Full wwPDB EM Validation Report ⓘ

Nov 28, 2023 – 03:39 pm GMT

PDB ID	:	8Q84
EMDB ID	:	EMD-18246
Title	:	Outer kinetochore Dam1 protomer dimer Ndc80-Nuf2 coiled-coil complex
Authors	:	Muir, K.W.; Barford, D.
Deposited on	:	2023-08-17
Resolution	:	3.15 Å(reported)
Based on initial model	:	.

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

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

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

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

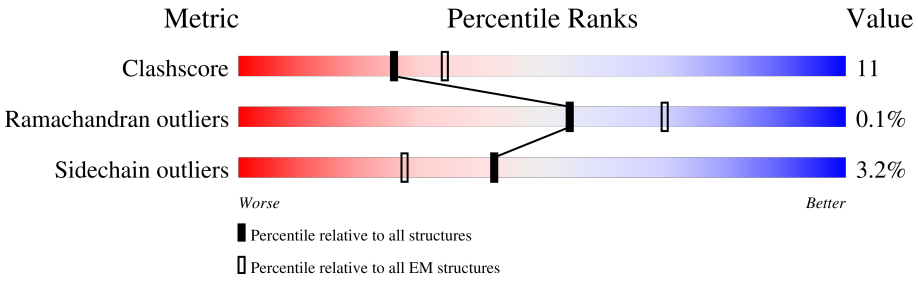
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



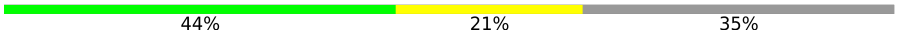
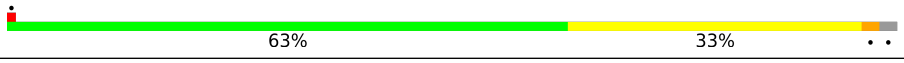
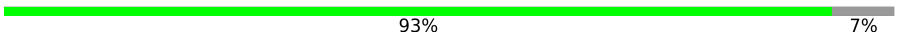
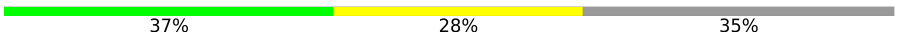
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	691	25% 42% 57%
1	F	691	26% 42% 57%
2	B	451	30% 52% 47%
2	G	451	31% 51% • 48%
3	I	343	20% 7% • 72%
3	U	343	19% 7% • 72%
3	e	343	• 97%
4	J	247	34% 13% 53%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	V	247	
5	K	133	
5	W	133	
6	L	94	
6	X	94	
7	M	72	
7	Y	72	
8	N	94	
8	Z	94	
9	O	295	
9	a	295	
10	P	292	
10	b	292	
11	Q	69	
11	c	69	
12	R	165	
12	d	165	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21802 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 Kinetochore protein NDC80.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	294	Total	C	N	O	0	0
			1463	875	294	294		
1	F	294	Total	C	N	O	0	0
			1463	875	294	294		

- Molecule 2 is a protein called Kinetochore protein NUF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	237	Total	C	N	O	0	0
			1180	706	237	237		
2	G	236	Total	C	N	O	0	0
			1175	703	236	236		

- Molecule 3 is a protein called DASH complex subunit DAM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	95	Total	C	N	O	S	0	0
			757	474	126	153	4		
3	U	95	Total	C	N	O	S	0	0
			757	474	126	153	4		
3	e	11	Total	C	N	O		0	0
			82	50	14	18			

- Molecule 4 is a protein called DASH complex subunit DUO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	117	Total	C	N	O	S	0	0
			935	580	167	185	3		
4	V	117	Total	C	N	O	S	0	0
			935	580	167	185	3		

- Molecule 5 is a protein called DASH complex subunit DAD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	106	Total	C	N	O	S	0	0
			837	519	139	174	5		
5	W	106	Total	C	N	O	S	0	0
			837	519	139	174	5		

- Molecule 6 is a protein called DASH complex subunit DAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	61	Total	C	N	O	S	0	0
			485	304	79	101	1		
6	X	68	Total	C	N	O	S	0	0
			535	334	86	114	1		

- Molecule 7 is a protein called DASH complex subunit DAD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	72	Total	C	N	O	S	0	0
			571	351	106	111	3		
7	Y	72	Total	C	N	O	S	0	0
			571	351	106	111	3		

- Molecule 8 is a protein called DASH complex subunit DAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	92	Total	C	N	O	S	0	0
			744	461	130	152	1		
8	Z	94	Total	C	N	O	S	0	0
			761	471	132	156	2		

- Molecule 9 is a protein called DASH complex subunit SPC34.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	235	Total	C	N	O	S	0	0
			1929	1213	342	367	7		
9	a	234	Total	C	N	O	S	0	0
			1925	1211	341	366	7		

- Molecule 10 is a protein called DASH complex subunit ASK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	65	Total	C	N	O	S	0	0
			527	332	83	108	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	70	Total	C	N	O	S	0	0
			561	352	88	116	5		

- Molecule 11 is a protein called DASH complex subunit HSK3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	64	Total	C	N	O	S	0	0
			527	327	94	101	5		
11	c	64	Total	C	N	O	S	0	0
			527	327	94	101	5		

- Molecule 12 is a protein called DASH complex subunit SPC19.

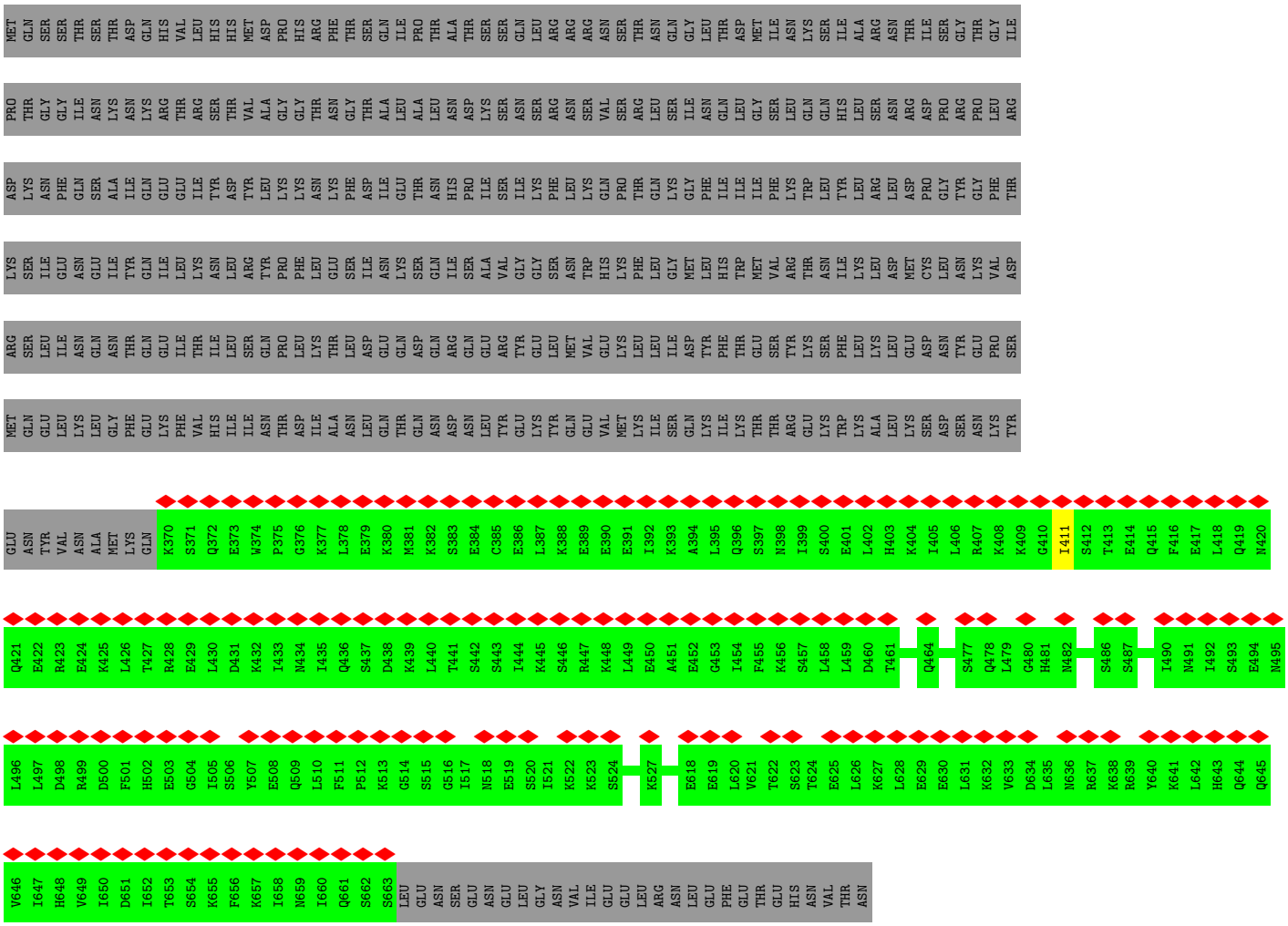
Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	108	Total	C	N	O	S	0	0
			859	532	149	172	6		
12	d	108	Total	C	N	O	S	0	0
			859	532	149	172	6		

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.

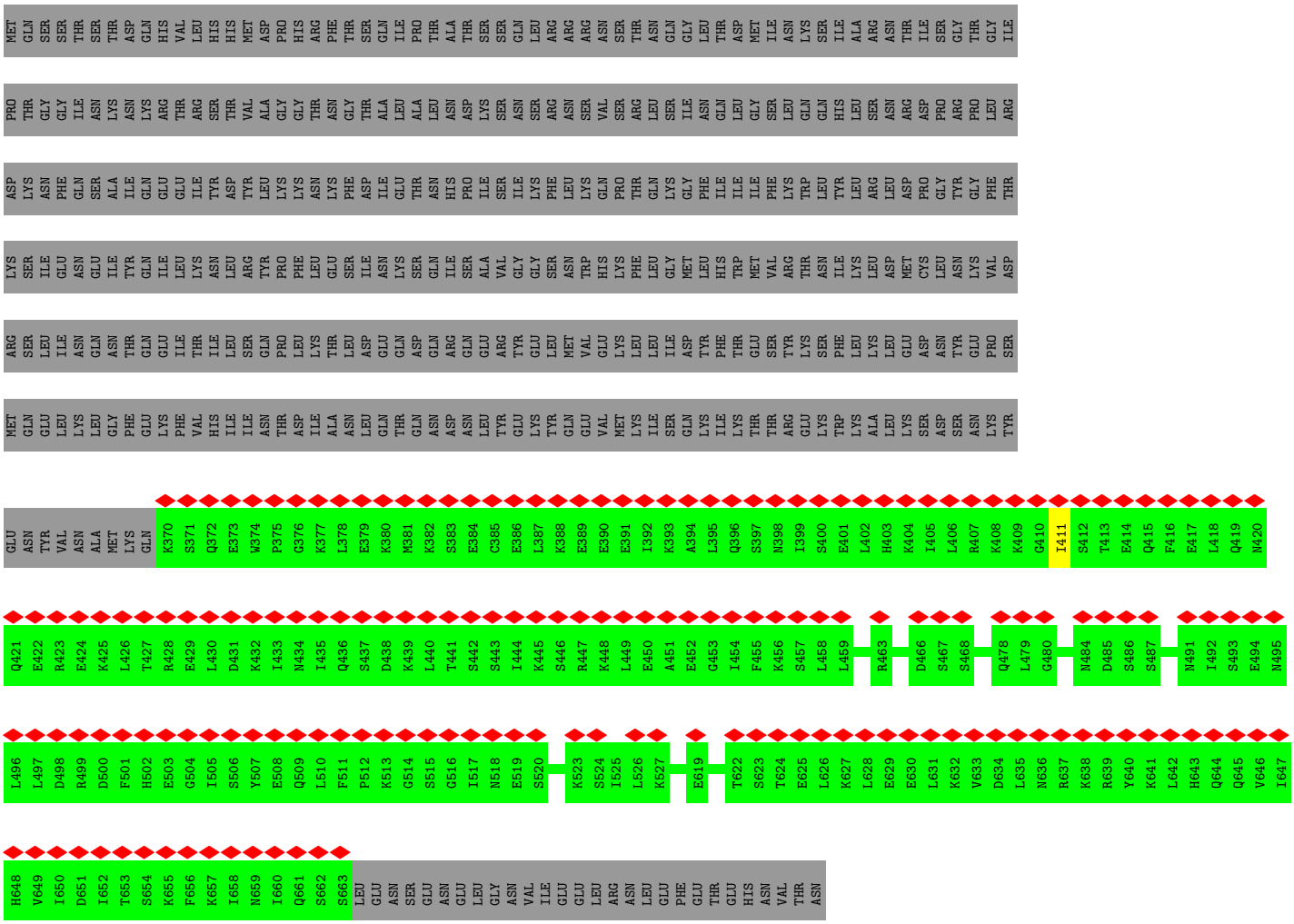
• Molecule 1: Kinetochore protein NDC80

Chain A:



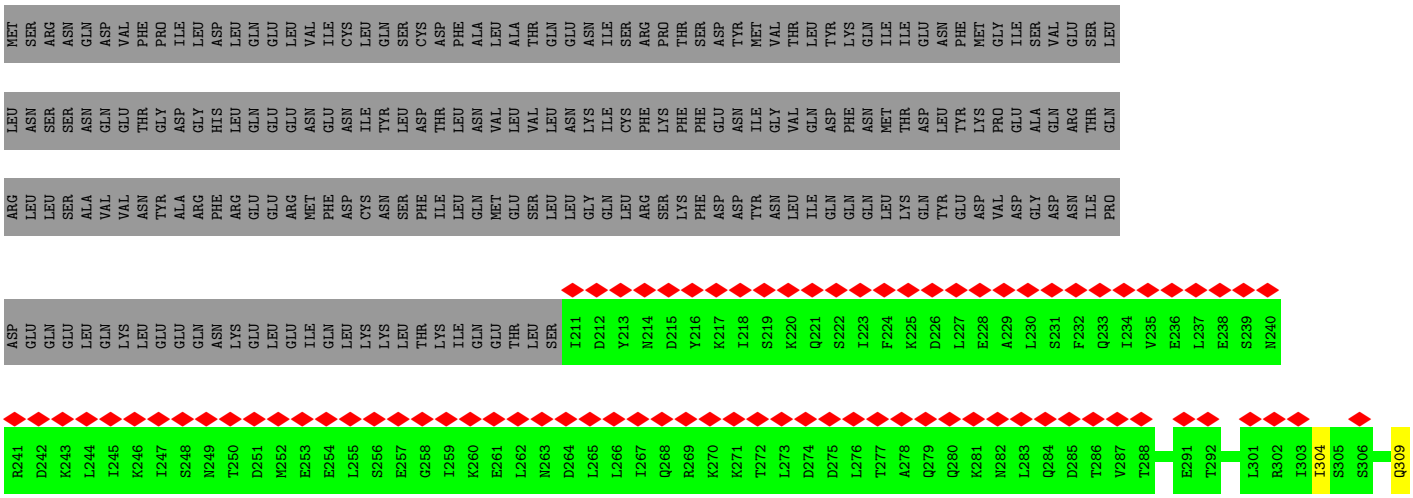
• Molecule 1: Kinetochore protein NDC80

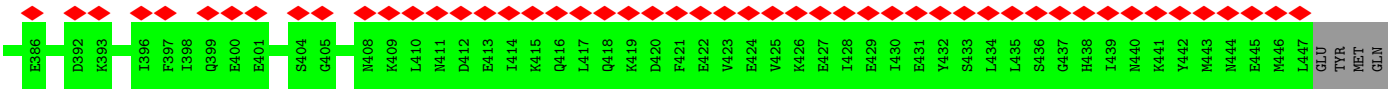
Chain F:



• Molecule 2: Kinetochore protein NUF2

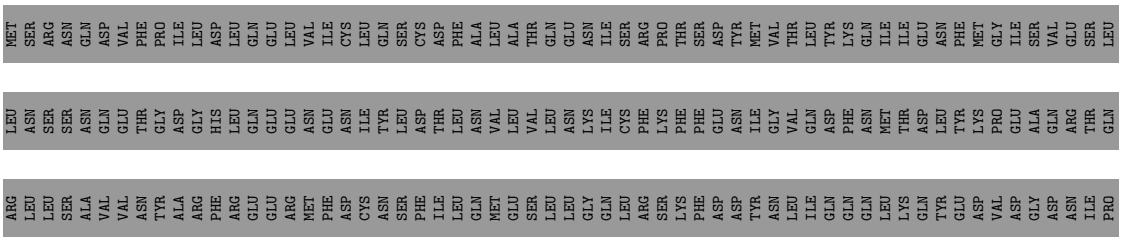
Chain B:

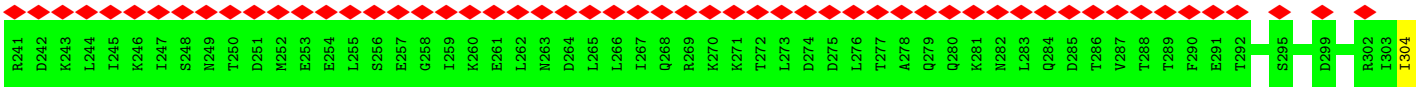


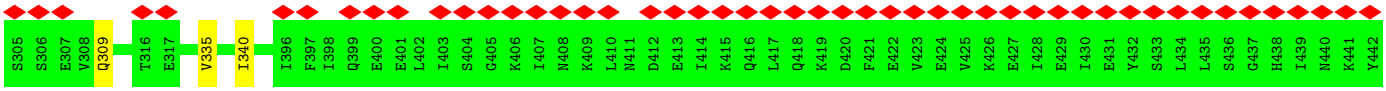


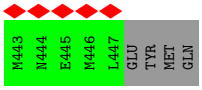
• Molecule 2: Kinetochore protein NUF2

Chain G:







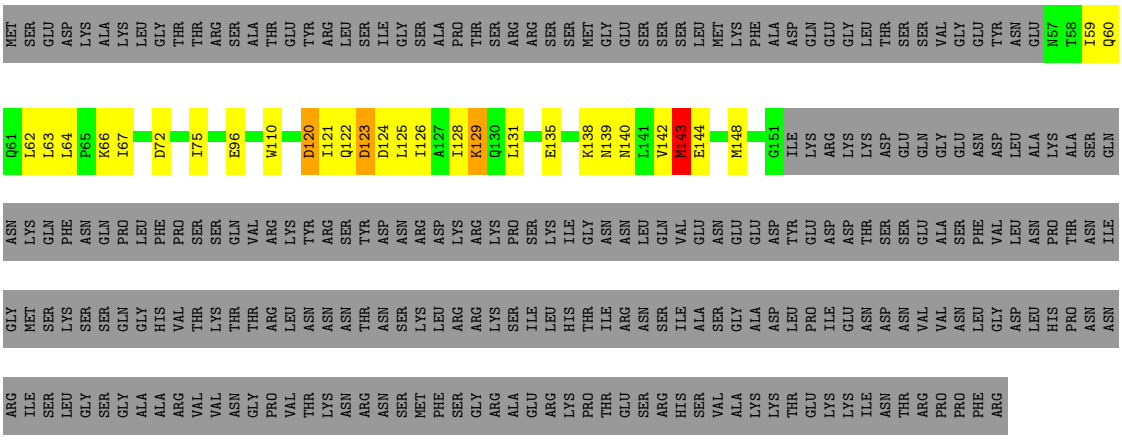


• Molecule 3: DASH complex subunit DAM1

Chain I:

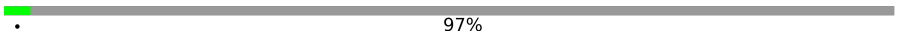
• Molecule 3: DASH complex subunit DAM1

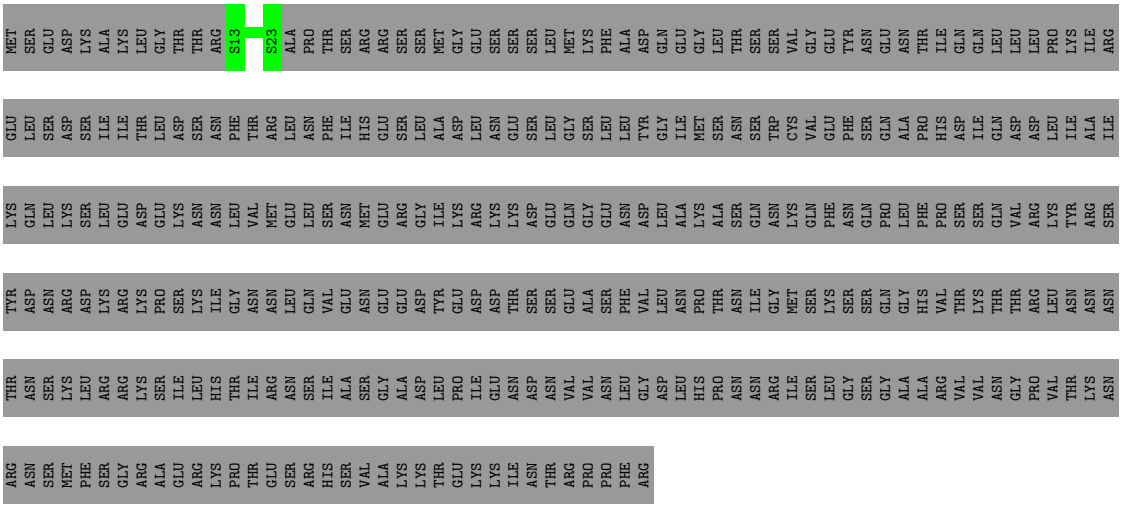
Chain U:



• Molecule 3: DASH complex subunit DAM1

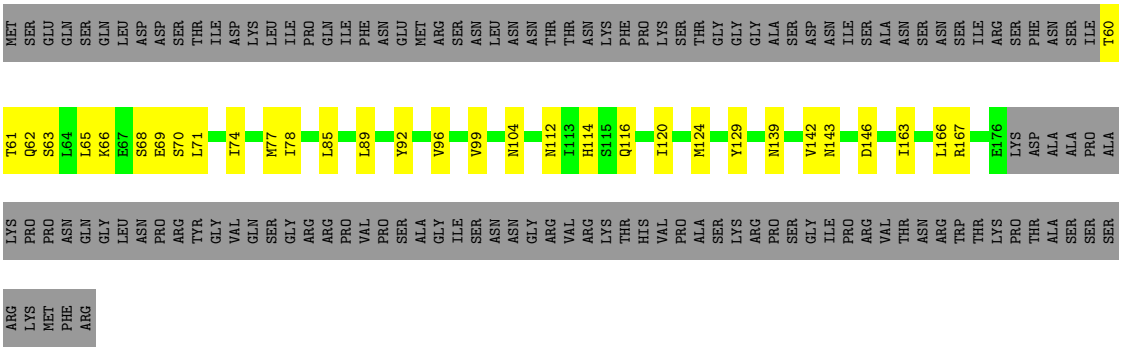
Chain e:





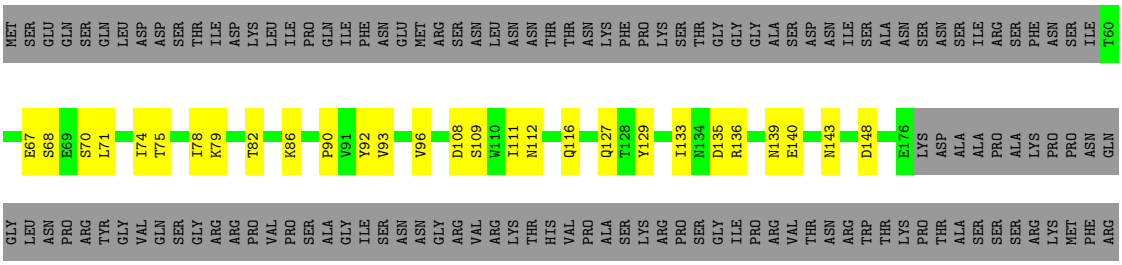
• Molecule 4: DASH complex subunit DUO1

Chain J:



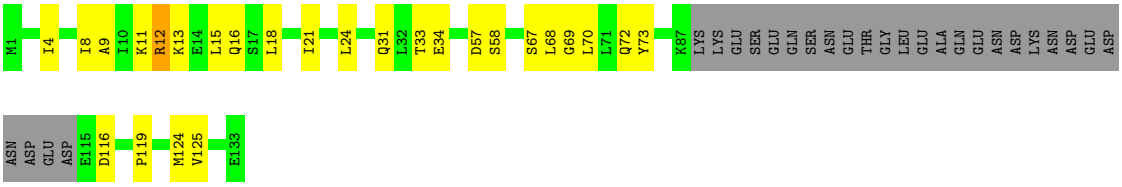
• Molecule 4: DASH complex subunit DUO1

Chain V:



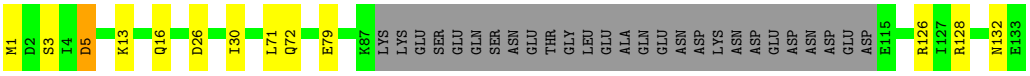
• Molecule 5: DASH complex subunit DAD2

Chain K:



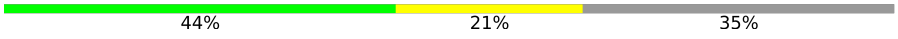
• Molecule 5: DASH complex subunit DAD2

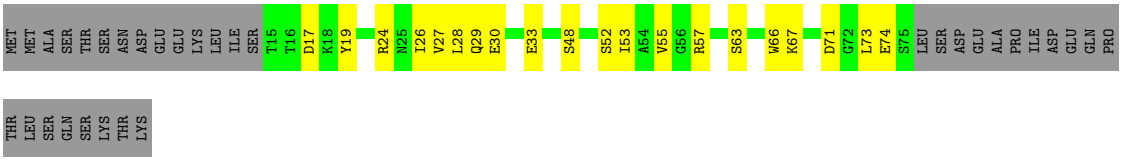
Chain W:



• Molecule 6: DASH complex subunit DAD1

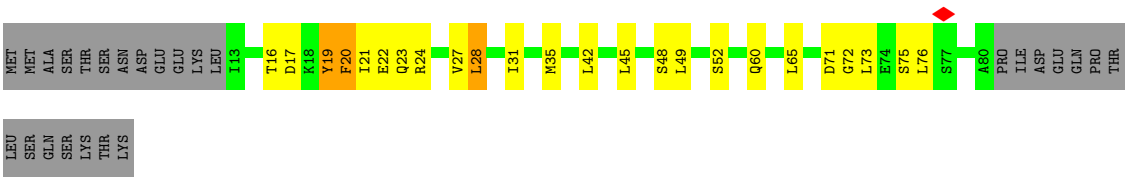
Chain L:





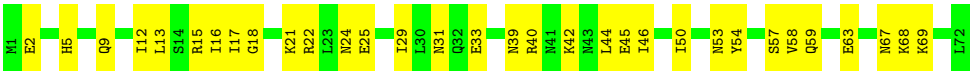
• Molecule 6: DASH complex subunit DAD1

Chain X:



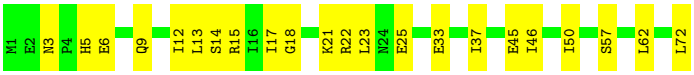
• Molecule 7: DASH complex subunit DAD4

Chain M:



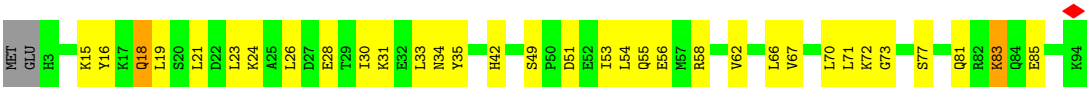
• Molecule 7: DASH complex subunit DAD4

Chain Y:



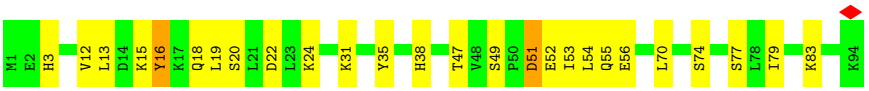
• Molecule 8: DASH complex subunit DAD3

Chain N:



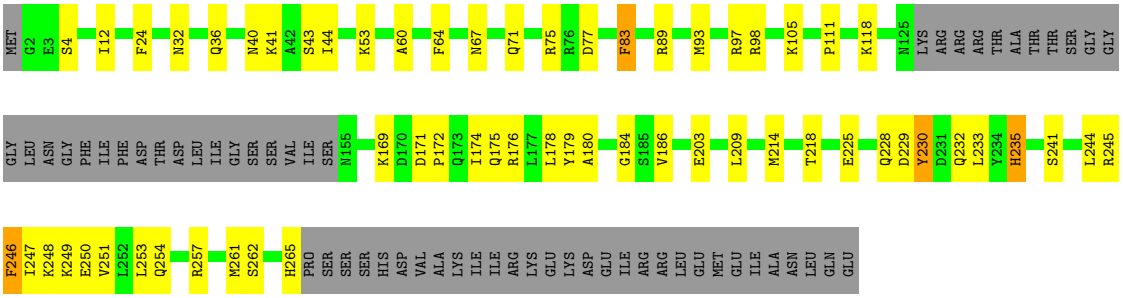
• Molecule 8: DASH complex subunit DAD3

Chain Z:



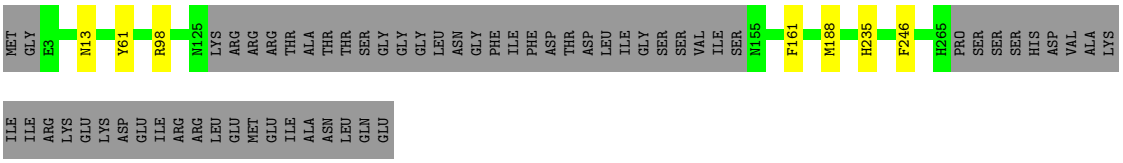
• Molecule 9: DASH complex subunit SPC34

Chain O:



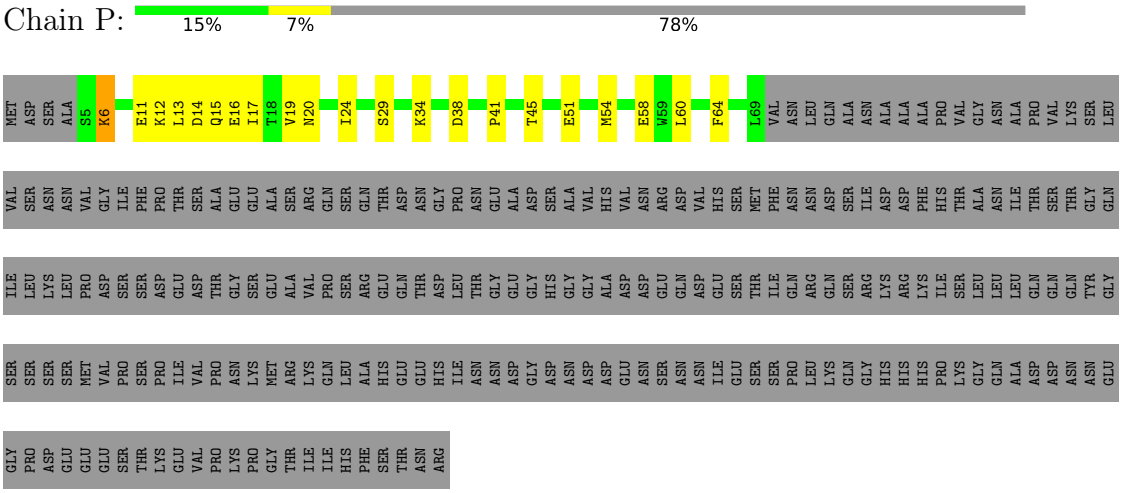
• Molecule 9: DASH complex subunit SPC34

Chain a:



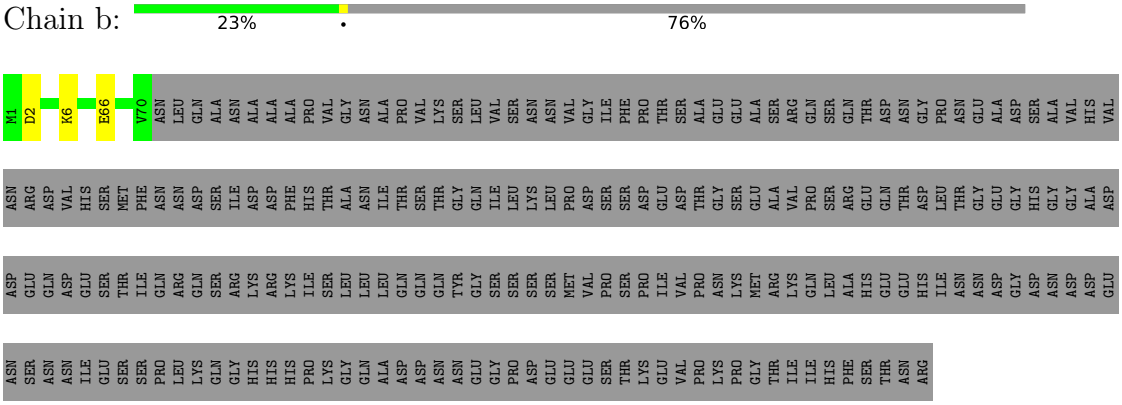
• Molecule 10: DASH complex subunit ASK1

Chain P:



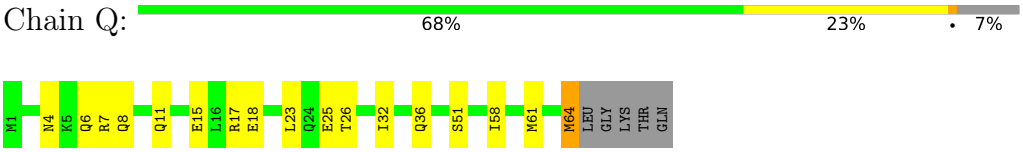
• Molecule 10: DASH complex subunit ASK1

Chain b:



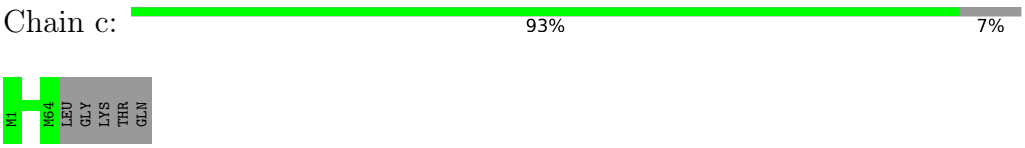
• Molecule 11: DASH complex subunit HSK3

Chain Q:



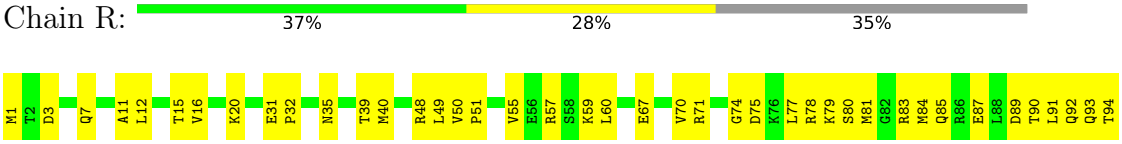
• Molecule 11: DASH complex subunit HSK3

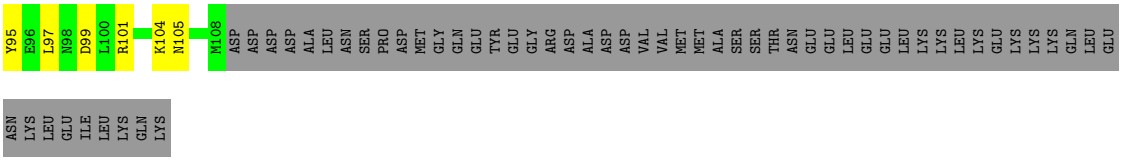
Chain c:



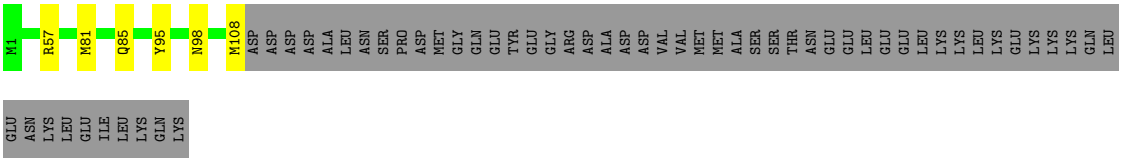
• Molecule 12: DASH complex subunit SPC19

Chain R:





• Molecule 12: DASH complex subunit SPC19



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248732	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.815	Depositor
Minimum map value	-0.855	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.22	0/1462	0.34	0/2041
1	F	0.22	0/1462	0.35	0/2041
2	B	0.21	0/1179	0.35	0/1646
2	G	0.21	0/1174	0.36	0/1639
3	I	0.25	0/766	0.57	2/1034 (0.2%)
3	U	0.29	0/766	0.70	3/1034 (0.3%)
3	e	0.27	0/82	0.61	0/109
4	J	0.25	0/945	0.51	0/1275
4	V	0.26	0/945	0.52	1/1275 (0.1%)
5	K	0.27	0/844	0.58	0/1135
5	W	0.27	0/844	0.50	0/1135
6	L	0.26	0/490	0.49	0/662
6	X	0.30	0/540	0.61	1/730 (0.1%)
7	M	0.28	0/577	0.51	0/779
7	Y	0.26	0/577	0.48	0/779
8	N	0.33	0/751	0.59	0/1007
8	Z	0.29	0/768	0.62	0/1029
9	O	0.26	0/1962	0.53	0/2638
9	a	0.26	0/1958	0.51	0/2633
10	P	0.28	0/535	0.49	0/722
10	b	0.27	0/569	0.54	0/768
11	Q	0.27	0/534	0.53	0/716
11	c	0.26	0/534	0.46	0/716
12	R	0.27	0/864	0.62	0/1161
12	d	0.26	0/864	0.61	0/1161
All	All	0.26	0/21992	0.51	7/29865 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	143	MET	CA-CB-CG	6.21	123.86	113.30
3	U	120	ASP	CB-CG-OD2	6.00	123.70	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	143	MET	CA-CB-CG	5.96	123.42	113.30
3	U	123	ASP	CB-CG-OD1	5.45	123.21	118.30
4	V	108	ASP	CB-CG-OD1	5.33	123.10	118.30
3	I	141	LEU	CA-CB-CG	-5.21	103.31	115.30
6	X	28	LEU	CA-CB-CG	5.01	126.83	115.30

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	1463	0	607	0	0
1	F	1463	0	607	0	0
2	B	1180	0	483	1	0
2	G	1175	0	481	2	0
3	I	757	0	753	19	0
3	U	757	0	753	21	0
3	e	82	0	79	0	0
4	J	935	0	952	31	0
4	V	935	0	952	24	0
5	K	837	0	837	29	0
5	W	837	0	837	9	0
6	L	485	0	475	15	0
6	X	535	0	522	19	0
7	M	571	0	578	25	0
7	Y	571	0	578	14	0
8	N	744	0	754	38	0
8	Z	761	0	772	26	0
9	O	1929	0	1929	60	0
9	a	1925	0	1926	0	0
10	P	527	0	513	22	0
10	b	561	0	548	0	0
11	Q	527	0	520	13	0
11	c	527	0	520	0	0
12	R	859	0	897	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	d	859	0	897	0	0
All	All	21802	0	18770	337	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 11.

All (337) 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)
8:N:18:GLN:HA	8:N:21:LEU:HD12	1.65	0.77
9:O:176:ARG:HB3	9:O:186:VAL:HG21	1.67	0.76
7:M:17:ILE:HG13	11:Q:11:GLN:HE22	1.49	0.76
4:V:68:SER:O	8:Z:15:LYS:NZ	2.19	0.76
4:J:104:ASN:ND2	8:N:56:GLU:OE2	2.20	0.75
11:Q:8:GLN:HA	11:Q:11:GLN:HE21	1.51	0.75
9:O:247:ILE:O	12:R:95:TYR:OH	2.05	0.73
9:O:174:ILE:HD13	9:O:209:LEU:HD11	1.69	0.72
12:R:101:ARG:HA	12:R:104:LYS:HE2	1.71	0.72
3:I:121:ILE:HD12	3:I:121:ILE:H	1.54	0.71
4:V:79:LYS:NZ	8:Z:22:ASP:OD1	2.18	0.71
3:U:60:GLN:HA	3:U:63:LEU:HG	1.73	0.71
5:K:24:LEU:HD21	12:R:12:LEU:HB3	1.72	0.70
12:R:90:THR:O	12:R:94:THR:HG23	1.92	0.69
3:I:141:LEU:HD13	4:J:167:ARG:NH2	2.08	0.69
8:N:66:LEU:HA	8:N:70:LEU:HD22	1.73	0.68
12:R:3:ASP:O	12:R:7:GLN:HG3	1.94	0.68
8:Z:13:LEU:HD22	8:Z:16:TYR:HE2	1.59	0.68
4:J:166:LEU:HB3	4:J:167:ARG:HH22	1.58	0.67
5:W:3:SER:OG	5:W:5:ASP:OD1	2.12	0.67
7:Y:3:ASN:HB3	7:Y:6:GLU:HG2	1.76	0.67
5:K:124:MET:HB3	12:R:49:LEU:HD12	1.75	0.67
9:O:67:ASN:O	9:O:71:GLN:N	2.28	0.67
9:O:261:MET:SD	12:R:101:ARG:NH1	2.67	0.67
9:O:203:GLU:OE1	12:R:83:ARG:NH1	2.28	0.66
5:K:13:LYS:O	5:K:16:GLN:NE2	2.28	0.66
9:O:218:THR:HG21	9:O:230:TYR:HB2	1.78	0.65
9:O:175:GLN:HB3	9:O:176:ARG:NH2	2.12	0.64
12:R:35:ASN:O	12:R:39:THR:HG23	1.98	0.64
12:R:93:GLN:O	12:R:97:LEU:HD22	1.99	0.63
3:I:128:ILE:HD11	4:J:129:TYR:HB2	1.80	0.63
4:J:163:ILE:O	4:J:167:ARG:HG2	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:57:SER:HB3	8:Z:70:LEU:HD12	1.81	0.63
5:K:4:ILE:HG21	10:P:6:LYS:HE2	1.80	0.62
9:O:254:GLN:NE2	12:R:99:ASP:OD1	2.32	0.62
7:M:45:GLU:OE2	7:M:45:GLU:N	2.27	0.62
9:O:97:ARG:HH12	10:P:54:MET:HE3	1.63	0.62
8:N:58:ARG:O	8:N:62:VAL:HG13	2.00	0.62
8:N:58:ARG:HH12	7:Y:15:ARG:CZ	2.12	0.62
9:O:174:ILE:HG23	9:O:175:GLN:OE1	2.00	0.62
3:I:61:GLN:O	3:I:65:PRO:HD2	2.00	0.60
9:O:247:ILE:O	9:O:251:VAL:HG13	2.00	0.60
4:J:163:ILE:O	4:J:167:ARG:NH1	2.34	0.60
8:N:53:ILE:HG22	8:N:54:LEU:H	1.67	0.60
9:O:40:ASN:H	9:O:43:SER:HB2	1.66	0.60
9:O:118:LYS:NZ	12:R:57:ARG:HE	2.00	0.60
8:N:54:LEU:O	8:N:58:ARG:CB	2.50	0.60
9:O:83:PHE:HE1	12:R:51:PRO:HD2	1.65	0.60
4:J:166:LEU:HB3	4:J:167:ARG:NH2	2.17	0.59
6:L:28:LEU:HD21	8:N:16:TYR:HE2	1.68	0.59
12:R:75:ASP:OD1	12:R:78:ARG:NH2	2.36	0.58
5:W:5:ASP:OD1	5:W:5:ASP:N	2.37	0.58
11:Q:23:LEU:HA	11:Q:26:THR:HG22	1.84	0.58
9:O:172:PRO:O	9:O:176:ARG:HG2	2.03	0.58
5:W:128:ARG:NH2	5:W:132:ASN:OD1	2.36	0.58
8:Z:12:VAL:HG12	8:Z:16:TYR:CZ	2.38	0.58
6:X:24:ARG:HH21	6:X:28:LEU:HD23	1.69	0.58
9:O:89:ARG:O	9:O:93:MET:HG2	2.04	0.57
9:O:248:LYS:O	9:O:251:VAL:HG22	2.03	0.57
12:R:80:SER:O	12:R:84:MET:HG3	2.03	0.57
7:Y:5:HIS:O	7:Y:9:GLN:HG2	2.04	0.57
7:Y:13:LEU:O	7:Y:17:ILE:HG12	2.04	0.57
2:G:304:ILE:O	2:G:309:GLN:N	2.29	0.57
8:N:53:ILE:O	8:N:56:GLU:N	2.30	0.57
10:P:20:ASN:O	10:P:24:ILE:HG12	2.04	0.57
4:V:136:ARG:NE	4:V:140:GLU:OE2	2.38	0.57
3:I:118:PRO:HB2	3:I:121:ILE:HG13	1.87	0.57
8:N:81:GLN:NE2	8:N:85:GLU:OE2	2.38	0.57
11:Q:17:ARG:NH2	12:R:7:GLN:OE1	2.38	0.56
5:W:79:GLU:OE1	5:W:79:GLU:N	2.35	0.56
9:O:175:GLN:HB3	9:O:176:ARG:HH22	1.70	0.56
9:O:251:VAL:HG12	12:R:95:TYR:HE1	1.69	0.56
7:Y:33:GLU:O	7:Y:37:ILE:HG12	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:79:ILE:HG22	8:Z:83:LYS:NZ	2.20	0.56
7:M:5:HIS:O	7:M:9:GLN:HG3	2.05	0.56
8:N:21:LEU:HA	8:N:24:LYS:NZ	2.20	0.56
9:O:250:GLU:HG3	12:R:95:TYR:OH	2.05	0.56
4:J:114:HIS:ND1	7:M:58:VAL:HG21	2.21	0.56
5:K:4:ILE:O	5:K:8:ILE:HG12	2.05	0.56
12:R:89:ASP:O	12:R:92:GLN:HG3	2.06	0.56
7:M:67:ASN:O	7:M:69:LYS:NZ	2.38	0.56
8:Z:79:ILE:HG22	8:Z:83:LYS:HZ3	1.71	0.55
3:U:124:ASP:O	3:U:128:ILE:HG12	2.07	0.55
5:K:125:VAL:HG12	9:O:53:LYS:HB2	1.88	0.55
7:M:5:HIS:NE2	10:P:11:GLU:OE2	2.40	0.55
9:O:97:ARG:HG3	10:P:58:GLU:OE2	2.07	0.55
2:B:304:ILE:O	2:B:309:GLN:N	2.32	0.55
7:M:54:TYR:O	7:M:58:VAL:HG13	2.07	0.55
3:I:142:VAL:HA	3:I:145:LEU:HD12	1.89	0.55
7:M:46:ILE:O	7:M:50:ILE:HG23	2.06	0.55
8:N:58:ARG:HH22	7:Y:12:ILE:HG12	1.72	0.55
9:O:83:PHE:CE1	12:R:51:PRO:HD2	2.42	0.55
4:V:82:THR:O	4:V:86:LYS:HG2	2.07	0.55
5:K:31:GLN:NE2	12:R:20:LYS:HD2	2.22	0.54
7:M:59:GLN:O	7:M:63:GLU:HG2	2.07	0.54
7:M:25:GLU:O	7:M:29:ILE:HG12	2.06	0.54
9:O:83:PHE:CE1	12:R:50:VAL:HG13	2.42	0.54
12:R:101:ARG:HA	12:R:104:LYS:CE	2.37	0.54
4:V:74:ILE:O	4:V:78:ILE:HG12	2.07	0.54
8:N:31:LYS:O	8:N:35:TYR:HD1	1.91	0.54
3:U:125:LEU:O	3:U:129:LYS:HG2	2.07	0.54
3:I:78:ASP:O	3:I:82:THR:HG23	2.08	0.54
4:J:139:ASN:HA	4:J:142:VAL:HG22	1.90	0.54
8:Z:13:LEU:HA	8:Z:16:TYR:CD2	2.42	0.54
6:X:52:SER:HB2	8:Z:53:ILE:HG23	1.90	0.54
5:K:11:LYS:O	5:K:15:LEU:HD23	2.08	0.53
9:O:241:SER:O	9:O:245:ARG:HG3	2.07	0.53
5:K:15:LEU:HD22	10:P:17:ILE:HD11	1.90	0.53
6:L:17:ASP:OD1	6:L:17:ASP:N	2.41	0.53
4:V:71:LEU:HA	4:V:74:ILE:CG1	2.39	0.53
8:N:49:SER:OG	8:N:51:ASP:OD1	2.20	0.53
4:V:70:SER:O	4:V:74:ILE:HG12	2.09	0.53
5:K:24:LEU:HG	12:R:16:VAL:HG21	1.91	0.53
9:O:83:PHE:CZ	12:R:50:VAL:HG13	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:232:GLN:HA	9:O:235:HIS:HD1	1.74	0.53
11:Q:7:ARG:O	11:Q:11:GLN:HG3	2.09	0.53
4:V:75:THR:O	4:V:79:LYS:HG2	2.09	0.53
4:J:71:LEU:HD21	8:N:16:TYR:CE1	2.44	0.52
3:U:140:ASN:HA	3:U:143:MET:SD	2.49	0.52
4:V:67:GLU:O	4:V:71:LEU:HD13	2.09	0.52
4:J:65:LEU:O	4:J:68:SER:OG	2.26	0.52
7:M:9:GLN:HA	7:M:12:ILE:HG22	1.90	0.52
7:M:53:ASN:ND2	8:N:77:SER:OG	2.43	0.52
9:O:246:PHE:O	9:O:250:GLU:HG2	2.09	0.52
9:O:261:MET:O	9:O:265:HIS:N	2.37	0.52
12:R:87:GLU:O	12:R:91:LEU:HD12	2.08	0.52
6:X:17:ASP:O	6:X:21:ILE:HG12	2.09	0.52
3:U:62:LEU:O	3:U:66:LYS:HE2	2.10	0.52
6:L:24:ARG:O	6:L:28:LEU:HD23	2.09	0.52
7:M:44:LEU:HD11	10:P:54:MET:HG2	1.91	0.52
8:N:19:LEU:O	8:N:23:LEU:HD23	2.09	0.52
6:X:42:LEU:HD13	6:X:45:LEU:HD23	1.92	0.52
8:Z:38:HIS:ND1	8:Z:47:THR:OG1	2.43	0.52
6:L:53:ILE:O	6:L:57:ARG:HG3	2.10	0.51
9:O:262:SER:OG	12:R:101:ARG:NH2	2.43	0.51
4:J:62:GLN:OE1	4:J:62:GLN:N	2.26	0.51
8:N:83:LYS:HG3	5:W:1:MET:HB3	1.91	0.51
7:M:13:LEU:O	7:M:17:ILE:HG12	2.10	0.51
4:J:85:LEU:HD13	4:J:89:LEU:HD22	1.93	0.51
5:K:18:LEU:HD23	5:K:21:ILE:HD12	1.92	0.51
9:O:174:ILE:O	9:O:178:LEU:HG	2.10	0.51
9:O:40:ASN:O	9:O:44:ILE:HG23	2.10	0.51
8:Z:22:ASP:OD2	8:Z:22:ASP:N	2.41	0.51
10:P:13:LEU:O	10:P:17:ILE:HG12	2.11	0.51
10:P:60:LEU:HD12	10:P:64:PHE:HE2	1.76	0.51
12:R:67:GLU:O	12:R:70:VAL:HG12	2.12	0.50
4:V:112:ASN:O	4:V:116:GLN:HG2	2.11	0.50
6:L:74:GLU:N	6:L:74:GLU:OE1	2.44	0.50
4:V:116:GLN:HE22	7:Y:72:LEU:HD23	1.76	0.50
3:I:88:HIS:CE1	9:O:24:PHE:HB3	2.47	0.50
6:L:63:SER:O	6:L:67:LYS:HG2	2.12	0.50
12:R:67:GLU:O	12:R:71:ARG:HG2	2.10	0.50
4:J:146:ASP:OD2	4:J:146:ASP:N	2.39	0.50
7:M:24:ASN:ND2	11:Q:15:GLU:OE1	2.44	0.50
6:L:48:SER:HB2	8:N:53:ILE:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:92:TYR:O	4:V:96:VAL:HG12	2.12	0.50
4:J:71:LEU:HD23	8:N:15:LYS:HG2	1.93	0.50
8:N:54:LEU:O	8:N:58:ARG:HB3	2.11	0.50
12:R:71:ARG:HA	12:R:71:ARG:NH1	2.27	0.50
6:L:26:ILE:O	6:L:29:GLN:HG3	2.12	0.50
7:M:13:LEU:O	7:M:16:ILE:HG22	2.12	0.50
3:U:131:LEU:O	3:U:135:GLU:HG2	2.12	0.50
7:Y:46:ILE:O	7:Y:50:ILE:HG23	2.11	0.49
4:V:129:TYR:CE2	4:V:133:ILE:HD11	2.47	0.49
6:X:16:THR:HA	8:Z:3:HIS:CE1	2.47	0.49
5:K:69:GLY:HA2	5:K:72:GLN:HG2	1.95	0.49
9:O:245:ARG:HB2	9:O:245:ARG:NH1	2.28	0.49
4:J:139:ASN:O	4:J:143:ASN:N	2.28	0.49
12:R:11:ALA:O	12:R:15:THR:HG23	2.13	0.49
12:R:94:THR:HA	12:R:97:LEU:HD23	1.94	0.49
3:U:122:GLN:O	3:U:126:ILE:HG22	2.12	0.49
6:X:16:THR:HA	8:Z:3:HIS:ND1	2.27	0.49
3:U:62:LEU:HD21	6:X:28:LEU:HD13	1.94	0.49
3:I:121:ILE:H	3:I:121:ILE:CD1	2.25	0.49
3:U:120:ASP:OD2	3:U:123:ASP:HB3	2.13	0.49
4:V:135:ASP:OD2	4:V:135:ASP:N	2.45	0.49
4:V:148:ASP:OD1	4:V:148:ASP:N	2.39	0.49
6:X:71:ASP:OD1	6:X:71:ASP:N	2.46	0.49
4:V:136:ARG:O	4:V:140:GLU:HG2	2.13	0.49
3:U:72:ASP:O	3:U:75:ILE:HG13	2.13	0.48
3:I:130:GLN:O	3:I:134:LEU:HG	2.13	0.48
5:K:34:GLU:HA	5:K:34:GLU:OE1	2.14	0.48
9:O:253:LEU:O	9:O:257:ARG:HG3	2.14	0.48
5:K:21:ILE:HG22	10:P:24:ILE:HD12	1.95	0.48
5:K:24:LEU:CD2	12:R:12:LEU:HB3	2.40	0.48
12:R:87:GLU:O	12:R:90:THR:OG1	2.22	0.48
8:Z:53:ILE:O	8:Z:56:GLU:N	2.24	0.48
10:P:15:GLN:O	10:P:19:VAL:HG12	2.14	0.48
8:Z:12:VAL:HG12	8:Z:16:TYR:CE1	2.49	0.48
9:O:169:LYS:HZ3	9:O:171:ASP:HB3	1.78	0.48
12:R:39:THR:OG1	12:R:40:MET:N	2.47	0.48
3:U:144:GLU:O	3:U:148:MET:HG2	2.13	0.48
4:V:71:LEU:O	4:V:75:THR:OG1	2.19	0.48
8:Z:53:ILE:HG22	8:Z:54:LEU:H	1.79	0.48
9:O:253:LEU:HB2	9:O:257:ARG:HH21	1.78	0.48
11:Q:32:ILE:O	11:Q:36:GLN:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:141:LEU:HD23	3:I:141:LEU:HA	1.73	0.47
4:J:71:LEU:HB3	8:N:15:LYS:HE3	1.96	0.47
6:X:31:ILE:O	6:X:35:MET:HG2	2.14	0.47
4:J:60:THR:O	4:J:63:SER:OG	2.28	0.47
9:O:229:ASP:OD1	9:O:232:GLN:NE2	2.34	0.47
3:U:138:LYS:O	3:U:142:VAL:HG13	2.14	0.47
6:X:71:ASP:OD1	6:X:75:SER:HB3	2.13	0.47
2:G:335:VAL:O	2:G:340:ILE:N	2.38	0.47
3:I:60:GLN:HE21	3:I:61:GLN:HG3	1.80	0.47
7:M:39:ASN:O	7:M:42:LYS:NZ	2.48	0.47
8:N:31:LYS:HB3	8:N:35:TYR:HE1	1.80	0.47
9:O:251:VAL:HG12	12:R:95:TYR:CE1	2.49	0.47
6:X:23:GLN:O	6:X:27:VAL:HG22	2.14	0.47
8:Z:49:SER:O	8:Z:53:ILE:HG13	2.15	0.47
4:J:78:ILE:HD13	8:N:23:LEU:HD22	1.97	0.47
12:R:57:ARG:NH1	12:R:60:LEU:HD22	2.30	0.47
7:M:33:GLU:OE1	7:M:33:GLU:HA	2.15	0.47
4:J:116:GLN:HB3	11:Q:58:ILE:HD11	1.97	0.47
6:L:66:TRP:HE1	8:N:67:VAL:HG12	1.80	0.47
5:K:70:LEU:HD21	6:L:73:LEU:HD23	1.97	0.46
12:R:74:GLY:O	12:R:78:ARG:HG2	2.15	0.46
9:O:60:ALA:O	9:O:64:PHE:N	2.47	0.46
3:I:64:LEU:HD21	9:O:4:SER:HB3	1.96	0.46
7:Y:45:GLU:OE1	7:Y:45:GLU:N	2.33	0.46
4:J:124:MET:HG2	12:R:40:MET:SD	2.55	0.46
4:J:120:ILE:HD11	11:Q:51:SER:O	2.15	0.46
3:U:122:GLN:OE1	3:U:122:GLN:N	2.28	0.46
5:W:26:ASP:O	5:W:30:ILE:HG12	2.16	0.46
5:K:68:LEU:HD21	9:O:111:PRO:HG2	1.96	0.46
7:M:24:ASN:ND2	11:Q:18:GLU:OE1	2.48	0.46
12:R:79:LYS:HZ2	12:R:83:ARG:NH1	2.13	0.46
5:K:125:VAL:N	12:R:50:VAL:O	2.37	0.46
7:M:2:GLU:OE2	7:M:2:GLU:N	2.31	0.46
7:M:18:GLY:O	7:M:22:ARG:HG2	2.16	0.46
8:N:31:LYS:O	8:N:34:ASN:N	2.49	0.46
10:P:41:PRO:O	10:P:45:THR:HG23	2.17	0.45
6:X:19:TYR:HA	6:X:22:GLU:OE1	2.16	0.45
9:O:172:PRO:O	9:O:176:ARG:NH1	2.49	0.45
3:I:88:HIS:NE2	4:J:99:VAL:HG21	2.32	0.45
7:M:12:ILE:HG13	7:M:15:ARG:NH2	2.31	0.45
9:O:98:ARG:HH21	10:P:51:GLU:HB3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:180:ALA:O	9:O:184:GLY:N	2.49	0.45
9:O:244:LEU:O	9:O:248:LYS:HG2	2.15	0.45
4:V:90:PRO:HA	4:V:93:VAL:HG22	1.98	0.45
3:I:98:LEU:O	3:I:102:LEU:HD23	2.16	0.45
9:O:246:PHE:HA	9:O:249:LYS:HG2	1.96	0.45
11:Q:6:GLN:HA	12:R:1:MET:SD	2.57	0.45
5:K:8:ILE:HG22	5:K:12:ARG:NE	2.31	0.45
12:R:71:ARG:HA	12:R:71:ARG:CZ	2.47	0.45
4:V:71:LEU:HA	4:V:74:ILE:HG12	1.98	0.45
3:I:60:GLN:NE2	3:I:61:GLN:HG3	2.31	0.45
5:K:18:LEU:HD12	10:P:17:ILE:HD12	1.99	0.45
3:U:110:TRP:HE1	5:W:126:ARG:HG3	1.81	0.45
11:Q:61:MET:O	11:Q:64:MET:HG3	2.17	0.45
4:J:63:SER:HA	4:J:66:LYS:HG2	1.99	0.44
6:X:60:GLN:HA	6:X:60:GLN:OE1	2.17	0.44
4:V:111:ILE:HG23	7:Y:62:LEU:HD21	1.98	0.44
5:W:13:LYS:HA	5:W:16:GLN:HG2	1.99	0.44
3:U:59:ILE:HA	3:U:62:LEU:HG	1.99	0.44
7:Y:23:LEU:HD12	7:Y:23:LEU:HA	1.87	0.44
8:N:21:LEU:HA	8:N:24:LYS:HZ1	1.81	0.44
8:N:54:LEU:O	8:N:58:ARG:HB2	2.17	0.44
9:O:41:LYS:O	9:O:44:ILE:HG12	2.18	0.44
6:X:73:LEU:HD23	6:X:73:LEU:H	1.82	0.44
8:Z:53:ILE:O	8:Z:55:GLN:N	2.50	0.44
8:N:28:GLU:OE1	8:N:28:GLU:HA	2.18	0.44
12:R:79:LYS:O	12:R:79:LYS:NZ	2.48	0.44
5:K:11:LYS:NZ	10:P:14:ASP:OD1	2.48	0.44
8:Z:13:LEU:HD22	8:Z:16:TYR:CE2	2.47	0.44
8:Z:20:SER:O	8:Z:24:LYS:HG2	2.17	0.44
5:K:13:LYS:HA	5:K:16:GLN:HG3	2.00	0.43
12:R:55:VAL:HG12	12:R:59:LYS:HZ2	1.83	0.43
3:I:103:TYR:O	3:I:106:MET:HG3	2.18	0.43
5:K:15:LEU:HD22	10:P:17:ILE:CD1	2.48	0.43
7:M:31:ASN:OD1	11:Q:26:THR:HB	2.19	0.43
8:N:83:LYS:O	8:N:83:LYS:HD3	2.19	0.43
4:V:127:GLN:HA	4:V:127:GLN:OE1	2.18	0.43
8:N:26:LEU:HG	8:N:30:ILE:HD13	2.01	0.43
6:X:20:PHE:CD2	6:X:21:ILE:HD13	2.54	0.43
5:K:33:THR:HG22	10:P:34:LYS:HE3	2.01	0.43
9:O:67:ASN:O	9:O:71:GLN:CA	2.66	0.43
8:Z:31:LYS:O	8:Z:35:TYR:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:71:LEU:HD23	5:W:71:LEU:H	1.83	0.42
9:O:250:GLU:HA	9:O:253:LEU:HG	2.01	0.42
9:O:261:MET:SD	12:R:105:ASN:HB3	2.59	0.42
12:R:85:GLN:NE2	12:R:89:ASP:OD2	2.52	0.42
4:V:71:LEU:HD22	8:Z:15:LYS:HD3	2.01	0.42
9:O:233:LEU:HD22	12:R:77:LEU:HD12	2.01	0.42
7:M:57:SER:OG	8:N:70:LEU:HG	2.19	0.42
4:J:70:SER:O	4:J:74:ILE:HG12	2.20	0.42
9:O:32:ASN:O	9:O:36:GLN:HG2	2.19	0.42
9:O:176:ARG:HG2	9:O:176:ARG:HH11	1.84	0.42
12:R:90:THR:O	12:R:93:GLN:HG3	2.20	0.42
3:I:96:GLU:OE2	3:I:96:GLU:HA	2.18	0.42
3:U:120:ASP:OD2	3:U:120:ASP:O	2.37	0.42
4:J:62:GLN:HA	4:J:65:LEU:HD12	2.01	0.42
4:J:112:ASN:O	4:J:116:GLN:HG2	2.19	0.42
8:Z:18:GLN:NE2	8:Z:22:ASP:OD1	2.52	0.42
5:K:57:ASP:OD1	5:K:58:SER:N	2.52	0.42
7:Y:18:GLY:O	7:Y:22:ARG:HG2	2.19	0.42
5:K:11:LYS:HB2	10:P:13:LEU:HD13	2.01	0.42
8:N:33:LEU:HD23	8:N:33:LEU:HA	1.82	0.42
3:U:63:LEU:HD12	3:U:64:LEU:N	2.35	0.42
6:L:27:VAL:O	6:L:30:GLU:HG3	2.20	0.42
8:N:51:ASP:HA	8:N:55:GLN:OE1	2.20	0.42
9:O:97:ARG:HH22	10:P:54:MET:HE2	1.84	0.42
12:R:78:ARG:HA	12:R:81:MET:HB2	2.02	0.42
4:V:139:ASN:O	4:V:143:ASN:N	2.32	0.41
6:X:49:LEU:HD13	6:X:49:LEU:HA	1.86	0.41
6:L:30:GLU:HA	6:L:33:GLU:HG3	2.02	0.41
3:U:139:ASN:HA	3:U:142:VAL:HG22	2.02	0.41
6:X:72:GLY:O	6:X:76:LEU:HG	2.20	0.41
6:L:71:ASP:N	6:L:71:ASP:OD1	2.53	0.41
4:J:77:MET:SD	4:J:78:ILE:N	2.94	0.41
10:P:12:LYS:O	10:P:16:GLU:HG2	2.21	0.41
10:P:60:LEU:HD12	10:P:64:PHE:CE2	2.54	0.41
8:Z:51:ASP:OD2	8:Z:52:GLU:N	2.54	0.41
5:K:73:TYR:CZ	5:K:119:PRO:HA	2.56	0.41
6:L:52:SER:OG	8:N:53:ILE:HG23	2.19	0.41
7:Y:21:LYS:O	7:Y:25:GLU:HG3	2.21	0.41
6:L:55:VAL:HG11	8:N:54:LEU:HD12	2.03	0.41
9:O:225:GLU:O	9:O:228:GLN:HG2	2.20	0.41
3:U:121:ILE:H	3:U:121:ILE:HG13	1.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:92:TYR:O	4:J:96:VAL:HG23	2.21	0.41
3:U:63:LEU:O	3:U:67:ILE:HG12	2.21	0.41
4:V:140:GLU:HG2	4:V:140:GLU:H	1.77	0.41
12:R:31:GLU:HB3	12:R:32:PRO:HD3	2.03	0.41
5:K:9:ALA:HA	5:K:12:ARG:HE	1.85	0.40
7:M:13:LEU:HD23	7:M:13:LEU:HA	1.89	0.40
4:J:60:THR:OG1	4:J:61:THR:N	2.54	0.40
8:N:72:LYS:O	8:N:73:GLY:C	2.59	0.40
3:U:66:LYS:HD3	3:U:66:LYS:N	2.36	0.40
3:I:132:LYS:HD2	3:I:132:LYS:O	2.21	0.40
9:O:75:ARG:NH2	9:O:77:ASP:OD2	2.39	0.40
6:X:24:ARG:HE	6:X:28:LEU:CD2	2.34	0.40
5:K:8:ILE:HG22	5:K:12:ARG:CZ	2.52	0.40
9:O:241:SER:HA	9:O:244:LEU:HB3	2.03	0.40
6:X:24:ARG:NH1	8:Z:16:TYR:CG	2.90	0.40
4:J:77:MET:HE2	9:O:12:ILE:HG21	2.04	0.40
8:N:71:LEU:HG	10:P:64:PHE:CE1	2.56	0.40
8:Z:15:LYS:O	8:Z:19:LEU:HD23	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	292/691 (42%)	291 (100%)	0	1 (0%)	41	73
1	F	292/691 (42%)	290 (99%)	1 (0%)	1 (0%)	41	73
2	B	235/451 (52%)	229 (97%)	6 (3%)	0	100	100
2	G	234/451 (52%)	228 (97%)	6 (3%)	0	100	100
3	I	93/343 (27%)	91 (98%)	2 (2%)	0	100	100
3	U	93/343 (27%)	92 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	e	9/343 (3%)	8 (89%)	1 (11%)	0	100	100
4	J	115/247 (47%)	113 (98%)	2 (2%)	0	100	100
4	V	115/247 (47%)	113 (98%)	2 (2%)	0	100	100
5	K	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
5	W	102/133 (77%)	98 (96%)	4 (4%)	0	100	100
6	L	59/94 (63%)	59 (100%)	0	0	100	100
6	X	66/94 (70%)	63 (96%)	3 (4%)	0	100	100
7	M	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
7	Y	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
8	N	90/94 (96%)	79 (88%)	11 (12%)	0	100	100
8	Z	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
9	O	231/295 (78%)	228 (99%)	3 (1%)	0	100	100
9	a	230/295 (78%)	222 (96%)	8 (4%)	0	100	100
10	P	63/292 (22%)	62 (98%)	1 (2%)	0	100	100
10	b	68/292 (23%)	67 (98%)	1 (2%)	0	100	100
11	Q	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
11	c	62/69 (90%)	62 (100%)	0	0	100	100
12	R	106/165 (64%)	105 (99%)	1 (1%)	0	100	100
12	d	106/165 (64%)	105 (99%)	1 (1%)	0	100	100
All	All	3057/6235 (49%)	2984 (98%)	71 (2%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	ILE
1	F	411	ILE

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	
3	I	89/309 (29%)	85 (96%)	4 (4%)	27	61
3	U	89/309 (29%)	86 (97%)	3 (3%)	37	68
3	e	9/309 (3%)	9 (100%)	0	100	100
4	J	109/222 (49%)	108 (99%)	1 (1%)	78	91
4	V	109/222 (49%)	108 (99%)	1 (1%)	78	91
5	K	95/120 (79%)	92 (97%)	3 (3%)	39	70
5	W	95/120 (79%)	93 (98%)	2 (2%)	53	78
6	L	56/87 (64%)	55 (98%)	1 (2%)	59	81
6	X	62/87 (71%)	58 (94%)	4 (6%)	17	48
7	M	66/66 (100%)	63 (96%)	3 (4%)	27	61
7	Y	66/66 (100%)	65 (98%)	1 (2%)	65	84
8	N	87/89 (98%)	84 (97%)	3 (3%)	37	68
8	Z	89/89 (100%)	85 (96%)	4 (4%)	27	61
9	O	217/269 (81%)	210 (97%)	7 (3%)	39	70
9	a	217/269 (81%)	210 (97%)	7 (3%)	39	70
10	P	62/259 (24%)	59 (95%)	3 (5%)	25	59
10	b	66/259 (26%)	63 (96%)	3 (4%)	27	61
11	Q	58/62 (94%)	55 (95%)	3 (5%)	23	55
11	c	58/62 (94%)	58 (100%)	0	100	100
12	R	101/153 (66%)	100 (99%)	1 (1%)	76	89
12	d	101/153 (66%)	95 (94%)	6 (6%)	19	51
All	All	1901/3581 (53%)	1841 (97%)	60 (3%)	42	70

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	63	LEU
3	I	89	GLU
3	I	129	LYS
3	I	143	MET
4	J	69	GLU
5	K	12	ARG
5	K	67	SER
5	K	116	ASP
6	L	19	TYR
7	M	21	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	M	40	ARG
7	M	68	LYS
8	N	18	GLN
8	N	42	HIS
8	N	83	LYS
9	O	83	PHE
9	O	105	LYS
9	O	179	TYR
9	O	214	MET
9	O	230	TYR
9	O	235	HIS
9	O	246	PHE
10	P	6	LYS
10	P	29	SER
10	P	38	ASP
11	Q	4	ASN
11	Q	25	GLU
11	Q	64	MET
12	R	48	ARG
3	U	96	GLU
3	U	129	LYS
3	U	143	MET
4	V	109	SER
5	W	5	ASP
5	W	72	GLN
6	X	19	TYR
6	X	20	PHE
6	X	48	SER
6	X	65	LEU
7	Y	14	SER
8	Z	16	TYR
8	Z	51	ASP
8	Z	74	SER
8	Z	77	SER
9	a	13	ASN
9	a	61	TYR
9	a	98	ARG
9	a	161	PHE
9	a	188	MET
9	a	235	HIS
9	a	246	PHE
10	b	2	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	b	6	LYS
10	b	66	GLU
12	d	57	ARG
12	d	81	MET
12	d	85	GLN
12	d	95	TYR
12	d	98	ASN
12	d	108	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	60	GLN
5	K	31	GLN
11	Q	11	GLN
9	a	254	GLN
10	b	22	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

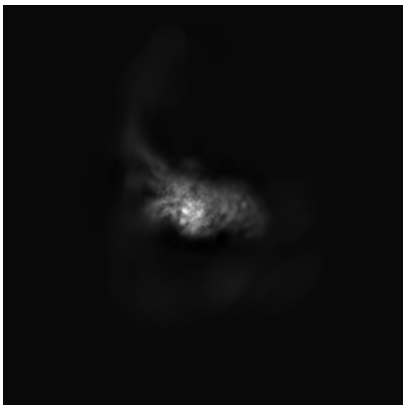
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18246. These allow visual inspection of the internal detail of the map and identification of artifacts.

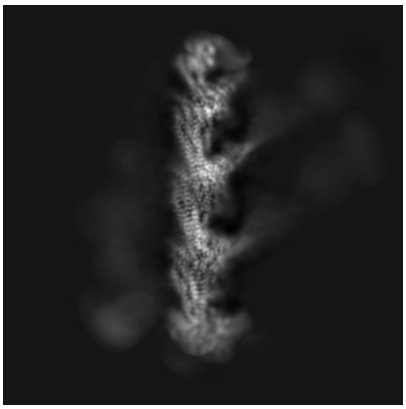
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

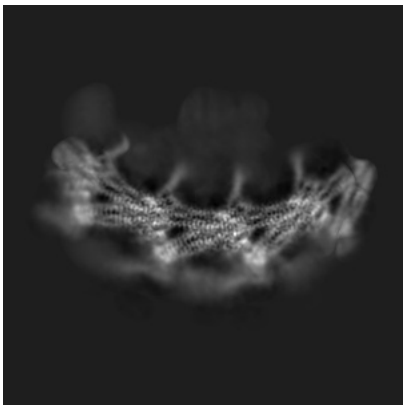
6.1.1 Primary map



X

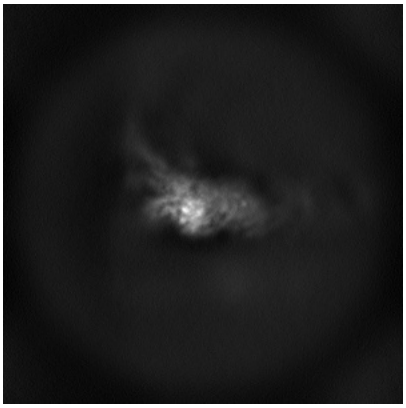


Y

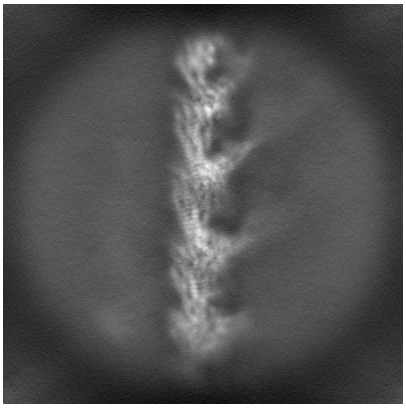


Z

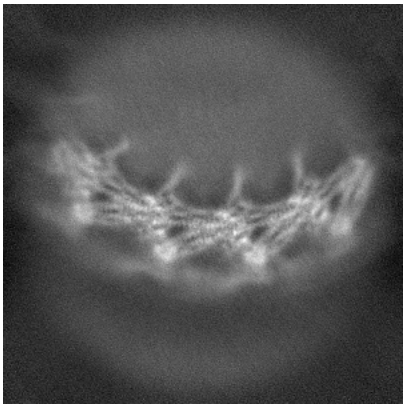
6.1.2 Raw map



X



Y



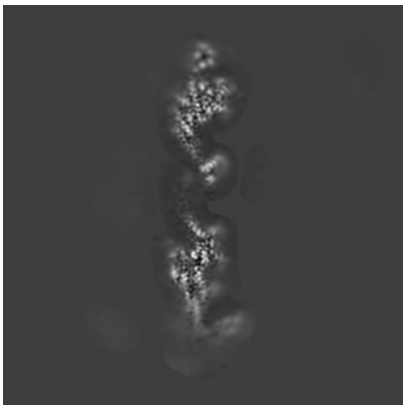
Z

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

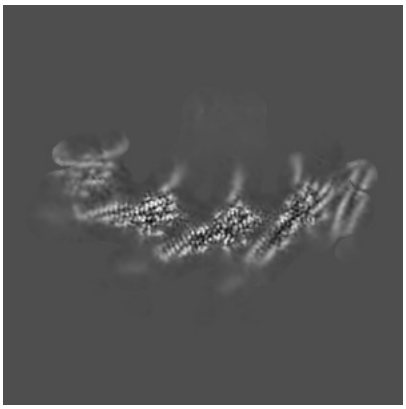
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200

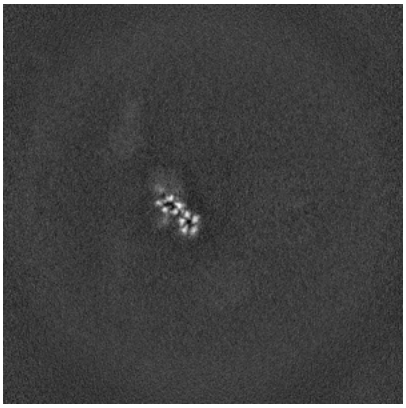


Y Index: 200

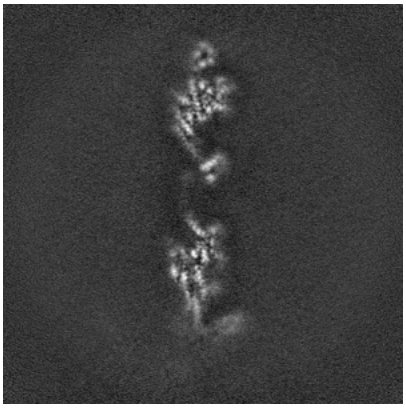


Z Index: 200

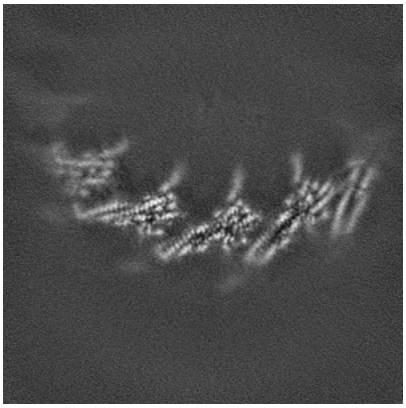
6.2.2 Raw map



X Index: 200



Y Index: 200

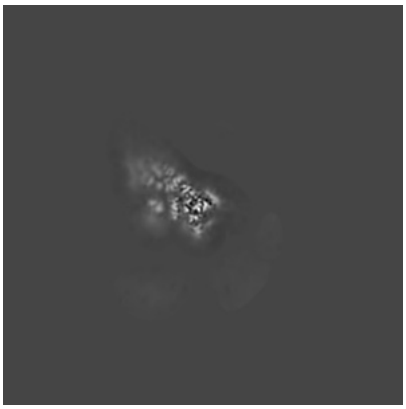


Z Index: 200

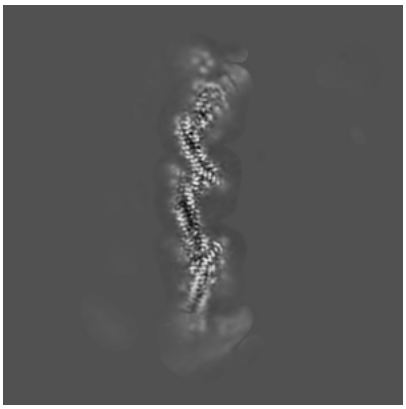
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

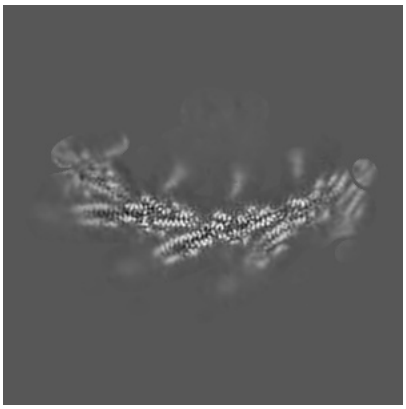
6.3.1 Primary map



X Index: 157

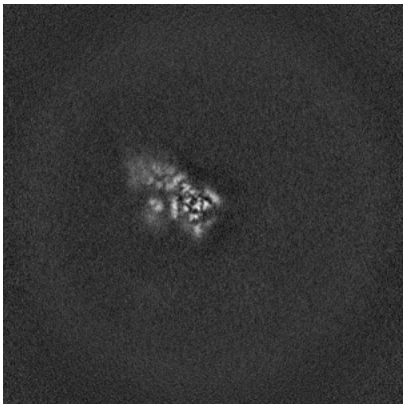


Y Index: 186

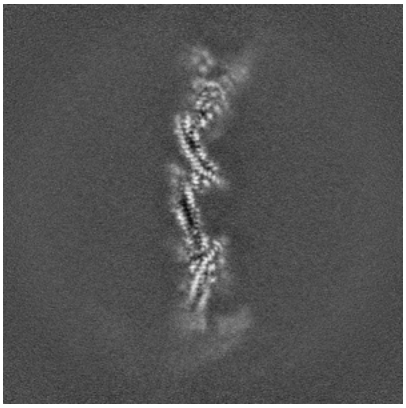


Z Index: 194

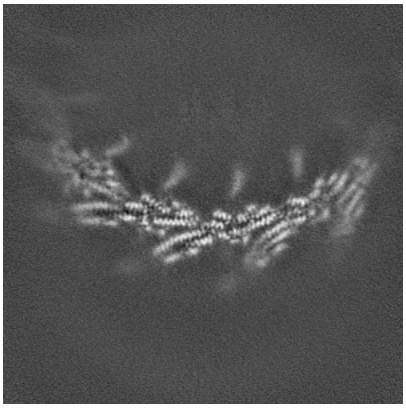
6.3.2 Raw map



X Index: 157



Y Index: 186

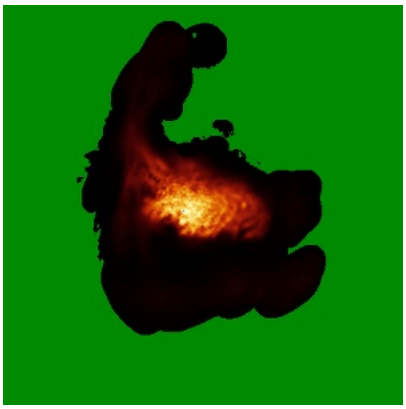


Z Index: 194

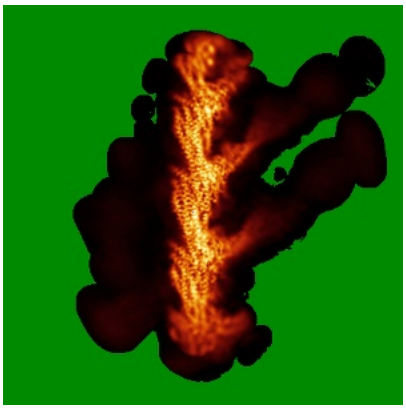
The images above show the largest variance slices of the map in three orthogonal directions.

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

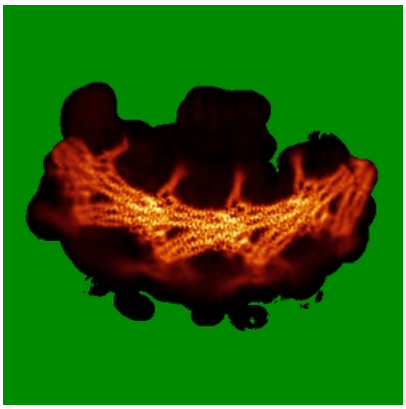
6.4.1 Primary map



X

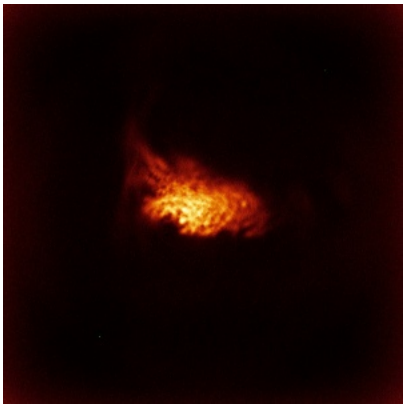


Y

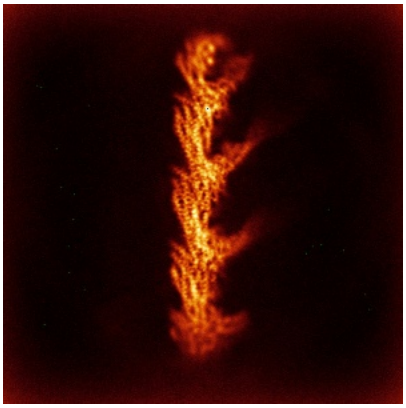


Z

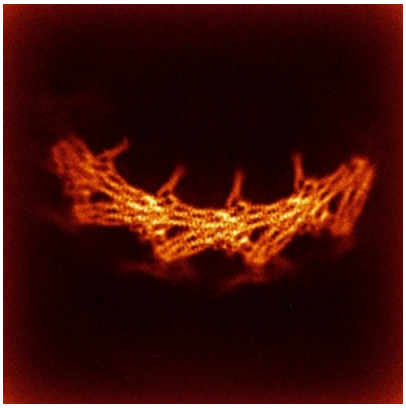
6.4.2 Raw map



X



Y



Z

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

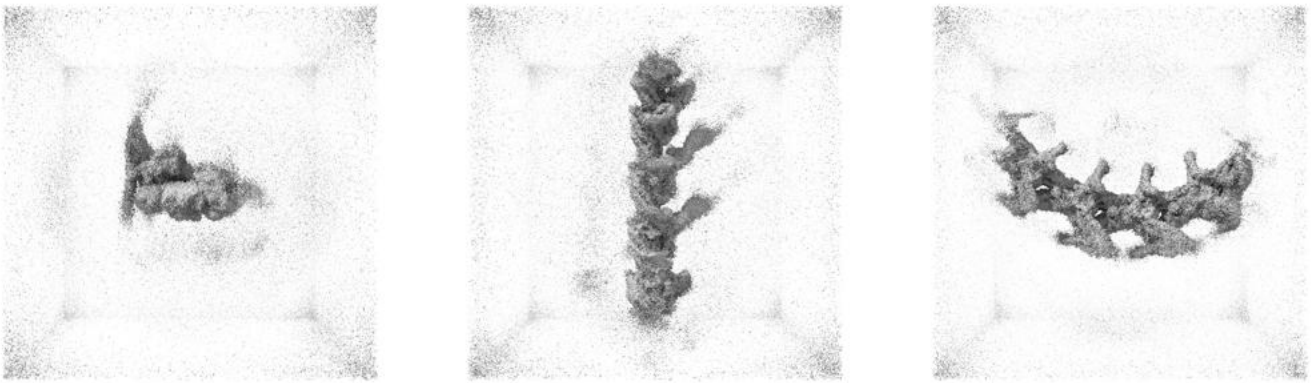
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

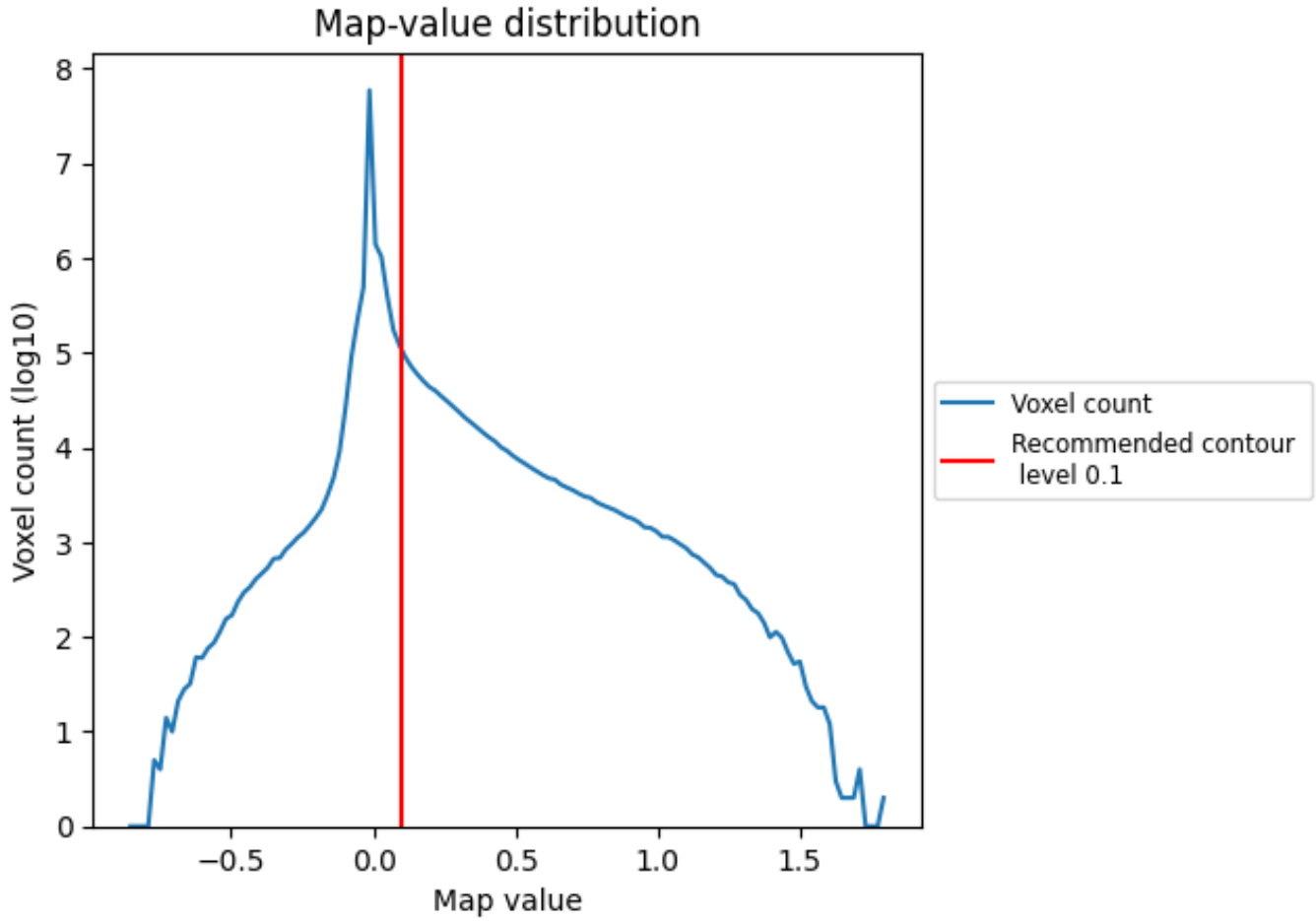
6.6 Mask visualisation (i)

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

7 Map analysis

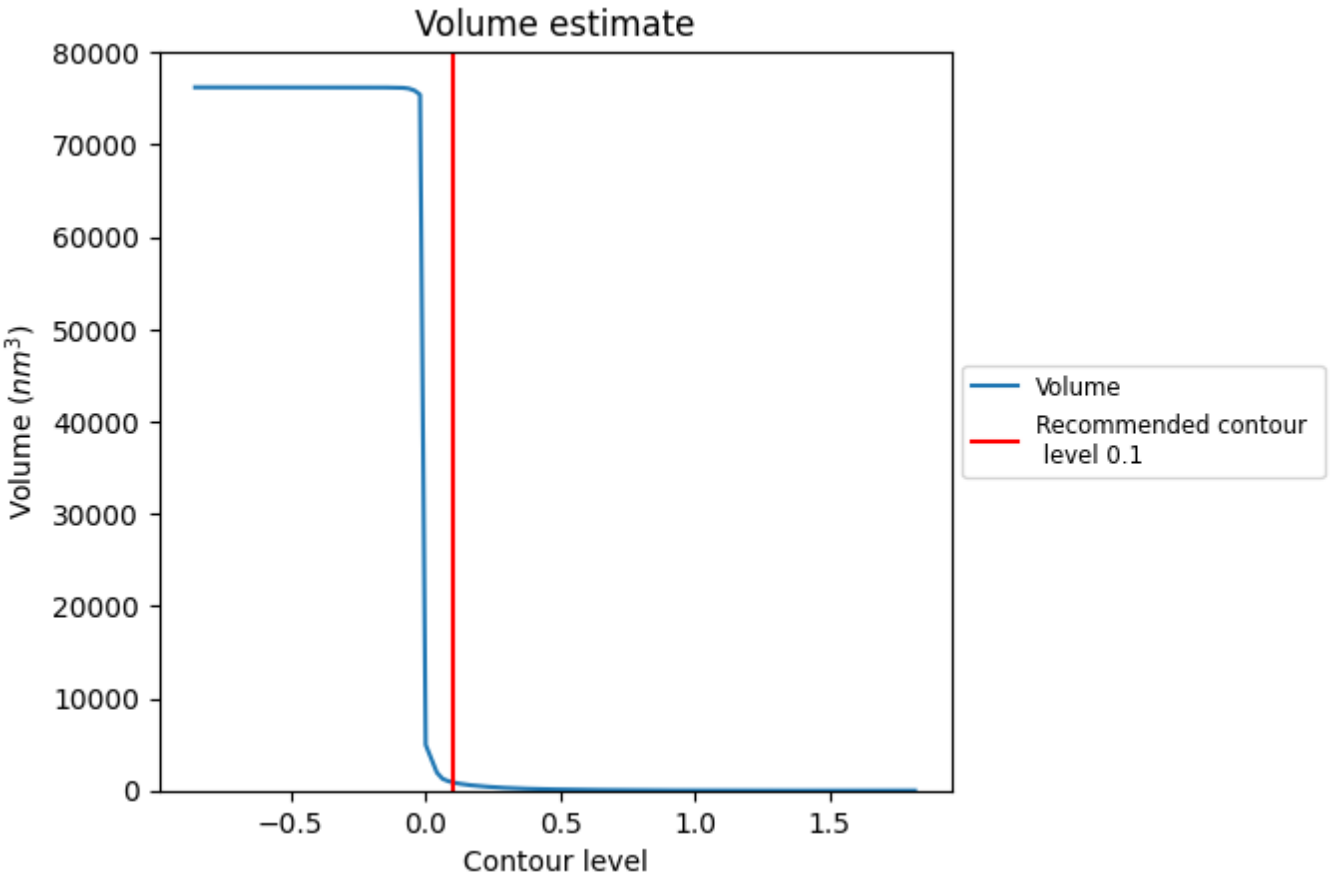
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

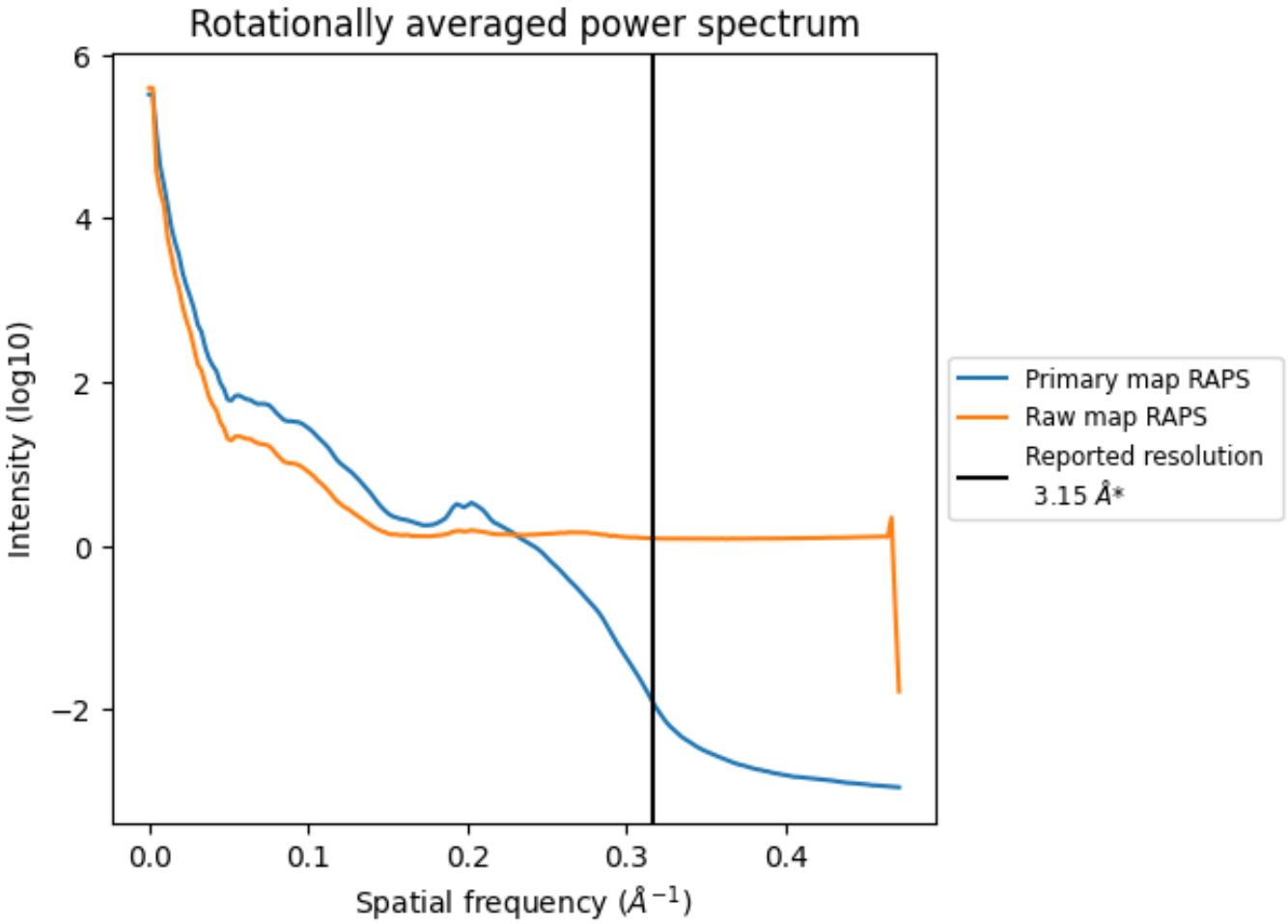
7.2 Volume estimate



The volume at the recommended contour level is 901 nm^3; this corresponds to an approximate mass of 814 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)

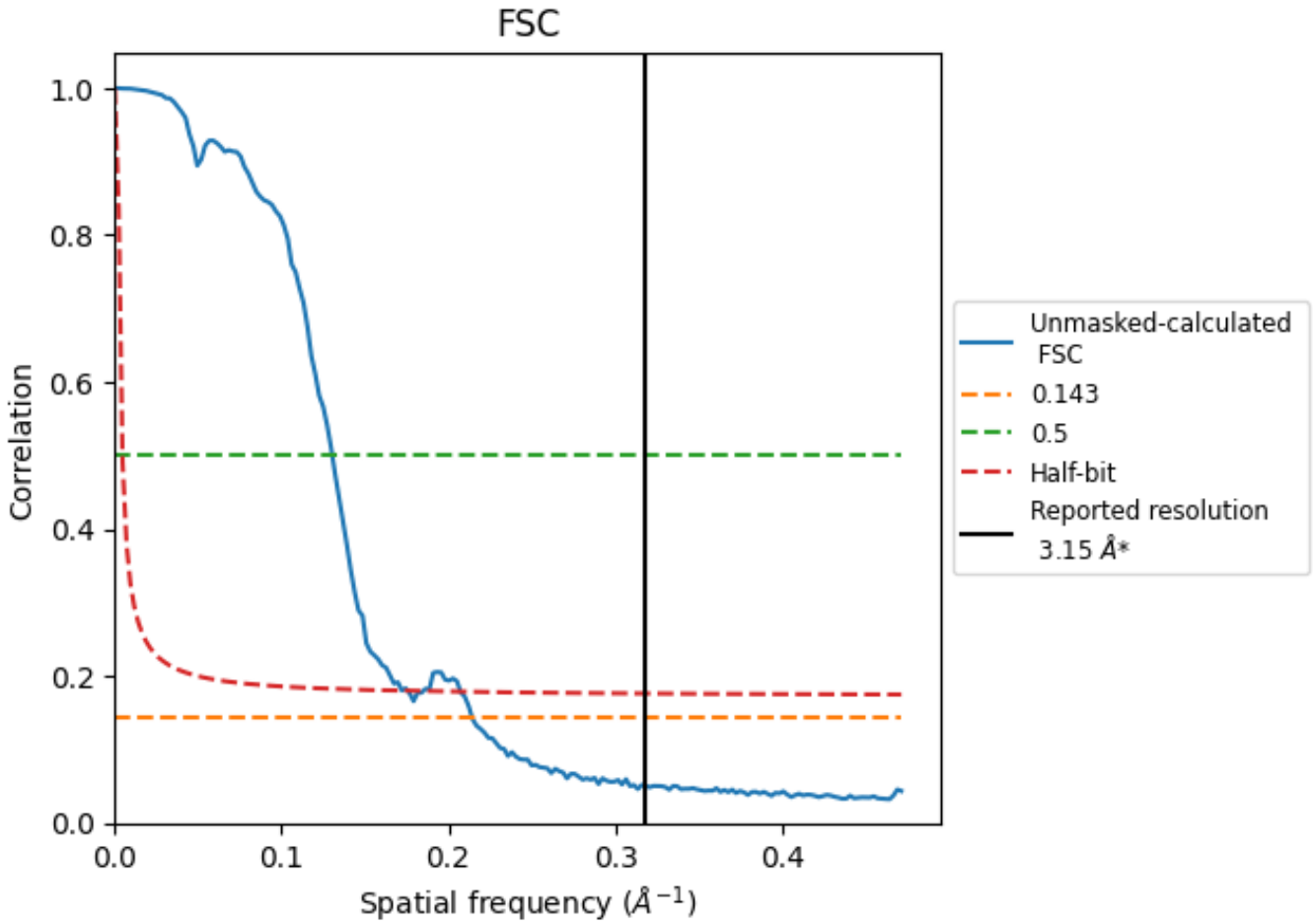


*Reported resolution corresponds to spatial frequency of 0.317 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8.2 Resolution estimates (i)

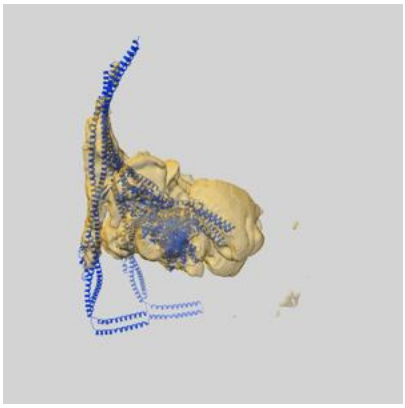
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.67	7.66	5.69

*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 4.67 differs from the reported value 3.15 by more than 10 %

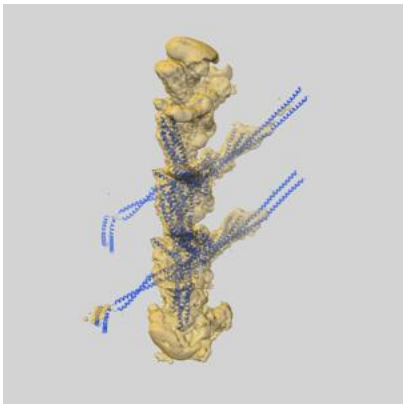
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18246 and PDB model 8Q84. Per-residue inclusion information can be found in section 3 on page 7.

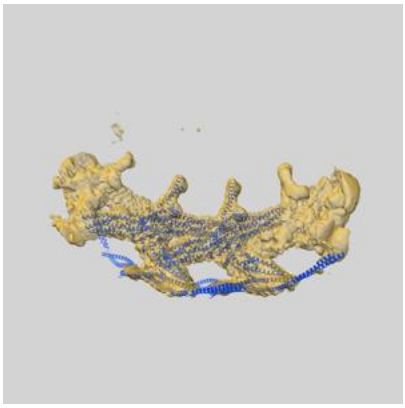
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

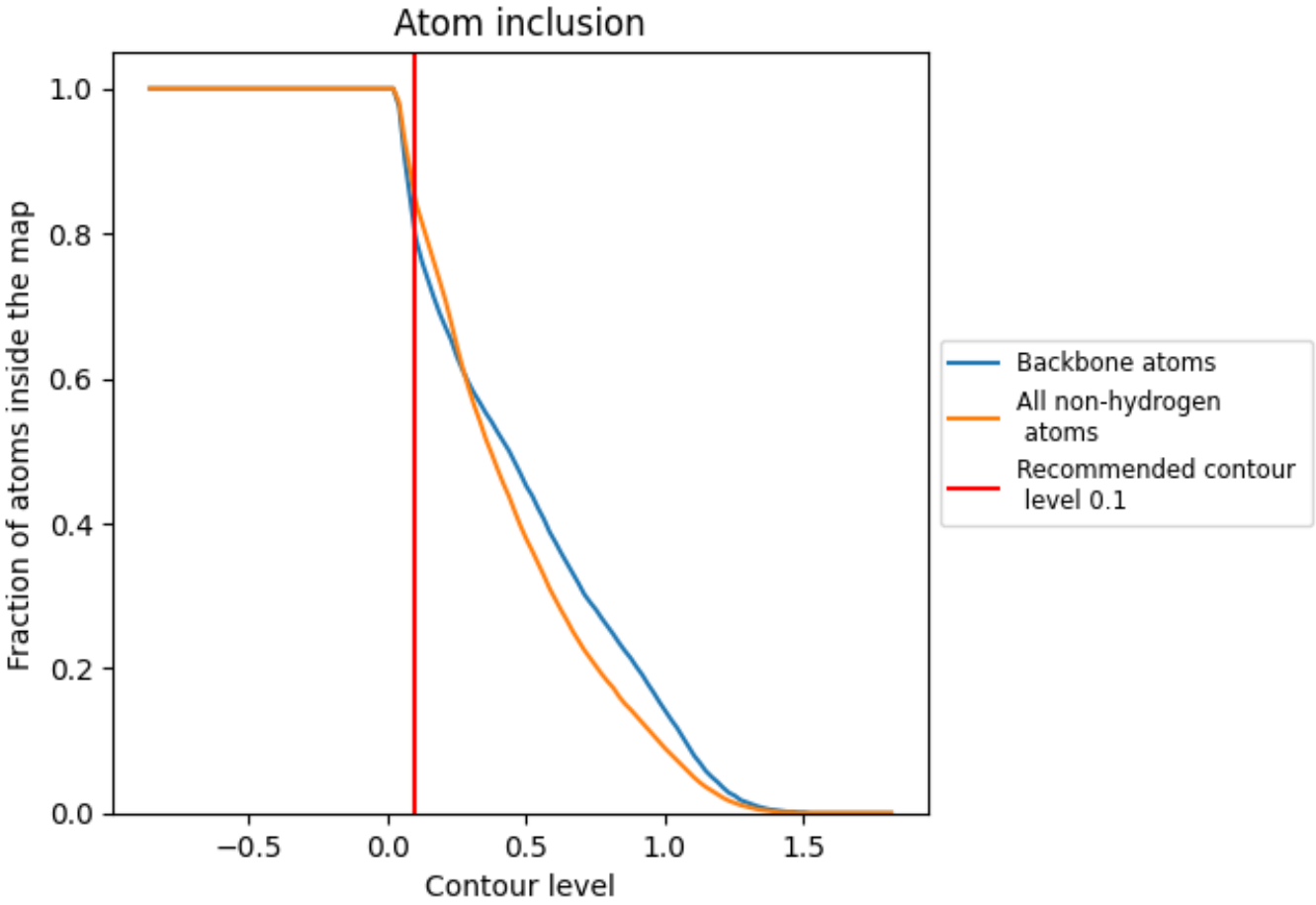
9.2 Q-score mapped to coordinate model

This section was not generated.

9.3 Atom inclusion mapped to coordinate model

This section was not generated.

9.4 Atom inclusion



At the recommended contour level, 80% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8480
A	0.4160
B	0.4420
F	0.3840
G	0.4140
I	0.9910
J	0.9980
K	0.9890
L	0.9960
M	0.9970
N	0.9760
O	0.9790
P	1.0000
Q	1.0000
R	0.9940
U	0.9960
V	0.9950
W	0.9950
X	0.9740
Y	1.0000
Z	0.9800
a	0.9880
b	0.9890
c	0.9960
d	0.9940
e	1.0000