



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 12:08 am GMT

PDB ID : 6R8Z
EMDB ID : EMD-4763
Title : Cryo-EM structure of NCP_THF2(-1)-UV-DDB
Authors : Matsumoto, S.; Cavadini, S.; Bunker, R.D.; Thoma, N.H.
Deposited on : 2019-04-02
Resolution : 3.90 Å(reported)
Based on initial models : 3EI4, 5Y0C, 4E54, 4ZUX

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.dev43
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.31.3

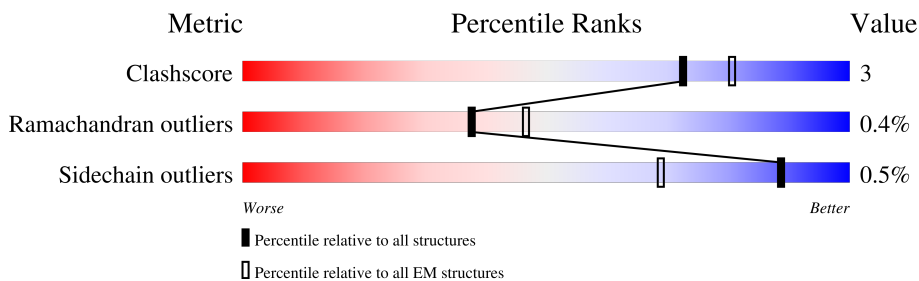
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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







Metric	Whole archive (#Entries)	EM structures (#Entries)
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 $\leq 5\%$. 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	139	
1	E	139	
2	B	106	
2	F	106	
3	C	133	
3	G	133	
4	D	129	
4	H	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	145	
6	J	145	
7	K	1163	
8	L	431	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 40831 atoms, of which 19214 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	101	Total	C	H	N	O	S	0	0
			1708	525	876	161	142	4		
1	E	101	Total	C	H	N	O	S	0	0
			1708	525	876	161	142	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P68431
A	-1	SER	-	expression tag	UNP P68431
A	0	HIS	-	expression tag	UNP P68431
E	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
E	0	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	86	Total	C	H	N	O	S	0	0
			1434	436	740	140	117	1		
2	F	82	Total	C	H	N	O	S	0	0
			1348	412	695	127	113	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62805
B	-1	SER	-	expression tag	UNP P62805
B	0	HIS	-	expression tag	UNP P62805
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
F	0	HIS	-	expression tag	UNP P62805

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	C	117	Total	C	H	N	O	0	0
			1878	571	969	181	157		
3	G	117	Total	C	H	N	O	0	0
			1878	571	969	181	157		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04908
C	-1	SER	-	expression tag	UNP P04908
C	0	HIS	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
G	0	HIS	-	expression tag	UNP P04908

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	97	Total	C	H	N	O	S	0	0
			1559	480	793	142	142	2		
4	H	97	Total	C	H	N	O	S	0	0
			1560	480	794	142	142	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
D	0	HIS	-	expression tag	UNP P06899
H	-2	GLY	-	expression tag	UNP P06899
H	-1	SER	-	expression tag	UNP P06899
H	0	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called Human alpha-satellite DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
5	I	145	Total	C	H	N	O	P	0	0
			4611	1421	1641	535	870	144		

- Molecule 6 is a DNA chain called Human alpha-satellite DNA (145-MER) with abasic sites at positions 97-98.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	J	145	4581	1410	1632	532	863	144	0	0

- Molecule 7 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	K	825	12900	4100	6422	1092	1250	36	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-22	MET	-	initiating methionine	UNP Q16531
K	-21	ALA	-	expression tag	UNP Q16531
K	-20	SER	-	expression tag	UNP Q16531
K	-19	TRP	-	expression tag	UNP Q16531
K	-18	SER	-	expression tag	UNP Q16531
K	-17	HIS	-	expression tag	UNP Q16531
K	-16	PRO	-	expression tag	UNP Q16531
K	-15	GLN	-	expression tag	UNP Q16531
K	-14	PHE	-	expression tag	UNP Q16531
K	-13	GLU	-	expression tag	UNP Q16531
K	-12	LYS	-	expression tag	UNP Q16531
K	-11	VAL	-	expression tag	UNP Q16531
K	-10	ASP	-	expression tag	UNP Q16531
K	-9	GLU	-	expression tag	UNP Q16531
K	-8	ASN	-	expression tag	UNP Q16531
K	-7	LEU	-	expression tag	UNP Q16531
K	-6	TYR	-	expression tag	UNP Q16531
K	-5	PHE	-	expression tag	UNP Q16531
K	-4	GLN	-	expression tag	UNP Q16531
K	-3	GLY	-	expression tag	UNP Q16531
K	-2	GLY	-	expression tag	UNP Q16531
K	-1	GLY	-	expression tag	UNP Q16531
K	0	ARG	-	expression tag	UNP Q16531

- Molecule 8 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	L	361	5666	1815	2807	515	513	16	0	0

There are 4 discrepancies between the modelled and reference sequences:

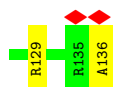
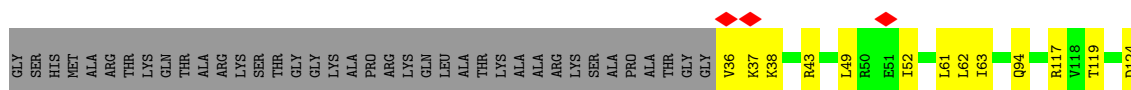
Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	expression tag	UNP Q92466
L	-2	GLY	-	expression tag	UNP Q92466
L	-1	GLY	-	expression tag	UNP Q92466
L	0	ARG	-	expression tag	UNP Q92466

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

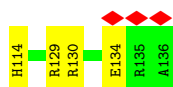
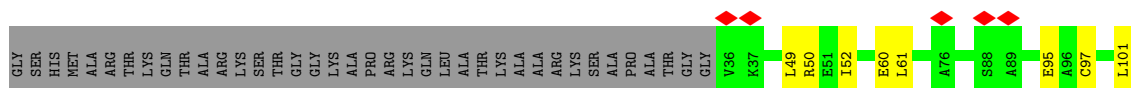
- Molecule 1: Histone H3.1

Chain A: 



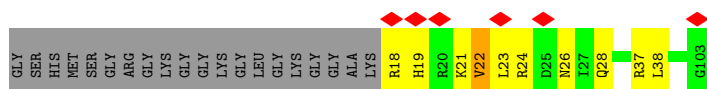
- Molecule 1: Histone H3.1

Chain E: 



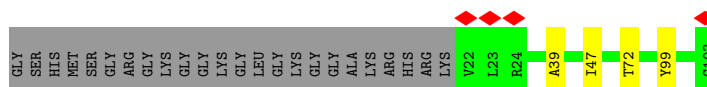
- Molecule 2: Histone H4

Chain B: 

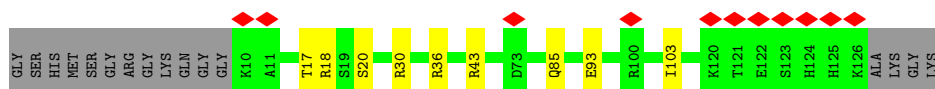
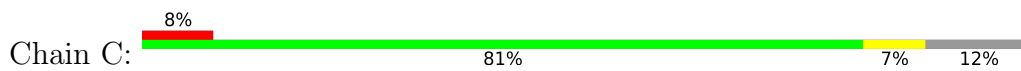


- Molecule 2: Histone H4

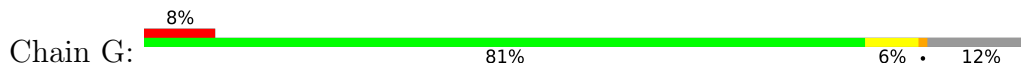
Chain F: 



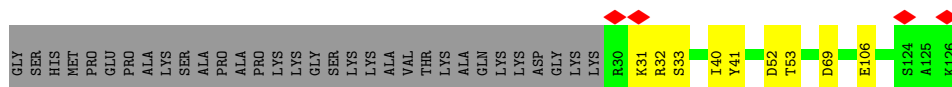
- Molecule 3: Histone H2A type 1-B/E



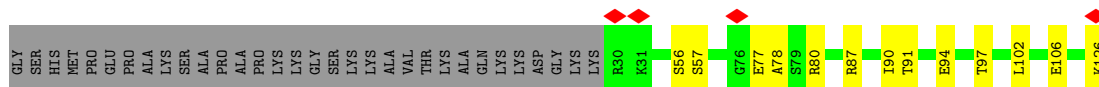
• Molecule 3: Histone H2A type 1-B/E



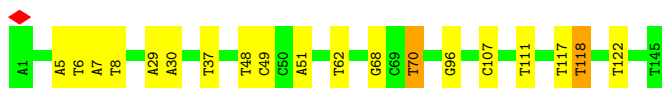
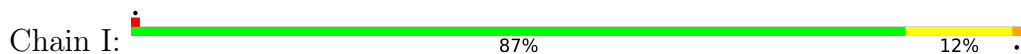
• Molecule 4: Histone H2B type 1-J



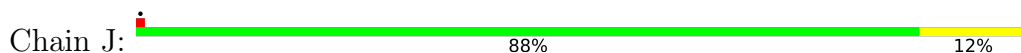
• Molecule 4: Histone H2B type 1-J



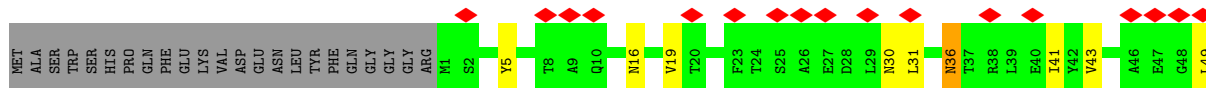
• Molecule 5: Human alpha-satellite DNA (145-MER)



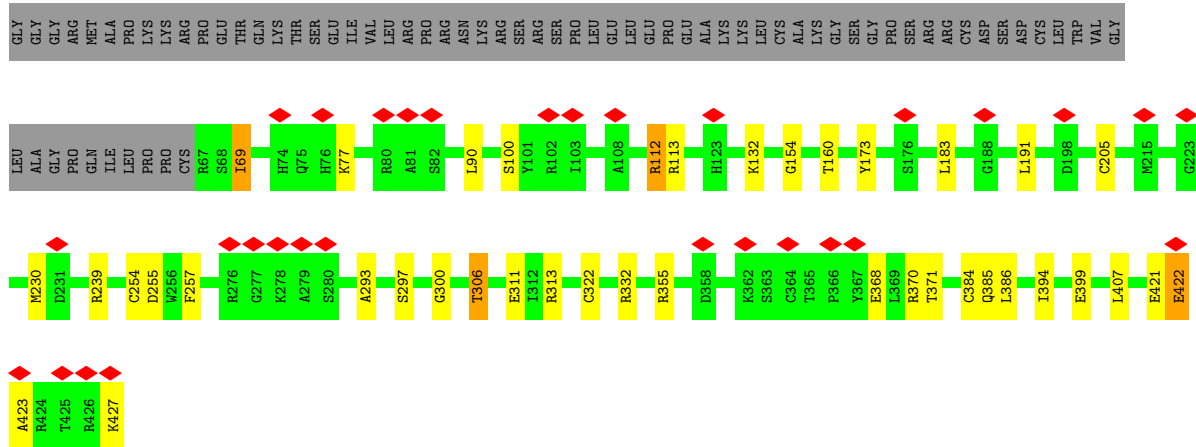
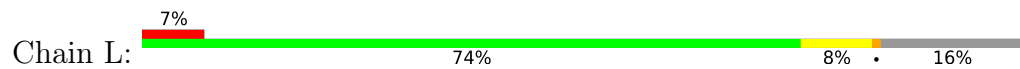
• Molecule 6: Human alpha-satellite DNA (145-MER) with abasic sites at positions 97-98



• Molecule 7: DNA damage-binding protein 1



• Molecule 8: DNA damage-binding protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	47.031	Depositor
Minimum map value	-16.739	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: 3DR

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	0.69	0/844	0.69	0/1130
1	E	0.68	0/844	0.71	0/1130
2	B	0.83	0/702	0.76	0/937
2	F	0.78	0/660	0.71	0/883
3	C	0.64	0/921	0.68	0/1239
3	G	0.65	0/921	0.74	2/1239 (0.2%)
4	D	0.76	0/777	0.67	0/1040
4	H	0.74	1/777 (0.1%)	0.64	0/1040
5	I	1.13	1/3331 (0.0%)	1.15	5/5140 (0.1%)
6	J	1.14	1/3283 (0.0%)	1.14	15/5062 (0.3%)
7	K	0.35	0/6595	0.59	0/8919
8	L	0.55	0/2938	0.68	1/3987 (0.0%)
All	All	0.77	3/22593 (0.0%)	0.84	23/31746 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
7	K	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	102	LEU	C-N	-7.38	1.17	1.34
6	J	132	DA	N7-C5	-5.11	1.36	1.39
5	I	118	DT	C5-C7	-5.06	1.47	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	79	DT	O4'-C1'-N1	6.43	112.50	108.00
6	J	87	DC	O4'-C4'-C3'	-6.29	101.98	104.50
3	G	117	LEU	CA-CB-CG	5.87	128.81	115.30
6	J	91	DT	N3-C4-O4	5.47	123.18	119.90
6	J	90	DT	N3-C4-O4	5.44	123.17	119.90
5	I	107	DC	O4'-C1'-N1	5.44	111.81	108.00
6	J	89	DT	N3-C4-O4	5.33	123.10	119.90
6	J	37	DT	N3-C4-O4	5.33	123.10	119.90
6	J	122	DT	N3-C4-O4	5.32	123.09	119.90
5	I	122	DT	N3-C4-O4	5.22	123.03	119.90
5	I	70	DT	N3-C4-O4	5.21	123.03	119.90
6	J	91	DT	C5-C4-O4	-5.20	121.26	124.90
3	G	116	LEU	CA-CB-CG	5.19	127.24	115.30
6	J	8	DT	N3-C4-O4	5.17	123.00	119.90
8	L	239	ARG	NE-CZ-NH1	5.16	122.88	120.30
6	J	122	DT	C5-C4-O4	-5.15	121.30	124.90
6	J	79	DT	O4'-C1'-C2'	-5.09	101.83	105.90
6	J	79	DT	N3-C4-O4	5.07	122.94	119.90
5	I	8	DT	N3-C4-O4	5.05	122.93	119.90
6	J	38	DT	N3-C4-O4	5.04	122.92	119.90
6	J	118	DT	N3-C4-O4	5.03	122.92	119.90
6	J	62	DT	N3-C4-O4	5.02	122.91	119.90
5	I	62	DT	N3-C4-O4	5.00	122.90	119.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	21	LYS	Peptide
2	B	23	LEU	Peptide
7	K	382	PHE	Mainchain
7	K	928	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	832	876	878	10	0
1	E	832	876	878	9	0
2	B	694	740	742	6	0
2	F	653	695	696	3	0
3	C	909	969	973	7	0
3	G	909	969	973	5	0
4	D	766	793	797	5	0
4	H	766	794	796	10	0
5	I	2970	1641	1641	13	0
6	J	2949	1632	1632	4	0
7	K	6478	6422	6445	64	0
8	L	2859	2807	2822	23	0
All	All	21617	19214	19273	137	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 3.

All (137) 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)
4:H:78:ALA:HB1	4:H:90:ILE:HD11	1.59	0.85
5:I:51:DA:OP1	8:L:332:ARG:NH2	2.17	0.77
7:K:929:SER:OG	7:K:954:MET:SD	2.45	0.74
3:C:43:ARG:NH2	5:I:37:DT:O3'	2.20	0.74
4:D:106:GLU:N	4:D:106:GLU:OE1	2.24	0.70
8:L:173:TYR:OH	8:L:230:MET:SD	2.50	0.70
4:H:106:GLU:N	4:H:106:GLU:OE1	2.26	0.69
4:H:78:ALA:CB	4:H:90:ILE:HD11	2.22	0.68
1:A:129:ARG:NH1	1:A:136:ALA:OXT	2.27	0.68
7:K:902:GLU:OE2	7:K:935:TYR:OH	2.11	0.68
7:K:973:ASN:OD1	7:K:999:HIS:ND1	2.28	0.67
7:K:337:ASN:ND2	7:K:339:ASP:O	2.28	0.67
7:K:310:ILE:N	7:K:384:GLU:OE2	2.28	0.66
3:G:93:GLU:N	3:G:93:GLU:OE1	2.28	0.66
7:K:816:LEU:HD13	7:K:831:VAL:HG22	1.78	0.66
3:C:17:THR:O	3:C:20:SER:OG	2.14	0.65
3:G:21:ARG:NH1	4:H:126:LYS:O	2.30	0.65
3:G:69:ASN:OD1	3:G:72:ARG:NH2	2.29	0.65
8:L:254:CYS:SG	8:L:255:ASP:N	2.70	0.64
7:K:318:ASP:OD2	7:K:319:ASN:ND2	2.31	0.64
7:K:118:THR:OG1	7:K:134:ARG:NH2	2.31	0.64
7:K:1133:VAL:O	7:K:1137:THR:HG23	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:113:GLN:O	3:G:116:LEU:HD23	1.99	0.62
4:H:94:GLU:OE1	4:H:94:GLU:N	2.31	0.62
3:C:85:GLN:OE1	3:C:103:ILE:HD12	1.98	0.62
7:K:381:ALA:O	7:K:385:GLY:N	2.33	0.62
7:K:945:ILE:O	7:K:990:GLN:NE2	2.33	0.61
1:A:61:LEU:HD13	1:A:94:GLN:NE2	2.15	0.61
3:C:93:GLU:N	3:C:93:GLU:OE1	2.34	0.61
4:H:91:THR:OG1	4:H:94:GLU:OE1	2.18	0.61
7:K:275:ASP:OD2	7:K:279:ARG:N	2.35	0.60
7:K:931:LEU:HD21	7:K:933:LEU:HD21	1.83	0.60
7:K:317:LEU:HD11	7:K:323:PHE:HB2	1.83	0.60
7:K:764:SER:O	7:K:805:HIS:ND1	2.34	0.60
8:L:293:ALA:HB3	8:L:306:THR:CG2	2.32	0.59
4:H:87:ARG:NH2	6:J:40:DG:OP2	2.35	0.59
1:E:129:ARG:NH2	1:E:134:GLU:O	2.35	0.59
7:K:36:ASN:OD1	7:K:60:LYS:NZ	2.36	0.58
1:E:60:GLU:N	1:E:60:GLU:OE1	2.36	0.58
7:K:906:TYR:CD1	8:L:423:ALA:HB1	2.39	0.58
3:C:36:ARG:NH2	6:J:113:DC:OP2	2.37	0.57
7:K:854:SER:OG	7:K:859:GLN:NE2	2.36	0.57
7:K:816:LEU:HD12	7:K:830:ILE:O	2.03	0.57
2:B:24:ARG:NH1	2:B:28:GLN:OE1	2.38	0.56
7:K:83:LYS:NZ	7:K:1073:TRP:O	2.31	0.56
1:E:61:LEU:HD21	1:E:95:GLU:OE2	2.05	0.56
7:K:1011:SER:OG	7:K:1013:VAL:HG22	2.06	0.56
7:K:19:VAL:O	7:K:31:LEU:HD12	2.06	0.55
7:K:166:ASP:OD2	7:K:167:VAL:N	2.39	0.55
1:E:50:ARG:NH1	5:I:7:DA:O3'	2.38	0.55
7:K:139:LEU:HD22	7:K:156:ASN:HB3	1.87	0.55
7:K:722:ARG:NH2	7:K:738:SER:OG	2.40	0.55
7:K:1114:TYR:CB	7:K:1124:ALA:HB2	2.37	0.54
7:K:1033:VAL:HG22	8:L:77:LYS:O	2.07	0.54
1:A:62:LEU:HD13	2:B:37:ARG:HB3	1.89	0.54
7:K:944:GLU:N	7:K:944:GLU:OE1	2.42	0.53
8:L:355:ARG:NH1	8:L:368:GLU:OE2	2.42	0.53
7:K:67:PHE:O	7:K:76:LEU:N	2.36	0.53
8:L:69:ILE:HD12	8:L:69:ILE:H	1.74	0.52
7:K:1114:TYR:HB2	7:K:1124:ALA:HB2	1.91	0.52
7:K:739:ARG:NH1	7:K:757:SER:OG	2.43	0.51
4:D:40:ILE:HD11	4:D:41:TYR:CZ	2.46	0.51
4:D:69:ASP:OD2	2:F:99:TYR:OH	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:953:TRP:CZ3	8:L:90:LEU:HD13	2.47	0.49
8:L:371:THR:OG1	8:L:386:LEU:O	2.25	0.49
1:E:97:CYS:O	1:E:101:LEU:HD23	2.12	0.49
7:K:30:ASN:ND2	7:K:43:VAL:HG22	2.27	0.49
8:L:384:CYS:SG	8:L:385:GLN:N	2.85	0.49
7:K:16:ASN:OD1	7:K:36:ASN:N	2.46	0.48
7:K:158:ARG:NH1	8:L:322:CYS:SG	2.86	0.48
7:K:264:VAL:HG21	7:K:272:LEU:HG	1.95	0.48
8:L:399:GLU:O	8:L:407:LEU:HD12	2.13	0.48
8:L:183:LEU:CD2	8:L:191:LEU:HD12	2.43	0.48
3:C:30:ARG:NE	5:I:29:DA:OP1	2.43	0.48
4:H:56:SER:OG	4:H:57:SER:N	2.47	0.48
5:I:117:DT:H2'	5:I:118:DT:H72	1.95	0.48
1:A:63:ILE:HD11	2:B:38:LEU:HD11	1.95	0.48
8:L:311:GLU:OE2	8:L:313:ARG:NE	2.41	0.48
7:K:392:ASN:OD1	7:K:393:GLY:N	2.47	0.47
7:K:342:GLU:OE1	7:K:342:GLU:N	2.44	0.47
8:L:113:ARG:O	8:L:132:LYS:N	2.48	0.47
7:K:246:LEU:HD13	7:K:297:LEU:CD2	2.45	0.47
1:A:43:ARG:NE	5:I:68:DG:OP1	2.48	0.46
1:A:49:LEU:HA	1:A:52:ILE:HD12	1.97	0.46
2:B:24:ARG:O	2:B:26:ASN:ND2	2.49	0.46
7:K:1022:THR:HG23	7:K:1024:THR:O	2.16	0.46
2:B:18:ARG:NH2	2:B:19:HIS:O	2.49	0.46
7:K:369:ARG:NH1	7:K:370:GLN:O	2.49	0.46
7:K:343:GLN:NE2	7:K:345:SER:OG	2.47	0.45
5:I:96:DG:H1	6:J:50:DC:H42	1.65	0.45
7:K:5:TYR:HB2	7:K:1043:LEU:HD11	1.97	0.45
7:K:188:ARG:NH1	7:K:216:ALA:O	2.49	0.45
2:B:22:VAL:O	2:B:22:VAL:HG23	2.18	0.44
4:D:52:ASP:O	4:D:53:THR:OG1	2.32	0.44
7:K:196:SER:OG	7:K:201:GLU:O	2.33	0.44
7:K:186:GLN:N	7:K:186:GLN:OE1	2.51	0.44
7:K:740:ILE:HD13	7:K:787:GLU:OE1	2.17	0.44
1:E:49:LEU:HA	1:E:52:ILE:HD12	1.99	0.43
7:K:931:LEU:HD13	7:K:947:ARG:NH2	2.33	0.43
8:L:160:THR:HG21	8:L:205:CYS:HA	2.00	0.43
8:L:100:SER:O	8:L:100:SER:OG	2.31	0.43
3:G:43:ARG:NH2	5:I:111:DT:O4'	2.52	0.43
4:H:77:GLU:OE1	4:H:80:ARG:NH2	2.46	0.43
7:K:847:ARG:NH1	7:K:863:GLU:OE2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:812:TYR:HB3	7:K:814:LEU:HD21	2.01	0.43
2:F:72:THR:HG22	4:H:97:THR:HG23	1.99	0.43
7:K:199:GLU:N	7:K:199:GLU:OE2	2.52	0.42
7:K:258:ILE:HD13	7:K:273:LEU:HD13	2.01	0.42
4:D:32:ARG:HE	4:D:33:SER:H	1.67	0.42
7:K:246:LEU:HD13	7:K:297:LEU:HG	2.01	0.42
1:A:117:ARG:NH2	1:A:124:ASP:OD2	2.52	0.42
7:K:112:ILE:HG21	8:L:257:PHE:HZ	1.84	0.42
7:K:931:LEU:HD13	7:K:947:ARG:HH21	1.85	0.42
7:K:246:LEU:HD11	7:K:299:ASP:HA	2.02	0.42
7:K:909:ILE:HG21	7:K:927:MET:CE	2.50	0.42
7:K:80:LEU:HD23	7:K:81:THR:O	2.19	0.42
7:K:49:LEU:HG	7:K:333:LEU:HD11	2.01	0.41
8:L:370:ARG:CZ	8:L:394:ILE:HD11	2.49	0.41
5:I:48:DT:H1'	5:I:49:DC:C5	2.55	0.41
6:J:104:DT:C2'	6:J:105:DT:H72	2.49	0.41
8:L:112:ARG:NH1	8:L:154:GLY:O	2.54	0.41
8:L:297:SER:OG	8:L:300:GLY:N	2.47	0.41
3:C:18:ARG:NH2	5:I:30:DA:OP2	2.53	0.41
5:I:5:DA:H2'	5:I:6:DT:H72	2.02	0.41
7:K:90:GLU:OE1	7:K:103:ARG:NH1	2.47	0.41
7:K:367:LEU:HD12	7:K:374:GLN:HB2	2.02	0.41
1:A:119:THR:N	5:I:70:DT:OP1	2.53	0.41
1:E:61:LEU:HD21	1:E:95:GLU:CD	2.40	0.41
5:I:117:DT:C2'	5:I:118:DT:H72	2.49	0.41
1:E:49:LEU:HD23	1:E:52:ILE:HD12	2.03	0.41
7:K:41:ILE:HD13	7:K:53:LYS:HB3	2.03	0.41
8:L:293:ALA:HB3	8:L:306:THR:HG23	2.03	0.41
1:A:36:VAL:HG12	1:A:38:LYS:H	1.86	0.40
2:F:39:ALA:CB	2:F:47:ILE:HD11	2.51	0.40
7:K:167:VAL:HG23	7:K:180:PHE:HB3	2.03	0.40
1:A:124:ASP:OD1	1:E:114:HIS:NE2	2.50	0.40
7:K:1114:TYR:HB3	7:K:1124:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	99/139 (71%)	97 (98%)	2 (2%)	0	100	100
1	E	99/139 (71%)	98 (99%)	1 (1%)	0	100	100
2	B	84/106 (79%)	76 (90%)	7 (8%)	1 (1%)	13	49
2	F	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
3	C	115/133 (86%)	111 (96%)	4 (4%)	0	100	100
3	G	115/133 (86%)	109 (95%)	6 (5%)	0	100	100
4	D	95/129 (74%)	90 (95%)	5 (5%)	0	100	100
4	H	95/129 (74%)	90 (95%)	5 (5%)	0	100	100
7	K	821/1163 (71%)	802 (98%)	16 (2%)	3 (0%)	34	71
8	L	359/431 (83%)	313 (87%)	43 (12%)	3 (1%)	19	57
All	All	1962/2608 (75%)	1864 (95%)	91 (5%)	7 (0%)	38	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	382	PHE
8	L	69	ILE
8	L	112	ARG
7	K	36	ASN
7	K	383	LYS
8	L	422	GLU
2	B	22	VAL

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/113 (78%)	87 (99%)	1 (1%)	73	84
1	E	88/113 (78%)	87 (99%)	1 (1%)	73	84
2	B	71/81 (88%)	71 (100%)	0	100	100
2	F	67/81 (83%)	67 (100%)	0	100	100
3	C	93/102 (91%)	93 (100%)	0	100	100
3	G	93/102 (91%)	92 (99%)	1 (1%)	73	84
4	D	83/107 (78%)	82 (99%)	1 (1%)	71	83
4	H	83/107 (78%)	83 (100%)	0	100	100
7	K	720/1018 (71%)	720 (100%)	0	100	100
8	L	313/372 (84%)	309 (99%)	4 (1%)	69	82
All	All	1699/2196 (77%)	1691 (100%)	8 (0%)	89	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
4	D	31	LYS
1	E	130	ARG
3	G	10	LYS
8	L	306	THR
8	L	421	GLU
8	L	422	GLU
8	L	427	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	26	ASN
2	F	28	GLN
4	H	96	GLN
7	K	93	GLN
7	K	319	ASN
7	K	859	GLN
7	K	990	GLN
7	K	1059	ASN
8	L	345	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	3DR	J	96	6	8,11,12	0.37	0	9,14,17	0.69	0
6	3DR	J	95	6	8,11,12	0.50	0	9,14,17	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	3DR	J	96	6	-	1/3/15/16	0/1/1/1
6	3DR	J	95	6	-	3/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	95	3DR	O4'-C4'-C5'-O5'
6	J	95	3DR	C3'-C4'-C5'-O5'
6	J	96	3DR	C4'-C5'-O5'-P
6	J	95	3DR	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	102:LEU	C	103:LEU	N	1.17

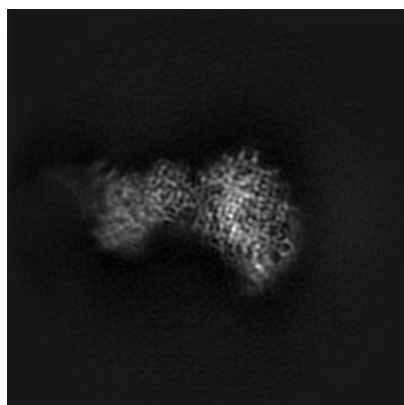
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4763. These allow visual inspection of the internal detail of the map and identification of artifacts.

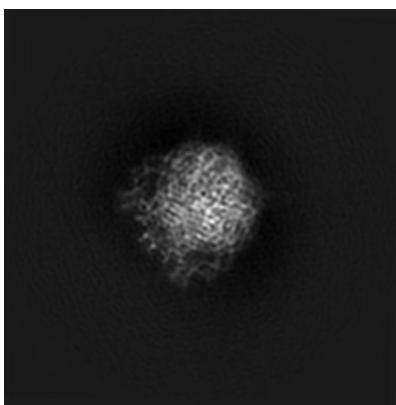
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

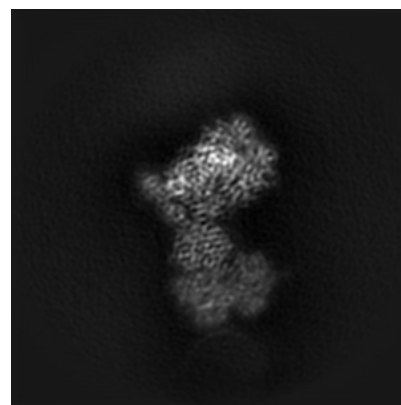
6.1.1 Primary map



X



Y

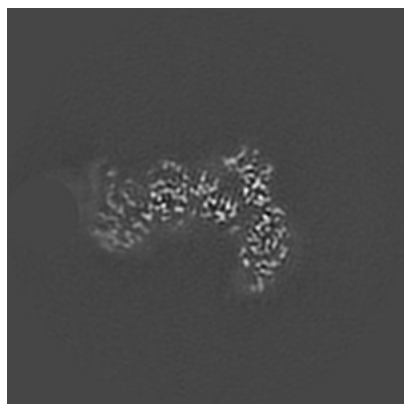


Z

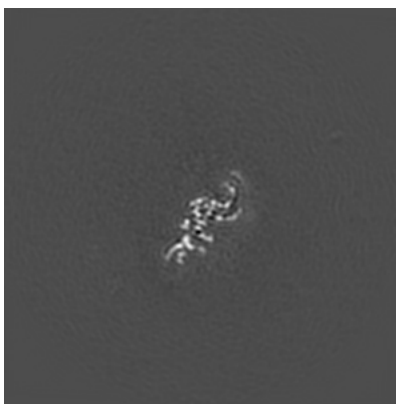
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

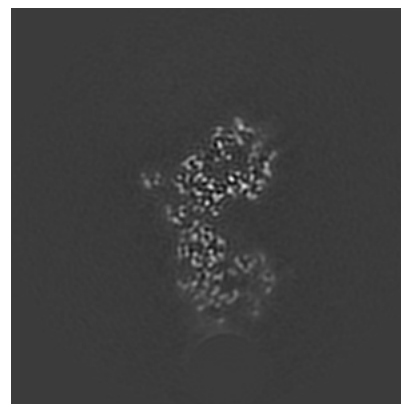
6.2.1 Primary map



X Index: 140



Y Index: 140

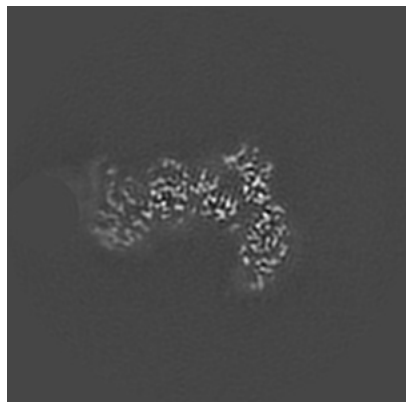


Z Index: 140

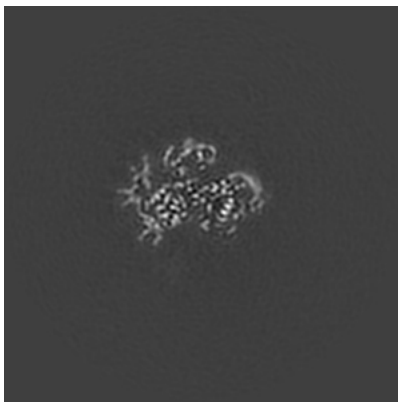
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

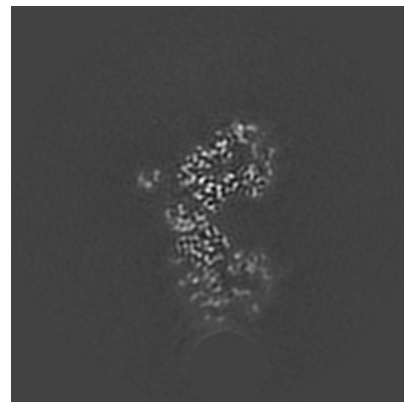
6.3.1 Primary map



X Index: 140



Y Index: 174

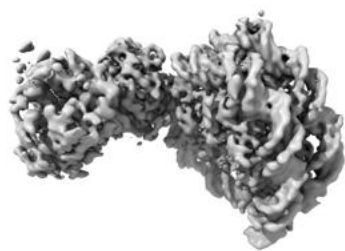


Z Index: 142

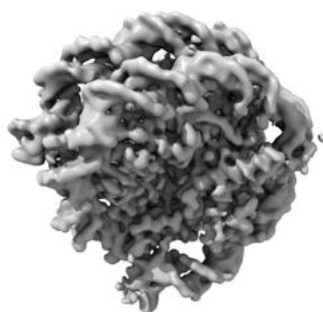
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

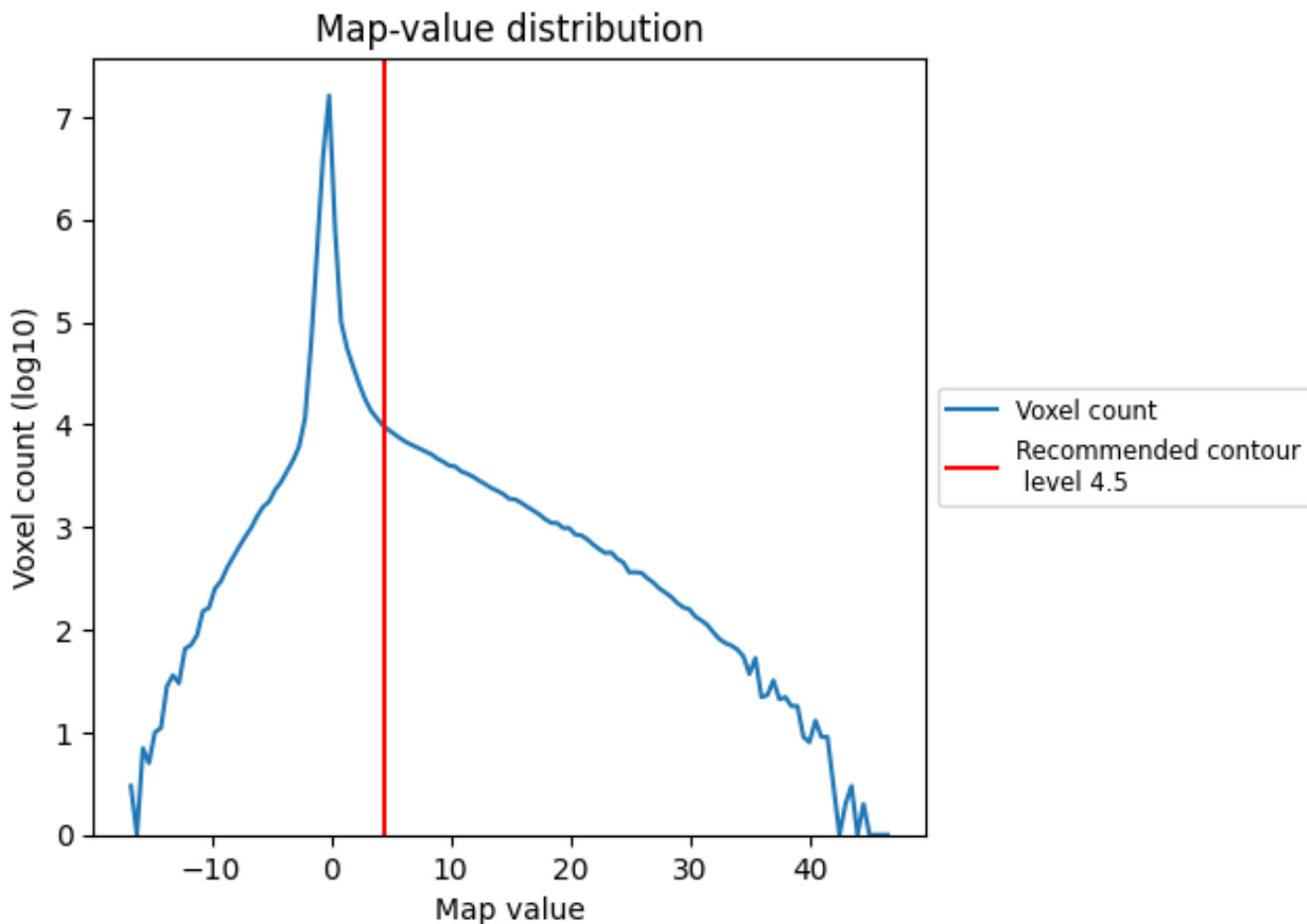
6.5 Mask visualisation

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

7 Map analysis [i](#)

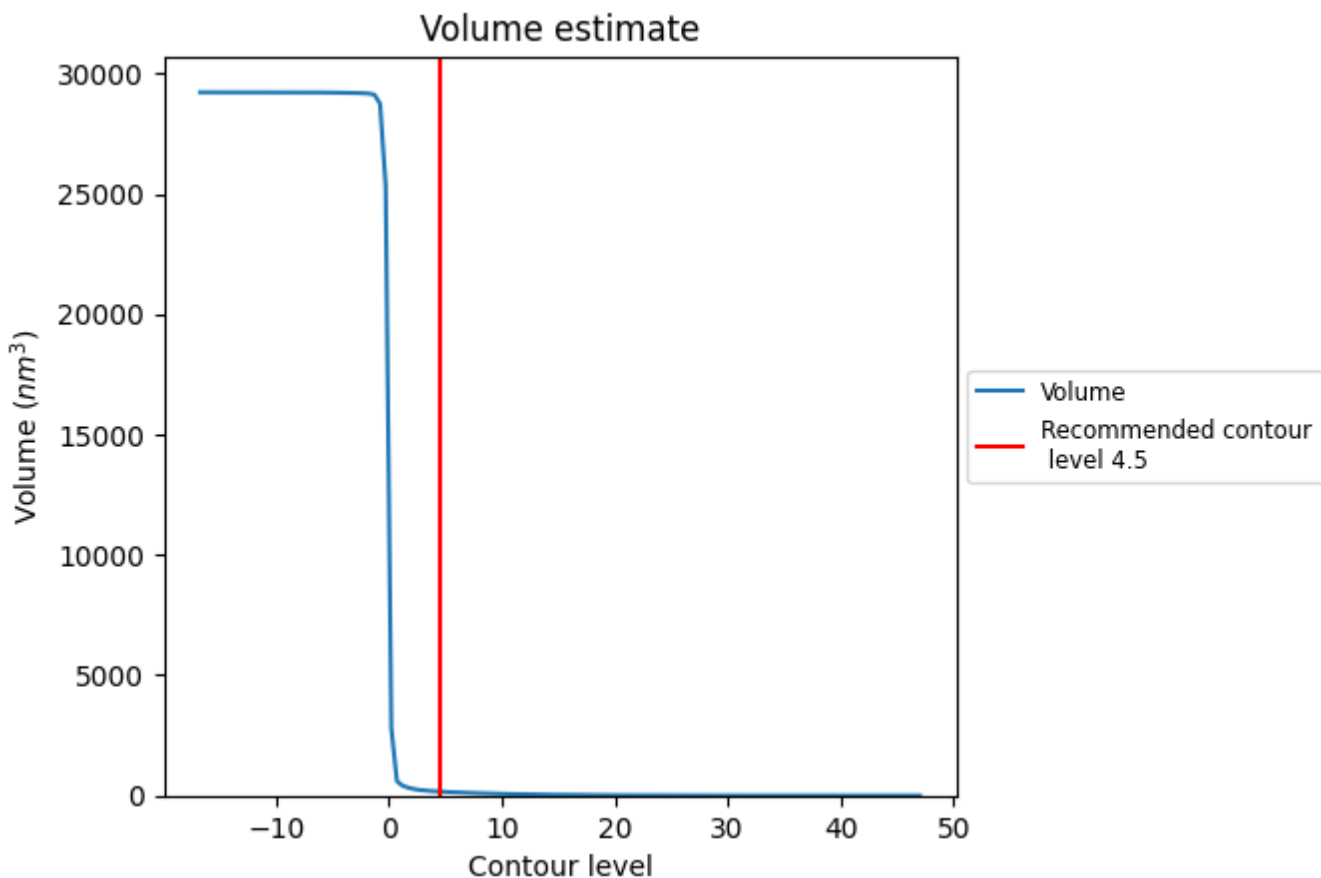
This section contains the results of statistical analysis of the map.

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.

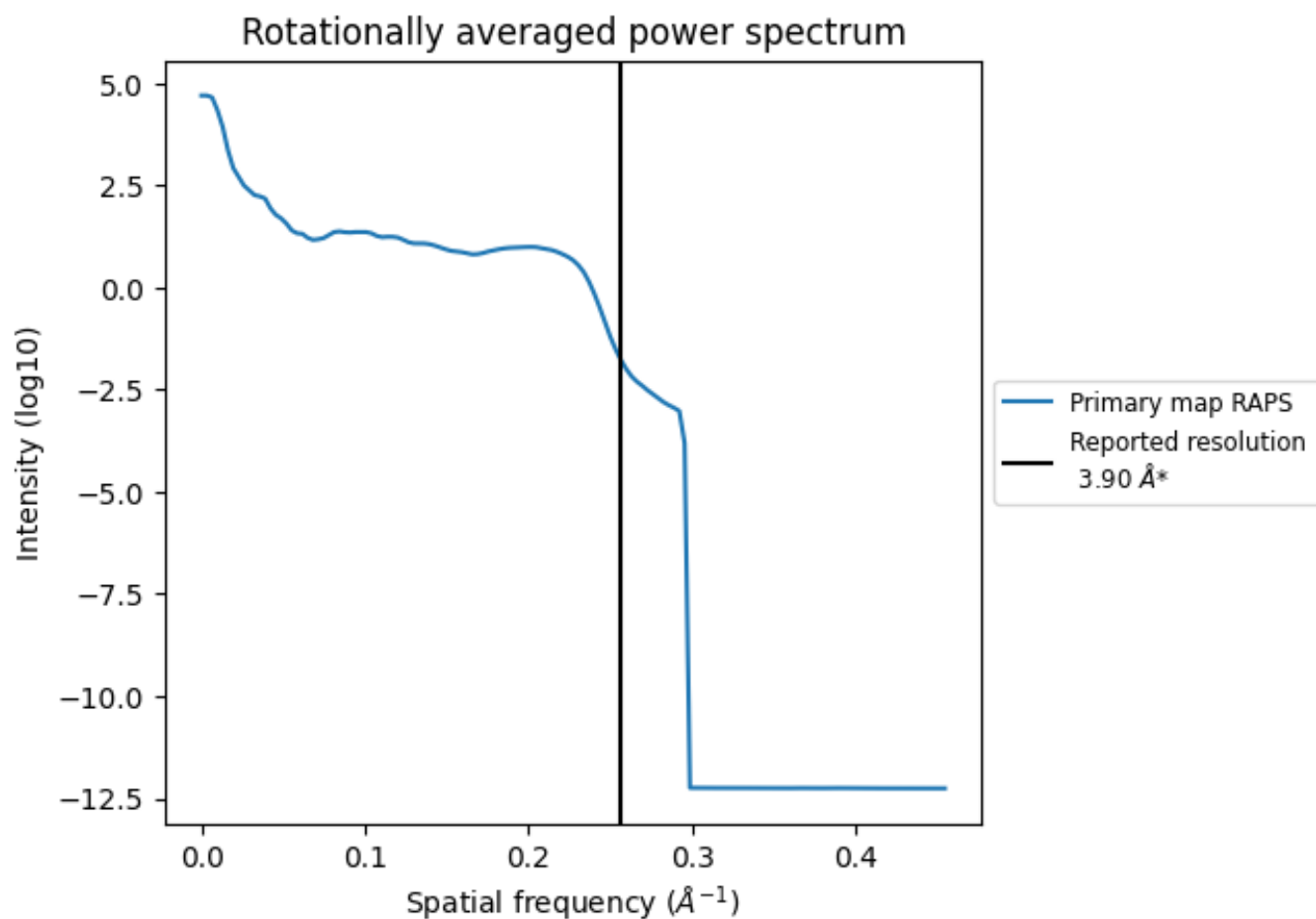
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm³; this corresponds to an approximate mass of 149 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

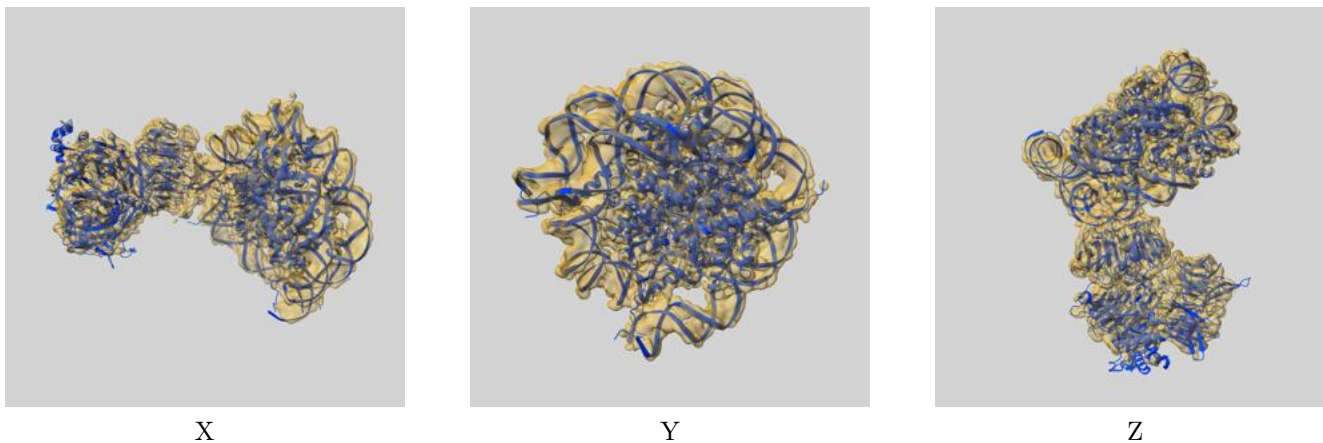
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

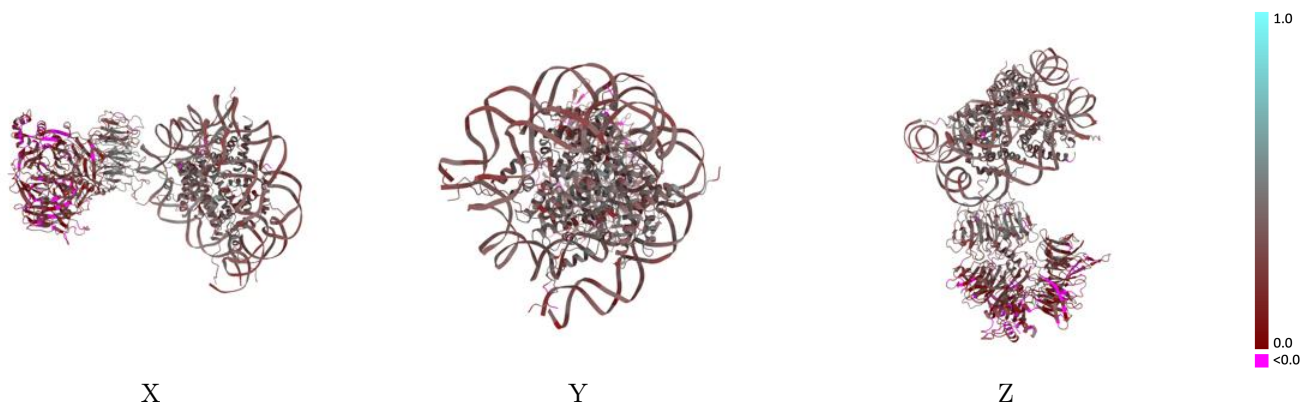
This section contains information regarding the fit between EMDB map EMD-4763 and PDB model 6R8Z. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



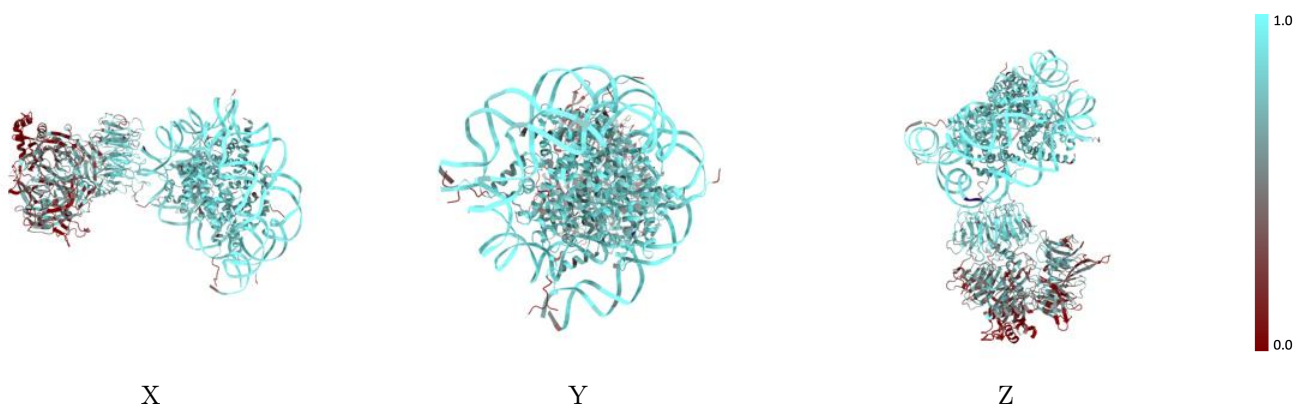
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



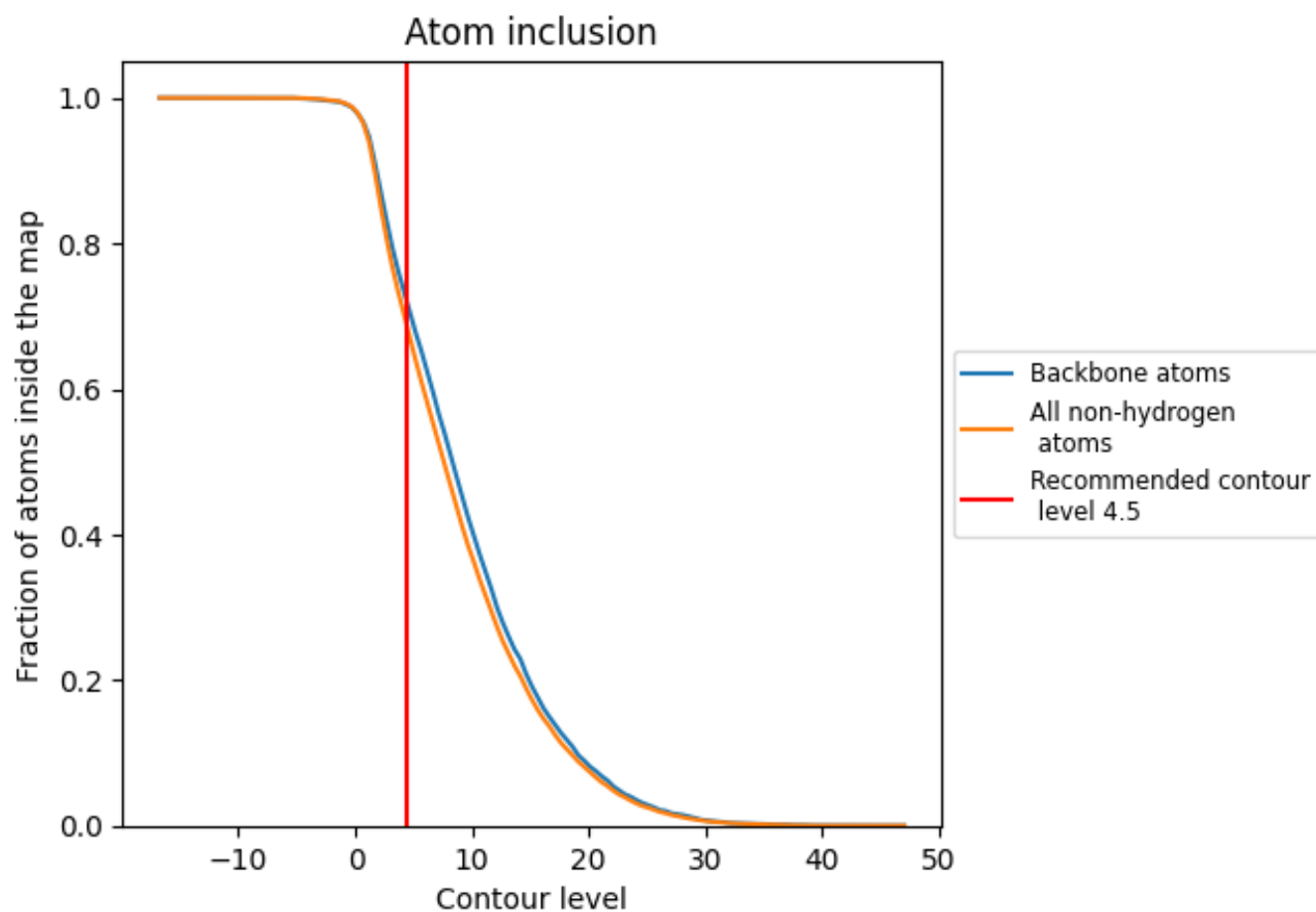
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 68% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6821	 0.3070
A	 0.8115	 0.3940
B	 0.8087	 0.3950
C	 0.7630	 0.3710
D	 0.8094	 0.3560
E	 0.8052	 0.3790
F	 0.8278	 0.3970
G	 0.7823	 0.3780
H	 0.8054	 0.3670
I	 0.8822	 0.3270
J	 0.8871	 0.3310
K	 0.4281	 0.1930
L	 0.7470	 0.3570

