Full wwPDB EM Validation Report ⓘ

Dec 6, 2020 – 05:21 am GMT

PDB ID	:	6R91
EMDB ID	:	EMD-4765
Title	:	Cryo-EM structure of NCP_THF2(-3)-UV-DDB
Authors	:	Matsumoto, S.; Cavadini, S.; Bunker, R.D.; Thoma, N.H.
Deposited on	:	2019-04-02
Resolution	:	4.10 Å(reported)
Based on initial models	:	4ZUX, 4E54, 3EI4, 5Y0C

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

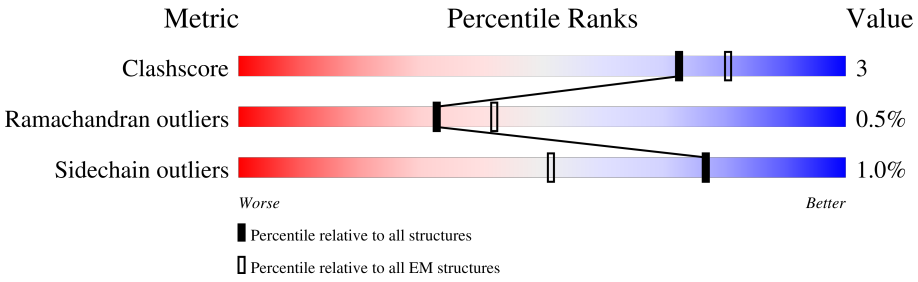
EMDB validation analysis	:	0.0.0.dev61
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

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 4.10 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	139	15% 61% 12% 27%
1	E	139	10% 59% 12% 29%
2	B	106	17% 62% 14% 24%
2	F	106	15% 68% 9% 23%
3	C	133	18% 75% 7% 17%
3	G	133	15% 77% 6% 17%
4	D	129	11% 62% 12% 25%
4	H	129	12% 63% 11% 25%

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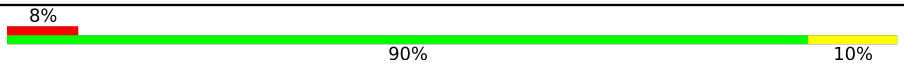
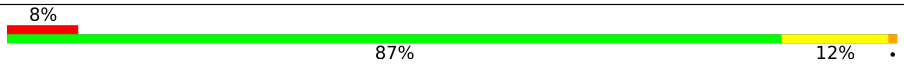
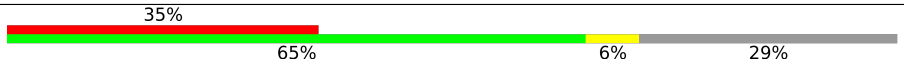
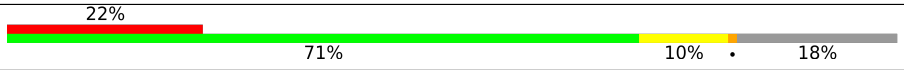
Mol	Chain	Length	Quality of chain
5	I	145	
6	J	145	
7	K	1163	
8	L	450	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 40556 atoms, of which 19079 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
1	A	101	Total	C	H	N	O	S	0	0
			1708	525	876	161	142	4		
1	E	98	Total	C	H	N	O	S	0	0
			1649	508	842	156	139	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
2	B	81	Total	C	H	N	O	S	0	0
			1331	407	685	126	112	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
3	C	110	Total	C	H	N	O	0	0
			1762	535	913	168	146		
3	G	111	Total	C	H	N	O	0	0
			1784	541	926	170	147		

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
4	D	97	Total	C	H	N	O	S	0	0
			1560	480	794	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
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
6	J	145	Total	C	H	N	O	P	0	0
			4581	1410	1633	529	865	144		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	825	Total	C	H	N	O	S	0	0
			12902	4100	6424	1092	1250	36		

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
8	L	367	Total	C	H	N	O	S	0	0
			5760	1845	2856	522	520	17		

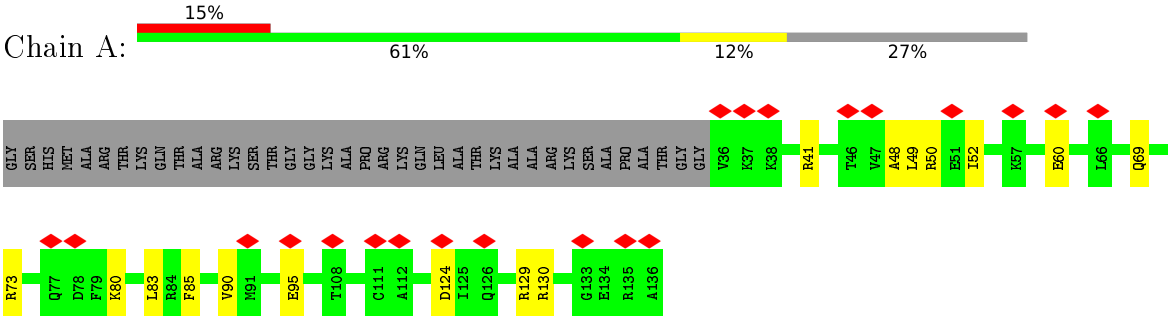
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-22	MET	-	initiating methionine	UNP Q92466
L	-21	ALA	-	expression tag	UNP Q92466
L	-20	SER	-	expression tag	UNP Q92466
L	-19	TRP	-	expression tag	UNP Q92466
L	-18	SER	-	expression tag	UNP Q92466
L	-17	HIS	-	expression tag	UNP Q92466
L	-16	PRO	-	expression tag	UNP Q92466
L	-15	GLN	-	expression tag	UNP Q92466
L	-14	PHE	-	expression tag	UNP Q92466
L	-13	GLU	-	expression tag	UNP Q92466
L	-12	LYS	-	expression tag	UNP Q92466
L	-11	VAL	-	expression tag	UNP Q92466
L	-10	ASP	-	expression tag	UNP Q92466
L	-9	GLU	-	expression tag	UNP Q92466
L	-8	ASN	-	expression tag	UNP Q92466
L	-7	LEU	-	expression tag	UNP Q92466
L	-6	TYR	-	expression tag	UNP Q92466
L	-5	PHE	-	expression tag	UNP Q92466
L	-4	GLN	-	expression tag	UNP Q92466
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

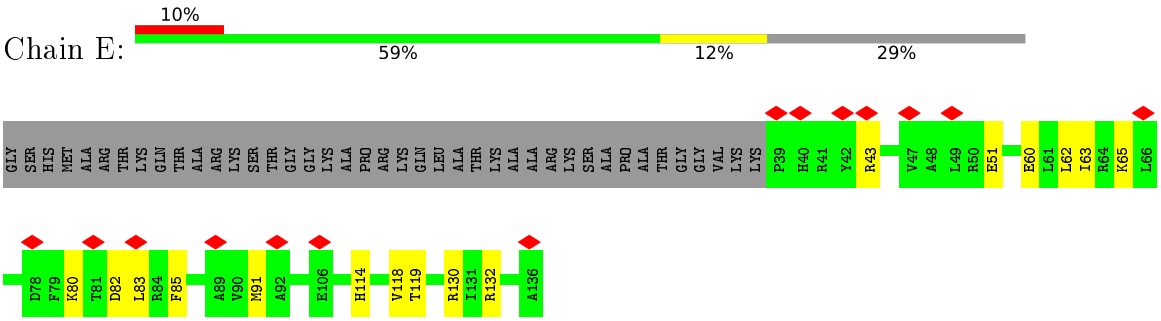
3 Residue-property plots (i)

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.

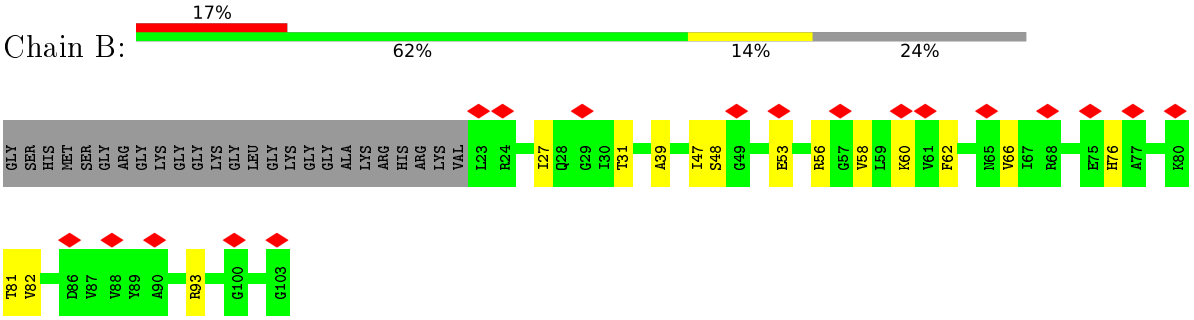
- Molecule 1: Histone H3.1



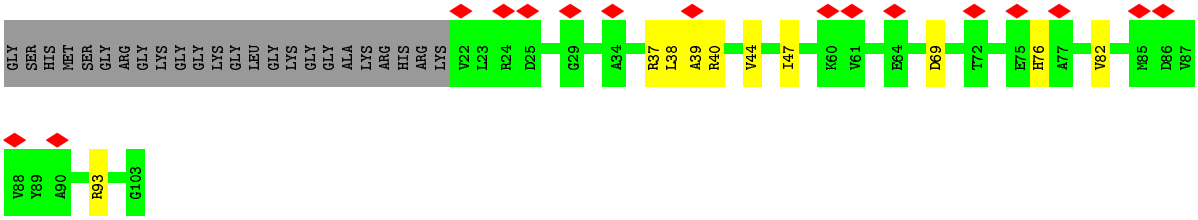
- Molecule 1: Histone H3.1



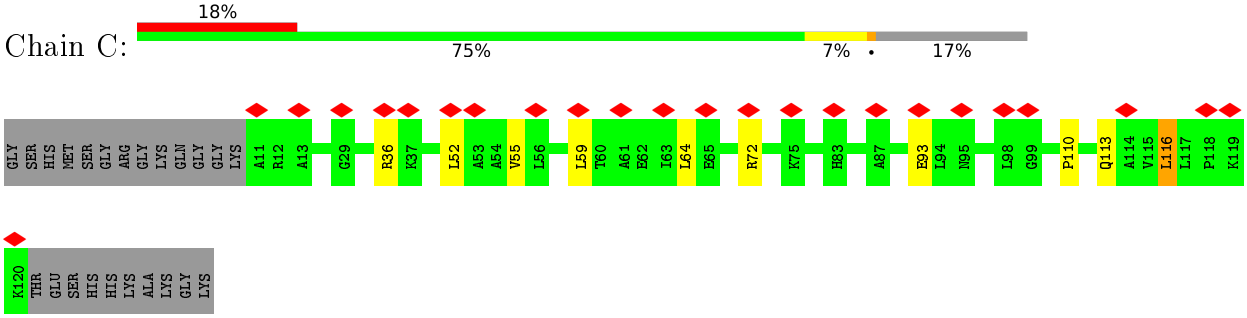
- Molecule 2: Histone H4



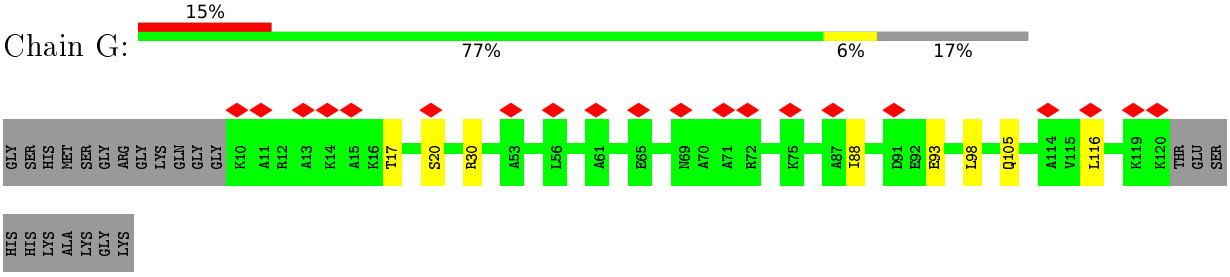
- Molecule 2: Histone H4



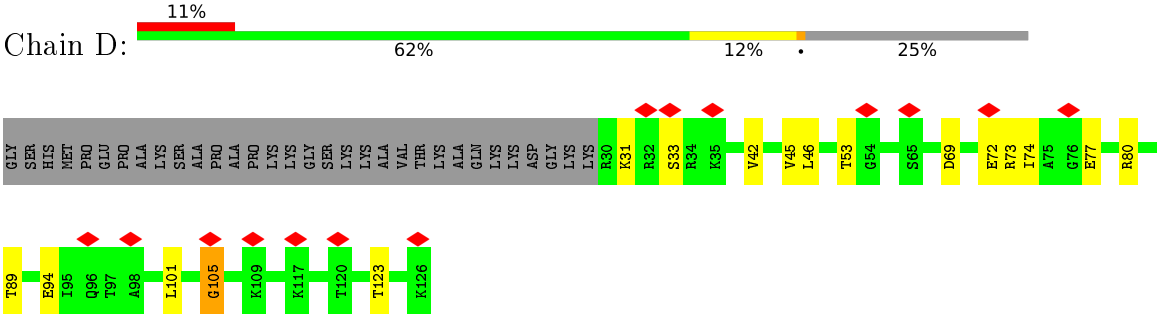
• Molecule 3: Histone H2A type 1-B/E



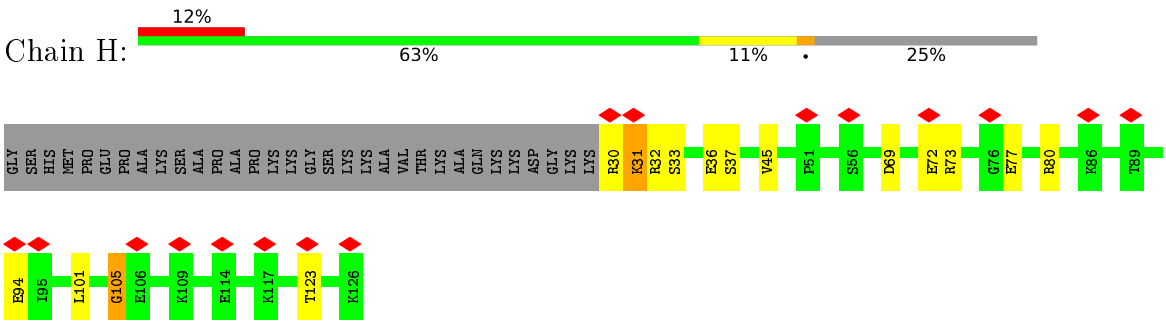
• Molecule 3: Histone H2A type 1-B/E



• Molecule 4: Histone H2B type 1-J

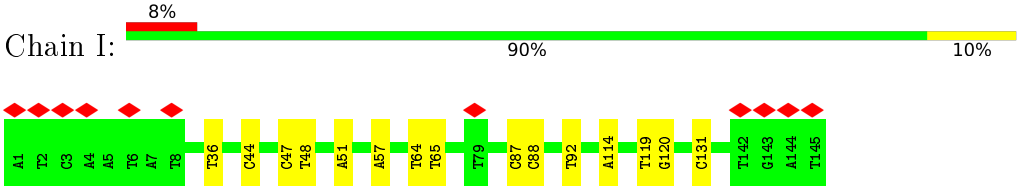


• Molecule 4: Histone H2B type 1-J



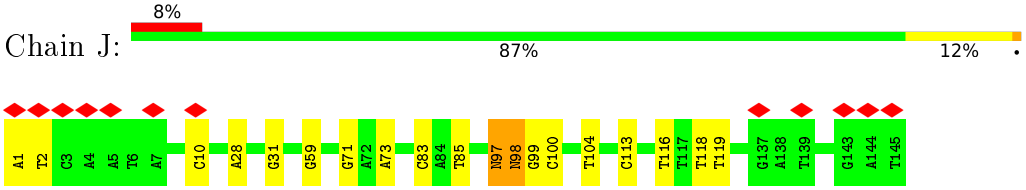
• Molecule 5: Human alpha-satellite DNA (145-MER)

Chain I:



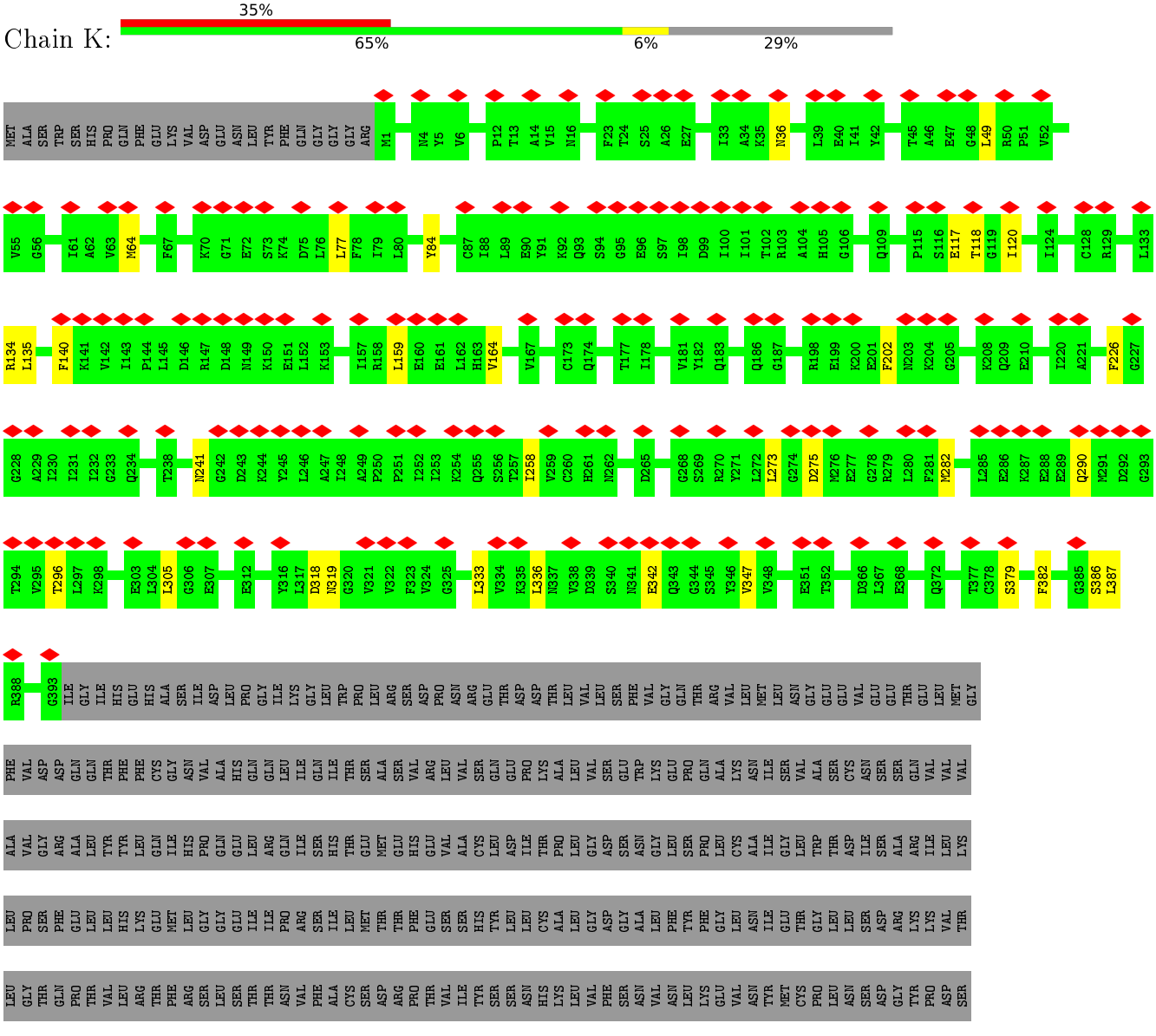
• Molecule 6: Human alpha-satellite DNA (145-MER) with abasic sites at positions 97-98

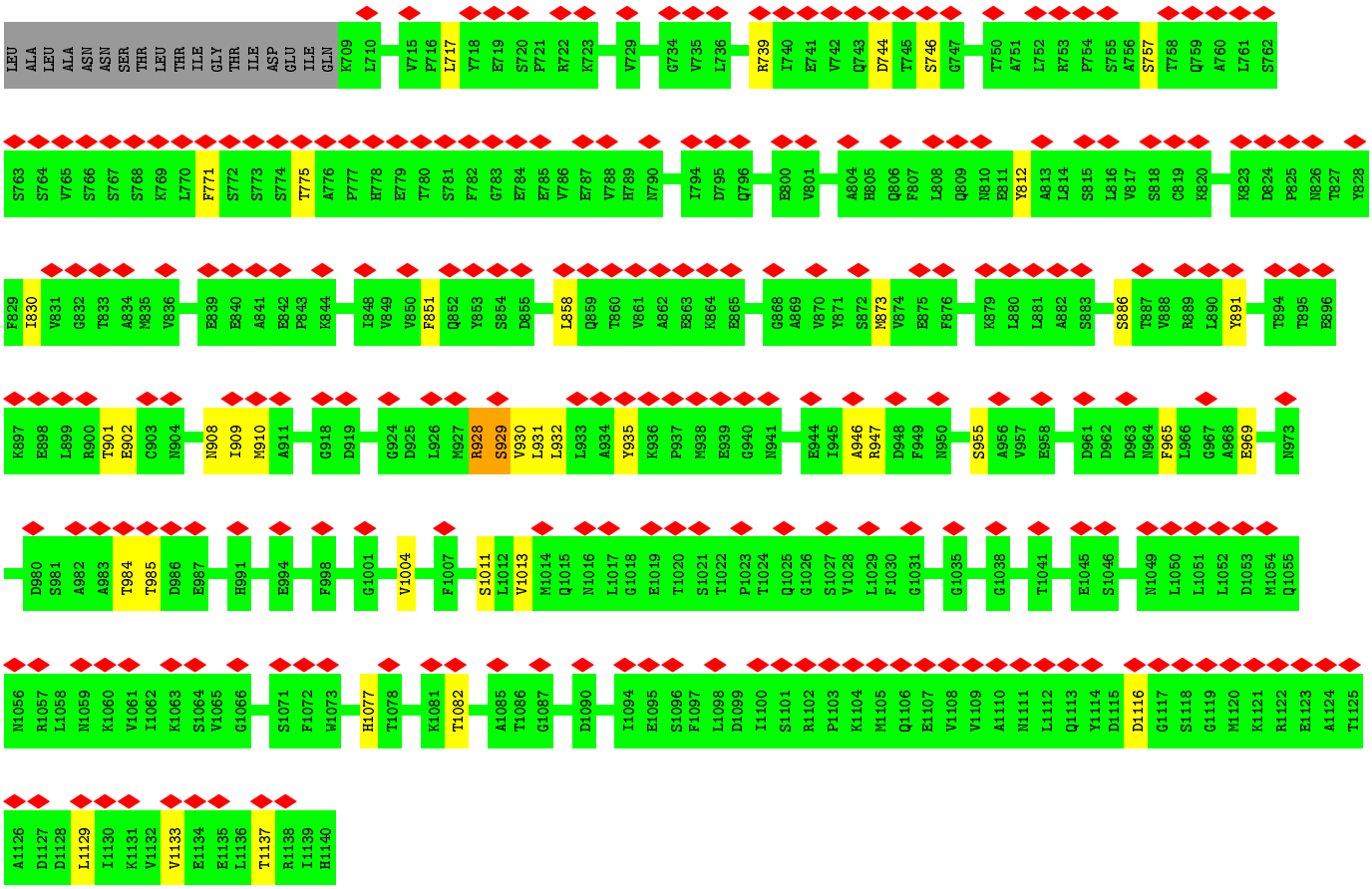
Chain J:



• Molecule 7: DNA damage-binding protein 1

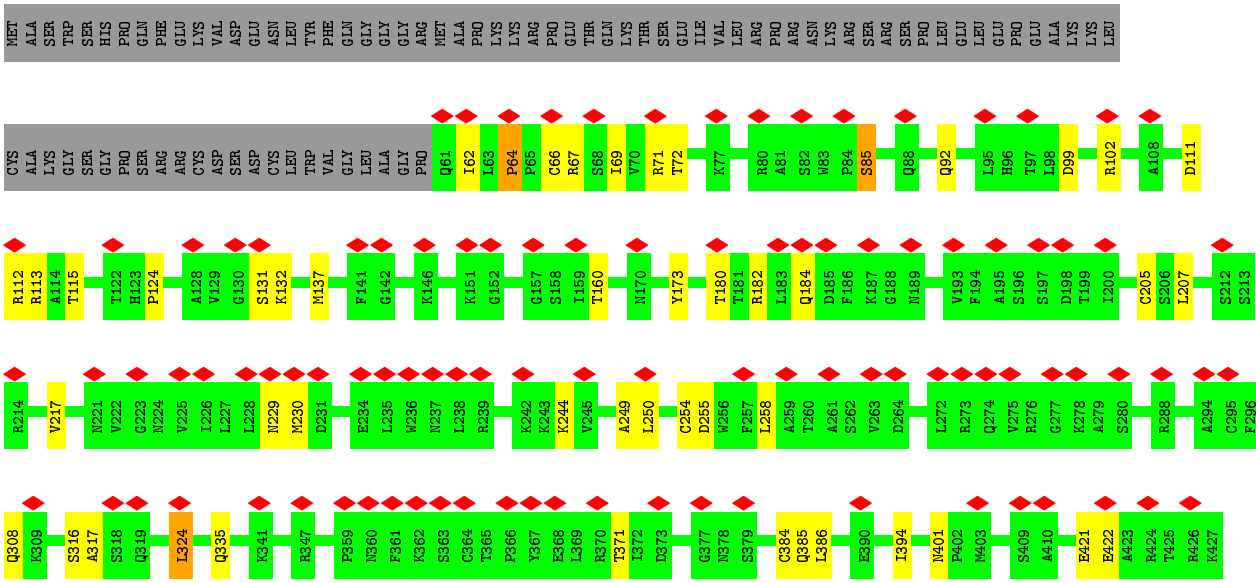
Chain K:





- Molecule 8: DNA damage-binding protein 2

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119309	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	45.498	Depositor
Minimum map value	-19.132	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.12	Depositor
Map size (Å)	330.24, 330.24, 330.24	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7199999, 1.7199999, 1.7199999	Depositor

5 Model quality

5.1 Standard geometry

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	0.32	0/844	0.72	1/1130 (0.1%)
1	E	0.36	0/819	0.80	2/1097 (0.2%)
2	B	0.36	0/653	0.77	0/873
2	F	0.37	0/660	0.76	0/883
3	C	0.33	0/859	0.76	1/1157 (0.1%)
3	G	0.33	0/868	0.71	1/1168 (0.1%)
4	D	0.35	0/777	0.69	1/1040 (0.1%)
4	H	0.35	0/777	0.69	1/1040 (0.1%)
5	I	0.79	1/3331 (0.0%)	1.09	3/5140 (0.1%)
6	J	0.79	0/3281	1.07	1/5059 (0.0%)
7	K	0.32	0/6595	0.66	2/8919 (0.0%)
8	L	0.33	0/2985	0.64	1/4053 (0.0%)
All	All	0.51	1/22449 (0.0%)	0.84	14/31559 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	K	0	1
8	L	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	87	DC	C1'-N1	5.46	1.56	1.49

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	116	LEU	CA-CB-CG	9.51	137.17	115.30
5	I	92	DT	O4'-C1'-N1	8.21	113.75	108.00
7	K	1116	ASP	CB-CG-OD1	6.88	124.49	118.30
7	K	275	ASP	CB-CG-OD1	6.22	123.90	118.30
5	I	92	DT	C1'-O4'-C4'	-5.98	104.12	110.10
1	E	132	ARG	NE-CZ-NH1	5.62	123.11	120.30
6	J	113	DC	O4'-C1'-N1	5.62	111.93	108.00
3	G	116	LEU	CA-CB-CG	5.61	128.21	115.30
4	D	105	GLY	N-CA-C	5.40	126.60	113.10
4	H	105	GLY	N-CA-C	5.40	126.59	113.10
8	L	137	MET	CG-SD-CE	5.25	108.60	100.20
1	E	82	ASP	CB-CG-OD1	5.19	122.97	118.30
5	I	131	DC	O4'-C1'-N1	5.16	111.61	108.00
1	A	41	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	K	928	ARG	Peptide
8	L	64	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	832	876	878	12	0
1	E	807	842	844	12	0
2	B	646	685	687	11	0
2	F	653	695	696	9	0
3	C	849	913	915	8	0
3	G	858	926	928	5	0
4	D	766	794	797	10	0
4	H	766	794	797	9	0
5	I	2970	1641	1641	14	0
6	J	2948	1633	1633	19	0
7	K	6478	6424	6445	42	0
8	L	2904	2856	2871	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21477	19079	19132	136	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 (136) 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)
6:J:98:3DR:C4'	6:J:98:3DR:O4'	1.67	1.27
6:J:97:3DR:O4'	6:J:97:3DR:C4'	1.66	1.16
5:I:48:DT:O2	8:L:335:GLN:OE1	2.02	0.78
8:L:66:CYS:O	8:L:92:GLN:NE2	2.19	0.76
8:L:173:TYR:OH	8:L:230:MET:SD	2.43	0.75
7:K:258:ILE:HD13	7:K:273:LEU:HD13	1.68	0.74
8:L:99:ASP:OD1	8:L:102:ARG:NH2	2.21	0.73
3:G:30:ARG:NH1	4:H:36:GLU:OE1	2.23	0.71
2:B:93:ARG:NH2	4:D:101:LEU:O	2.23	0.70
1:E:65:LYS:NZ	1:E:91:MET:SD	2.65	0.70
8:L:254:CYS:SG	8:L:255:ASP:N	2.66	0.69
8:L:371:THR:OG1	8:L:386:LEU:O	2.09	0.69
6:J:99:DG:OP2	8:L:244:LYS:NZ	2.25	0.69
7:K:226:PHE:O	7:K:241:ASN:ND2	2.30	0.64
1:E:119:THR:N	6:J:73:DA:OP1	2.32	0.63
3:C:64:LEU:HD11	4:D:42:VAL:HG13	1.79	0.62
5:I:51:DA:OP1	8:L:394:ILE:N	2.32	0.62
7:K:886:SER:OG	7:K:908:ASN:O	2.20	0.60
1:A:50:ARG:NH1	6:J:10:DC:OP1	2.34	0.60
2:F:76:HIS:NE2	4:H:94:GLU:OE1	2.28	0.59
8:L:62:ILE:HG22	8:L:64:PRO:HD3	1.84	0.59
3:G:17:THR:O	3:G:20:SER:OG	2.19	0.58
8:L:182:ARG:NE	8:L:184:GLN:OE1	2.37	0.58
7:K:902:GLU:OE2	7:K:935:TYR:OH	2.21	0.57
7:K:379:SER:OG	7:K:386:SER:OG	2.21	0.57
7:K:771:PHE:O	7:K:775:THR:OG1	2.12	0.57
3:G:93:GLU:N	3:G:93:GLU:OE1	2.38	0.57
7:K:342:GLU:OE1	7:K:342:GLU:N	2.36	0.57
1:A:73:ARG:NH1	5:I:47:DC:OP1	2.37	0.56
7:K:134:ARG:NH1	7:K:164:VAL:O	2.38	0.56
4:H:30:ARG:NH2	6:J:28:DA:O3'	2.39	0.56
3:C:93:GLU:N	3:C:93:GLU:OE1	2.39	0.56
1:E:62:LEU:HD13	2:F:37:ARG:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:739:ARG:NH1	7:K:757:SER:OG	2.37	0.55
2:F:39:ALA:HB1	2:F:44:VAL:HB	1.88	0.55
2:B:81:THR:N	6:J:104:DT:OP1	2.40	0.55
2:B:48:SER:OG	6:J:83:DC:OP1	2.24	0.54
1:A:95:GLU:OE2	3:G:105:GLN:N	2.39	0.54
8:L:113:ARG:O	8:L:132:LYS:N	2.41	0.53
4:D:77:GLU:OE1	4:D:80:ARG:NH2	2.41	0.53
7:K:336:LEU:CD2	7:K:347:VAL:HG22	2.39	0.53
8:L:69:ILE:O	8:L:72:THR:OG1	2.24	0.53
6:J:100:DC:OP1	8:L:308:GLN:NE2	2.42	0.53
7:K:812:TYR:OH	8:L:71:ARG:NH2	2.42	0.52
4:D:89:THR:N	5:I:36:DT:OP1	2.43	0.52
8:L:124:PRO:O	8:L:401:ASN:ND2	2.43	0.52
7:K:932:LEU:HD22	7:K:965:PHE:CZ	2.45	0.52
7:K:84:TYR:CE1	7:K:120:ILE:HD11	2.45	0.51
8:L:229:ASN:OD1	8:L:230:MET:N	2.44	0.51
2:F:93:ARG:NH2	4:H:101:LEU:O	2.44	0.51
4:H:77:GLU:OE1	4:H:80:ARG:NH2	2.41	0.50
1:A:80:LYS:HB3	1:A:83:LEU:HD11	1.93	0.50
3:C:72:ARG:NH2	4:D:53:THR:OG1	2.45	0.49
7:K:984:THR:HG23	7:K:985:THR:HG23	1.93	0.49
1:A:73:ARG:NH2	5:I:47:DC:OP2	2.46	0.49
2:B:53:GLU:OE2	2:B:56:ARG:NH1	2.45	0.49
3:C:64:LEU:HD13	4:D:46:LEU:HB2	1.93	0.49
6:J:118:DT:H2'	6:J:119:DT:H72	1.94	0.49
7:K:387:LEU:HG	7:K:717:LEU:HD11	1.95	0.49
7:K:64:MET:HG3	7:K:77:LEU:HD11	1.94	0.49
8:L:316:SER:HB2	8:L:324:LEU:HD13	1.94	0.49
7:K:1011:SER:OG	7:K:1013:VAL:HG22	2.12	0.49
7:K:282:MET:HB2	7:K:305:LEU:HD21	1.94	0.48
5:I:64:DT:H2'	5:I:65:DT:H72	1.96	0.48
3:G:88:ILE:HD13	3:G:98:LEU:HD12	1.95	0.48
7:K:931:LEU:HD13	7:K:947:ARG:NE	2.29	0.48
1:A:69:GLN:HG3	1:A:90:VAL:HG11	1.94	0.48
5:I:88:DC:O2	6:J:59:DG:N2	2.47	0.48
2:B:62:PHE:O	2:B:66:VAL:HG23	2.14	0.48
7:K:851:PHE:HB3	7:K:858:LEU:HD22	1.95	0.47
2:B:76:HIS:NE2	4:D:94:GLU:OE1	2.39	0.47
2:F:69:ASP:OD2	2:F:93:ARG:NH2	2.47	0.47
1:E:43:ARG:NH2	6:J:71:DG:OP1	2.47	0.47
8:L:160:THR:HG21	8:L:205:CYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:GLU:OE1	2:F:40:ARG:NE	2.46	0.47
3:C:113:GLN:O	3:C:116:LEU:HD23	2.15	0.47
1:E:60:GLU:OE1	1:E:60:GLU:N	2.47	0.46
7:K:830:ILE:HG22	7:K:873:MET:HE1	1.97	0.46
7:K:955:SER:OG	7:K:1004:VAL:O	2.16	0.46
7:K:318:ASP:OD1	7:K:319:ASN:ND2	2.49	0.46
7:K:931:LEU:HD12	7:K:946:ALA:O	2.17	0.45
5:I:114:DA:N6	6:J:31:DG:C6	2.84	0.45
2:B:27:ILE:HD13	2:B:60:LYS:NZ	2.31	0.45
1:E:80:LYS:HB3	1:E:83:LEU:HD11	1.98	0.45
7:K:159:LEU:HD23	7:K:202:PHE:HE2	1.81	0.45
7:K:744:ASP:OD2	7:K:746:SER:N	2.50	0.45
8:L:250:LEU:CD2	8:L:258:LEU:HD13	2.47	0.45
3:C:55:VAL:O	3:C:59:LEU:HD12	2.18	0.44
7:K:1077:HIS:ND1	7:K:1082:THR:HG22	2.32	0.44
7:K:140:PHE:HB2	7:K:159:LEU:HD21	1.99	0.44
4:H:32:ARG:NH2	5:I:120:DG:O3'	2.51	0.44
1:A:124:ASP:OD1	1:E:114:HIS:NE2	2.45	0.44
7:K:336:LEU:HD22	7:K:347:VAL:HG22	1.99	0.43
2:F:39:ALA:CB	2:F:47:ILE:HD11	2.48	0.43
7:K:159:LEU:HD23	7:K:202:PHE:CE2	2.53	0.43
6:J:98:3DR:C5'	6:J:98:3DR:O4'	2.56	0.43
2:B:31:THR:HG21	5:I:57:DA:H3'	2.01	0.43
7:K:891:TYR:CE1	7:K:901:THR:HG22	2.54	0.43
1:A:49:LEU:HA	1:A:52:ILE:HD12	2.01	0.43
7:K:118:THR:OG1	7:K:134:ARG:NH2	2.45	0.43
7:K:909:ILE:HG12	7:K:928:ARG:HD2	2.01	0.43
8:L:384:CYS:SG	8:L:385:GLN:N	2.92	0.43
1:A:60:GLU:N	1:A:60:GLU:OE1	2.51	0.43
2:B:39:ALA:HB3	2:B:47:ILE:HD11	2.00	0.43
7:K:1133:VAL:O	7:K:1137:THR:HG23	2.19	0.43
8:L:421:GLU:O	8:L:422:GLU:HG3	2.19	0.43
1:E:119:THR:HG1	6:J:73:DA:P	2.42	0.42
4:H:37:SER:N	5:I:119:DT:OP1	2.44	0.42
1:E:85:PHE:CE1	2:F:82:VAL:HG11	2.54	0.42
7:K:929:SER:OG	7:K:930:VAL:N	2.52	0.42
3:C:52:LEU:HD21	4:D:74:ILE:HG21	2.02	0.42
6:J:118:DT:C2'	6:J:119:DT:H72	2.50	0.42
7:K:117:GLU:OE2	8:L:85:SER:N	2.53	0.42
1:A:48:ALA:HB2	6:J:85:DT:P	2.59	0.42
4:D:89:THR:HG1	5:I:36:DT:P	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:115:THR:OG1	8:L:131:SER:O	2.38	0.42
8:L:250:LEU:HD23	8:L:258:LEU:HD13	2.02	0.42
8:L:207:LEU:HD12	8:L:217:VAL:O	2.20	0.41
8:L:249:ALA:O	8:L:258:LEU:HD12	2.19	0.41
1:E:63:ILE:HD11	2:F:38:LEU:HD11	2.03	0.41
5:I:64:DT:C2'	5:I:65:DT:H72	2.50	0.41
7:K:49:LEU:HG	7:K:333:LEU:HD11	2.01	0.41
3:C:36:ARG:NH2	6:J:116:DT:OP2	2.49	0.41
8:L:316:SER:OG	8:L:317:ALA:N	2.53	0.41
4:D:69:ASP:OD2	4:D:73:ARG:NH2	2.52	0.41
4:H:69:ASP:OD2	4:H:73:ARG:NH2	2.52	0.41
7:K:932:LEU:HD22	7:K:965:PHE:HZ	1.84	0.41
4:H:31:LYS:NZ	5:I:44:DC:OP1	2.39	0.41
7:K:120:ILE:HG23	7:K:135:LEU:HD23	2.03	0.41
7:K:290:GLN:NE2	7:K:296:THR:HG23	2.36	0.41
6:J:1:DA:H2'	6:J:2:DT:H72	2.03	0.41
7:K:1129:LEU:O	7:K:1133:VAL:HG23	2.21	0.40
1:A:129:ARG:NH1	2:B:58:VAL:HG22	2.36	0.40
1:A:85:PHE:CE1	2:B:82:VAL:HG11	2.57	0.40
1:E:118:VAL:HG12	1:E:118:VAL:O	2.21	0.40
7:K:909:ILE:HG22	7:K:910:MET:HG3	2.02	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	96/139 (69%)	95 (99%)	1 (1%)	0	100	100
2	B	79/106 (74%)	77 (98%)	2 (2%)	0	100	100
2	F	80/106 (76%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	108/133 (81%)	103 (95%)	4 (4%)	1 (1%)	17 54
3	G	109/133 (82%)	102 (94%)	7 (6%)	0	100 100
4	D	95/129 (74%)	91 (96%)	3 (3%)	1 (1%)	14 50
4	H	95/129 (74%)	91 (96%)	3 (3%)	1 (1%)	14 50
7	K	821/1163 (71%)	796 (97%)	22 (3%)	3 (0%)	34 71
8	L	365/450 (81%)	320 (88%)	42 (12%)	3 (1%)	19 58
All	All	1947/2627 (74%)	1849 (95%)	89 (5%)	9 (0%)	32 67

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	K	382	PHE
4	D	105	GLY
4	H	105	GLY
8	L	112	ARG
7	K	929	SER
8	L	67	ARG
7	K	36	ASN
8	L	111	ASP
3	C	110	PRO

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	85/113 (75%)	84 (99%)	1 (1%)	71 83
2	B	66/81 (82%)	66 (100%)	0	100 100
2	F	67/81 (83%)	67 (100%)	0	100 100
3	C	86/102 (84%)	86 (100%)	0	100 100
3	G	87/102 (85%)	87 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	83/107 (78%)	78 (94%)	5 (6%)	19 47
4	H	83/107 (78%)	78 (94%)	5 (6%)	19 47
7	K	720/1018 (71%)	719 (100%)	1 (0%)	93 97
8	L	319/390 (82%)	316 (99%)	3 (1%)	78 87
All	All	1684/2214 (76%)	1668 (99%)	16 (1%)	77 85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ARG
4	D	31	LYS
4	D	33	SER
4	D	45	VAL
4	D	72	GLU
4	D	123	THR
1	E	130	ARG
4	H	31	LYS
4	H	33	SER
4	H	45	VAL
4	H	72	GLU
4	H	123	THR
7	K	969	GLU
8	L	85	SER
8	L	180	THR
8	L	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	ASN
2	F	26	ASN
3	G	25	GLN
3	G	39	ASN
7	K	319	ASN
7	K	1059	ASN

5.3.3 RNA

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	97	6	8,11,12	5.81	6 (75%)	9,14,17	1.37	1 (11%)
6	3DR	J	98	6	8,11,12	5.85	4 (50%)	9,14,17	1.08	1 (11%)

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	97	6	-	1/3/15/16	0/1/1/1
6	3DR	J	98	6	-	0/3/15/16	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	98	3DR	O4'-C4'	13.86	1.67	1.44
6	J	97	3DR	O4'-C4'	13.53	1.66	1.44
6	J	97	3DR	C3'-C4'	-6.82	1.34	1.53
6	J	98	3DR	C3'-C4'	-6.79	1.34	1.53
6	J	97	3DR	O4'-C1'	-3.96	1.31	1.42
6	J	98	3DR	O4'-C1'	-3.87	1.31	1.42
6	J	97	3DR	C2'-C1'	3.32	1.60	1.51
6	J	98	3DR	C2'-C1'	3.17	1.59	1.51
6	J	97	3DR	C2'-C3'	2.24	1.56	1.52
6	J	97	3DR	O5'-C5'	-2.05	1.39	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	97	3DR	C1'-O4'-C4'	-2.69	104.14	108.48
6	J	98	3DR	O4'-C4'-C3'	2.02	106.70	103.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	97	3DR	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	97	3DR	1	0
6	J	98	3DR	2	0

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.

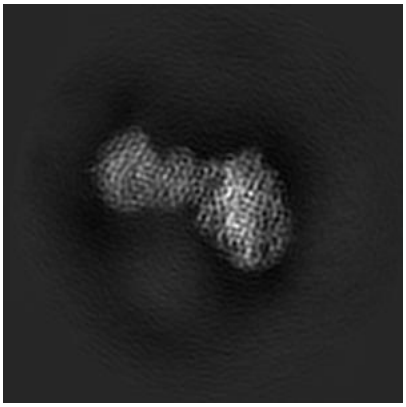
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4765. These allow visual inspection of the internal detail of the map and identification of artifacts.

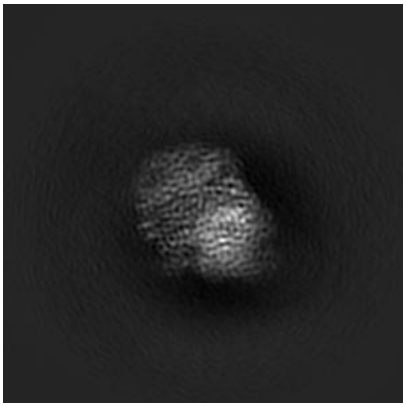
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

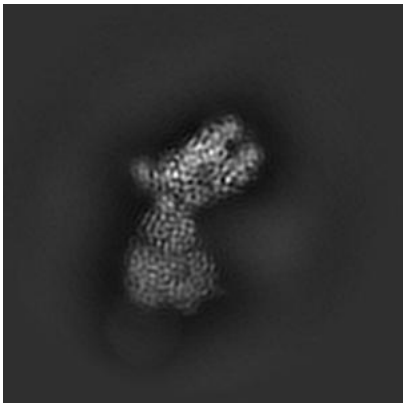
6.1.1 Primary map



X



Y

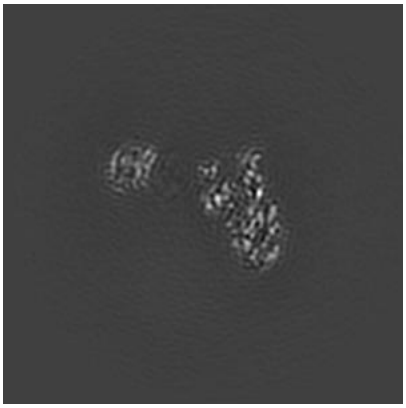


Z

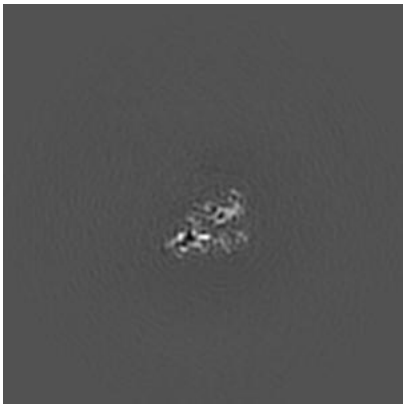
The images above show the map projected in three orthogonal directions.

6.2 Central slices

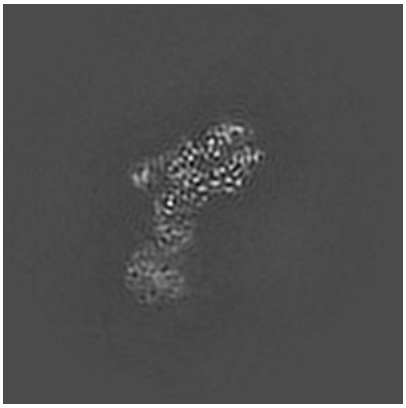
6.2.1 Primary map



X Index: 96



Y Index: 96

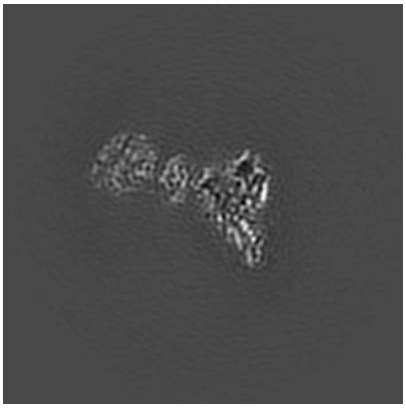


Z Index: 96

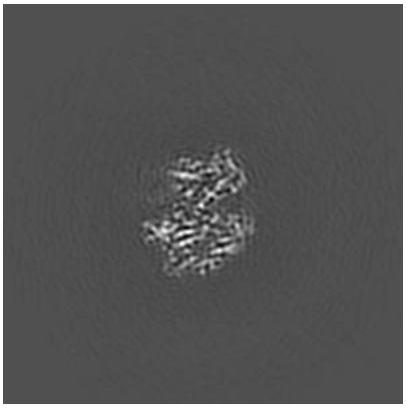
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

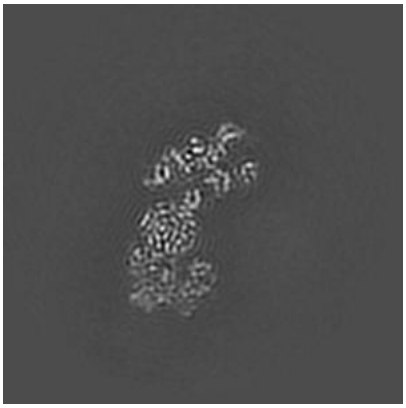
6.3.1 Primary map



X Index: 90



Y Index: 109

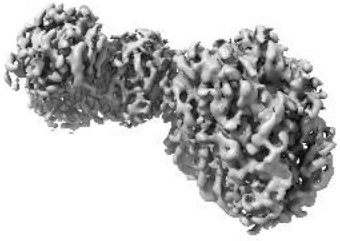


Z Index: 106

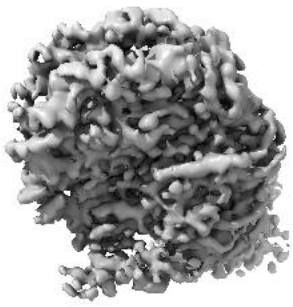
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

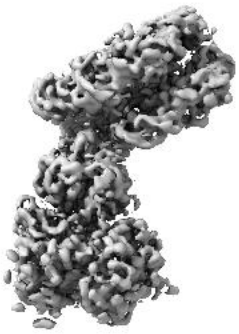
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

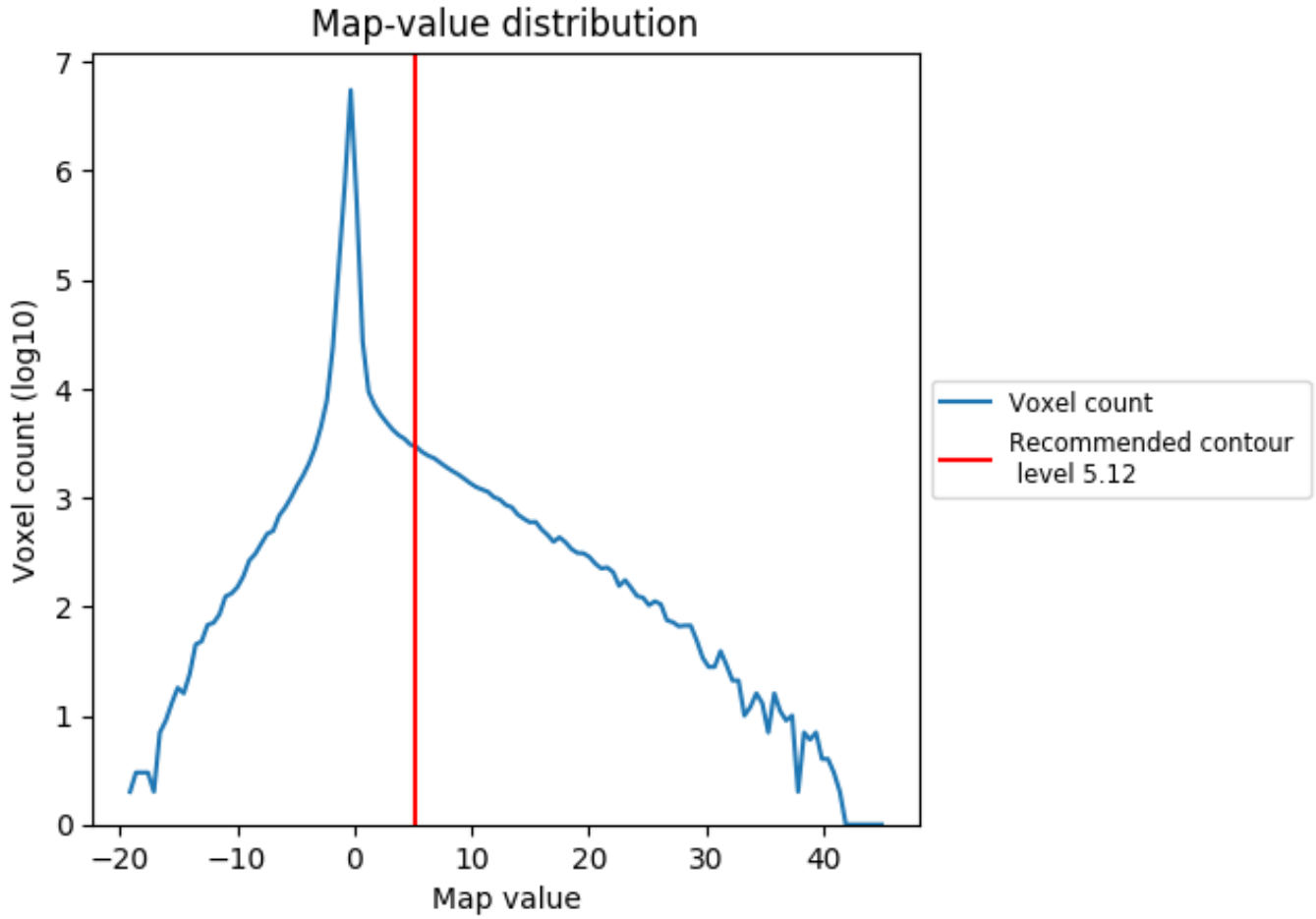
6.5 Mask visualisation (i)

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

7 Map analysis

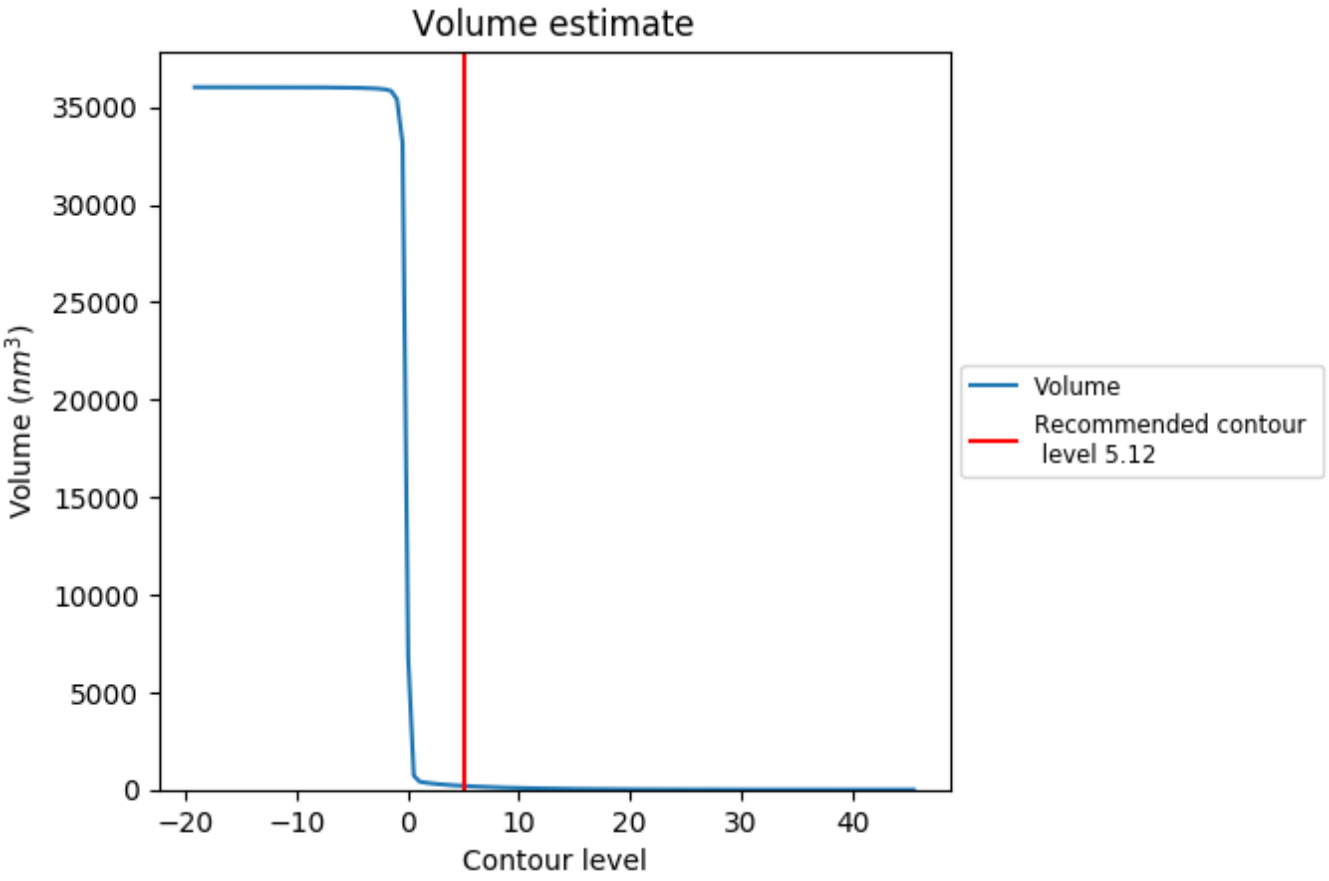
This section contains the results of statistical analysis of the map.

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.

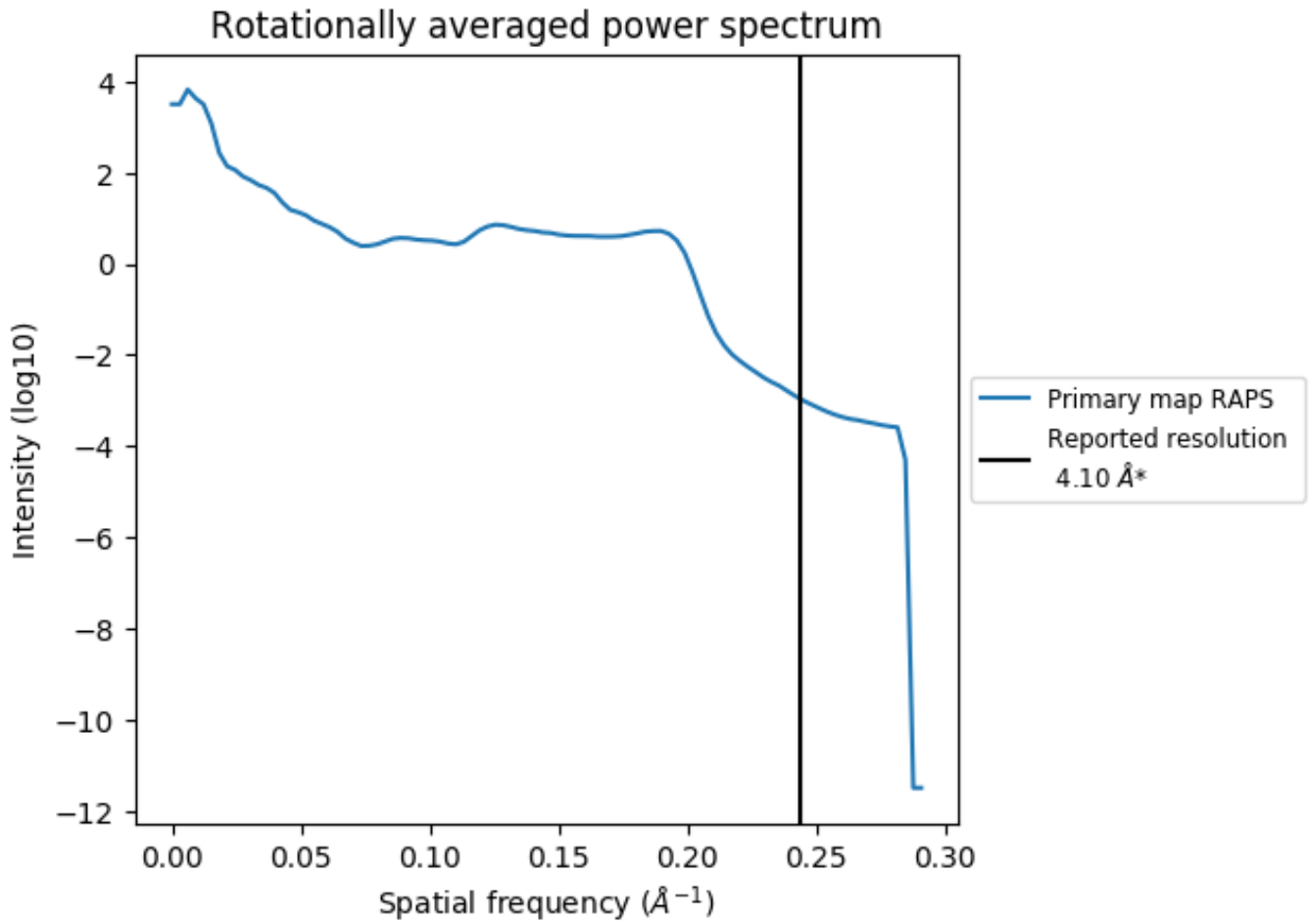
7.2 Volume estimate



The volume at the recommended contour level is 191 nm^3; this corresponds to an approximate mass of 172 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 0.244 Å^{-1}

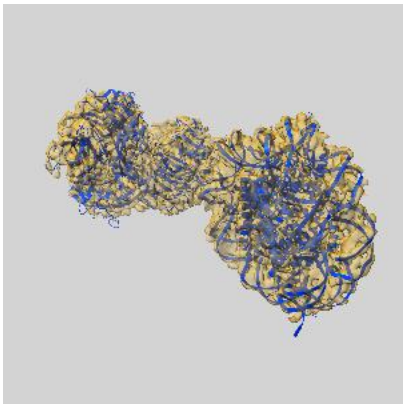
8 Fourier-Shell correlation

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

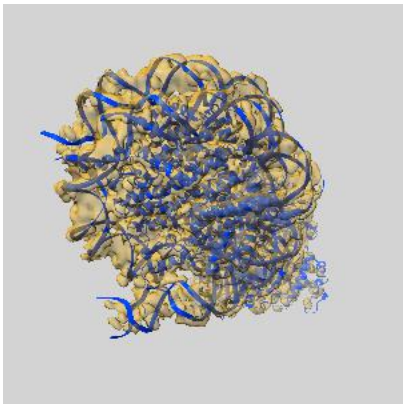
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4765 and PDB model 6R91. Per-residue inclusion information can be found in section 3 on page 8.

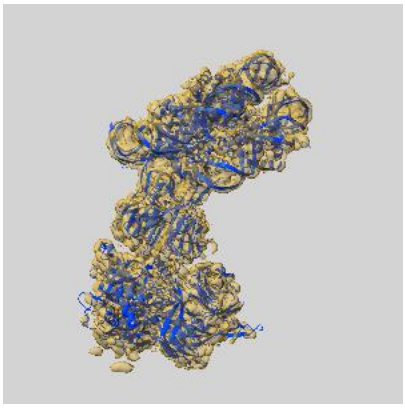
9.1 Map-model overlay



X



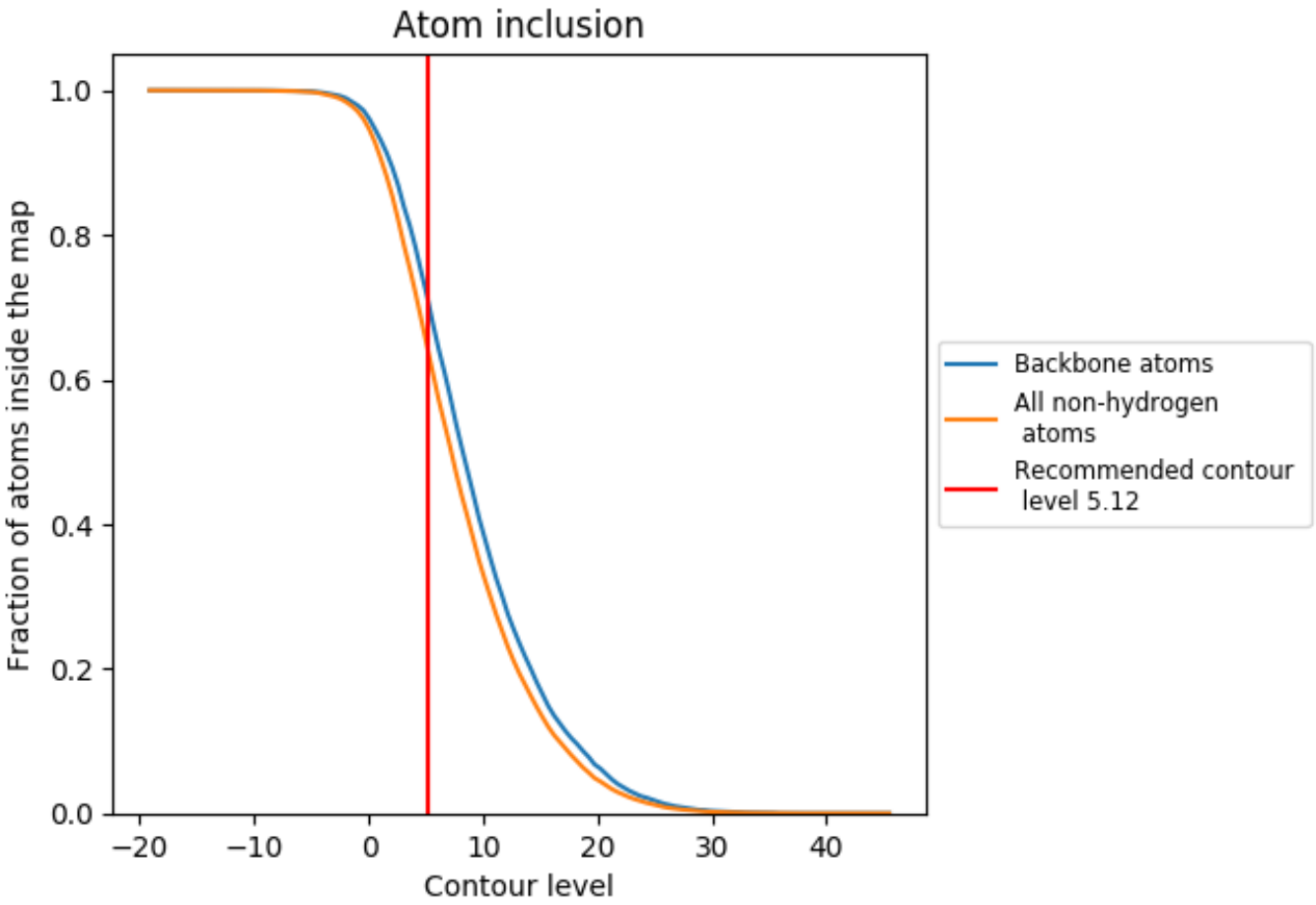
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.12 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 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.