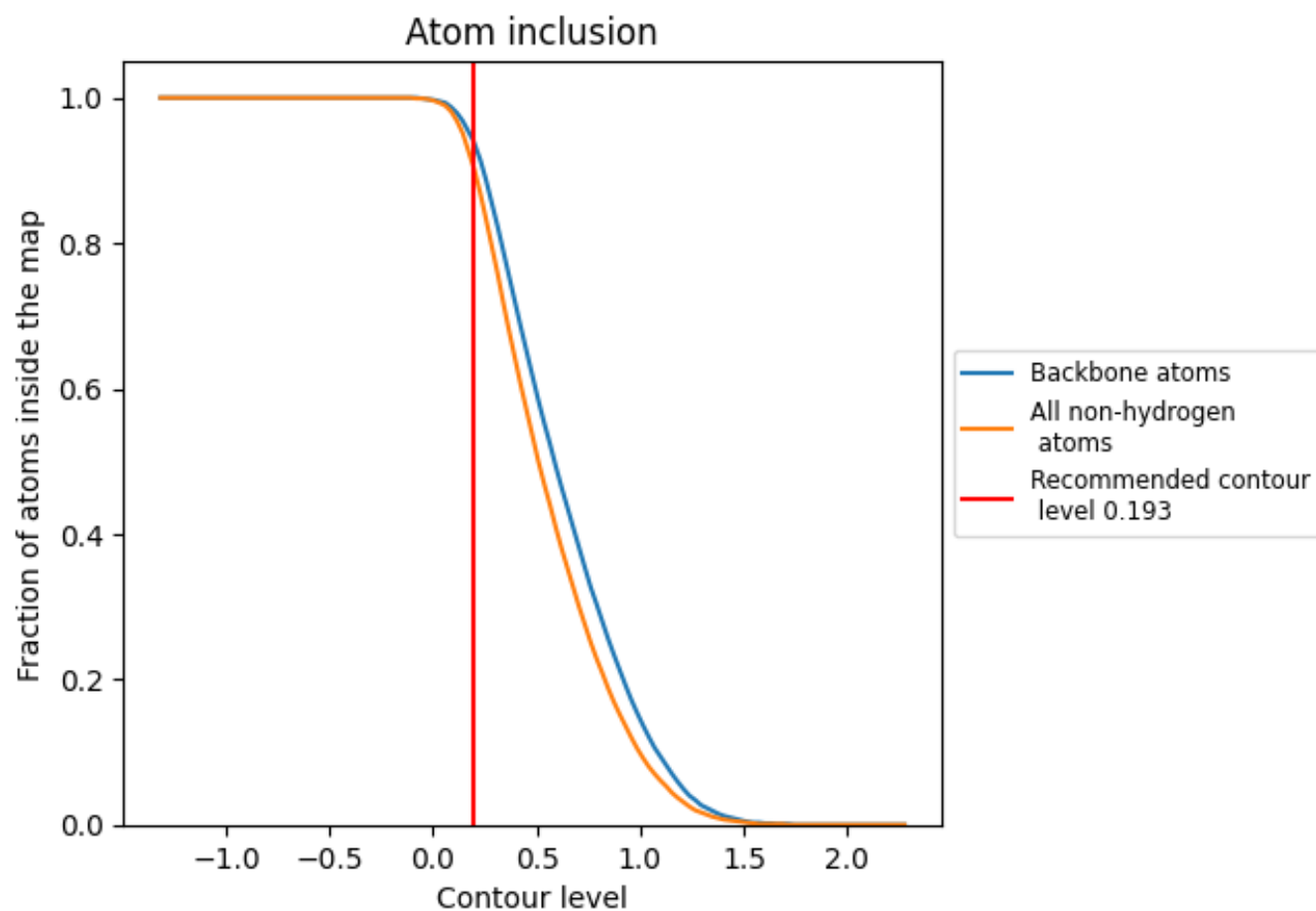
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.193).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.4850
A	 0.9370	 0.5290
B	 0.8550	 0.4190
C	 0.9800	 0.4850
D	 0.9810	 0.4800
E	 0.9530	 0.5580
F	 0.8680	 0.4310
G	 0.9510	 0.4370
H	 0.9260	 0.4180
I	 0.9550	 0.5570
J	 0.8610	 0.4350
K	 0.9710	 0.4890
L	 0.9760	 0.4670
M	 0.9490	 0.5490
N	 0.8190	 0.3970
O	 0.9510	 0.4510
P	 0.9650	 0.4590
Q	 0.8350	 0.3700
R	 0.8110	 0.3740

