



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 10:04 PM JST

PDB ID : 7F75  
EMDB ID : EMD-31485  
Title : Cryo-EM structure of Spx-dependent transcription activation complex  
Authors : Lin, W.; Feng, Y.; Shi, J.  
Deposited on : 2021-06-28  
Resolution : 4.20 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
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

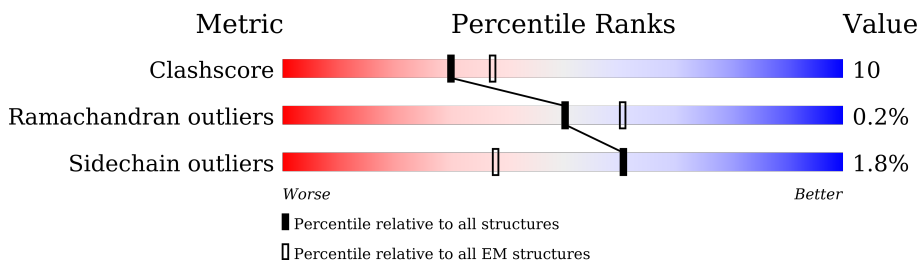
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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.






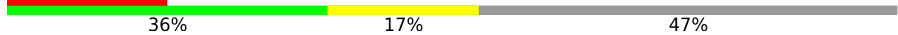
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	314	
1	B	314	
1	I	314	
2	C	1193	
3	D	1199	
4	E	67	
5	F	371	
6	H	69	

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Mol	Chain	Length	Quality of chain
7	G	131	 66% 31% ..
8	J	68	 50% 37% 13%
9	K	68	 56% 37% 7% 18%
10	L	173	 18% 36% 17% 47%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 26887 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	Total	C	N	O		0	0
			1540	961	266	313			
1	B	220	Total	C	N	O		0	0
			1538	968	263	307			
1	I	67	Total	C	N	O	S	0	0
			530	327	94	105	4		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1133	Total	C	N	O	S	0	0
			8041	5033	1380	1612	16		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1142	Total	C	N	O	S	0	0
			7891	4972	1391	1501	27		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	62	Total	C	N	O	S	0	0
			405	253	73	78	1		

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	272	Total	C	N	O	S	0	0
			2047	1289	361	391	6		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	69	Total	C	N	O	S	0	0
			542	348	86	107	1		

- Molecule 7 is a protein called transcriptional regulator Spx.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	129	Total	C	N	O	S	0	0
			1077	679	196	197	5		

- Molecule 8 is a DNA chain called trxA promoter DNA-Non template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	59	Total	C	N	O	P	0	0
			1225	582	240	345	58		

- Molecule 9 is a DNA chain called trxA promoter DNA-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	63	Total	C	N	O	P	0	0
			1285	615	225	382	63		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	92	Total	C	N	O	S	0	0
			763	489	122	150	2		

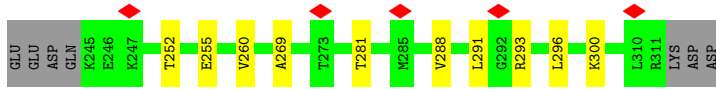
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	

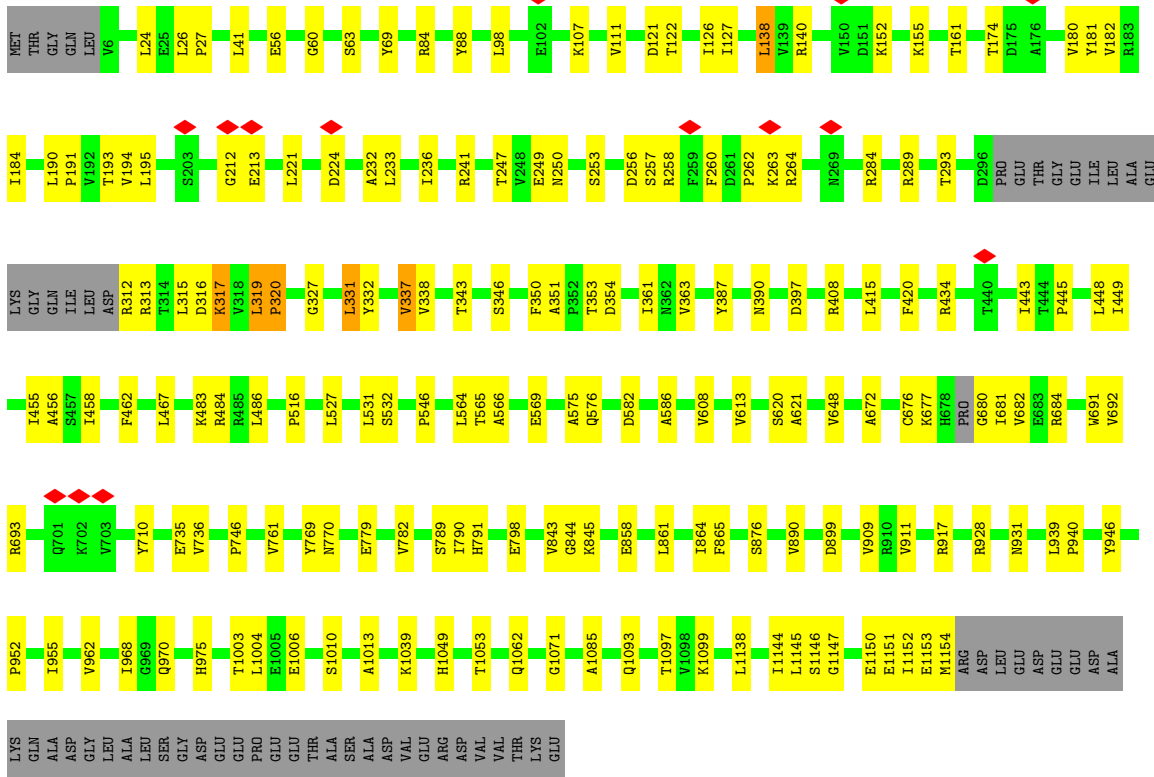
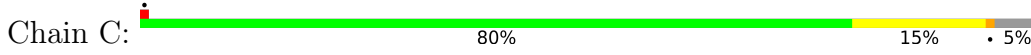
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	D	2	Total	Zn	0
			2	2	

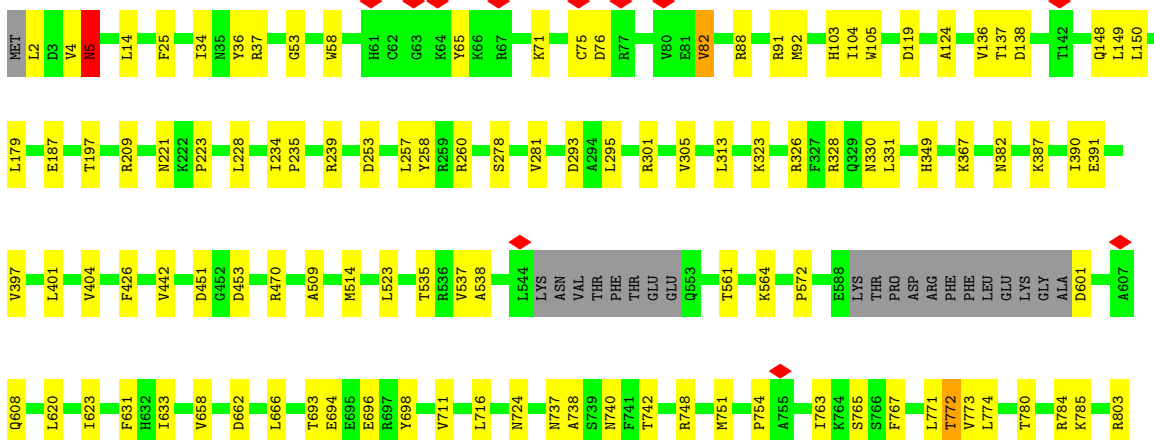
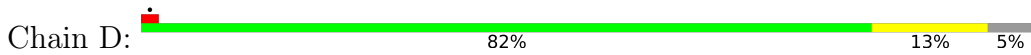


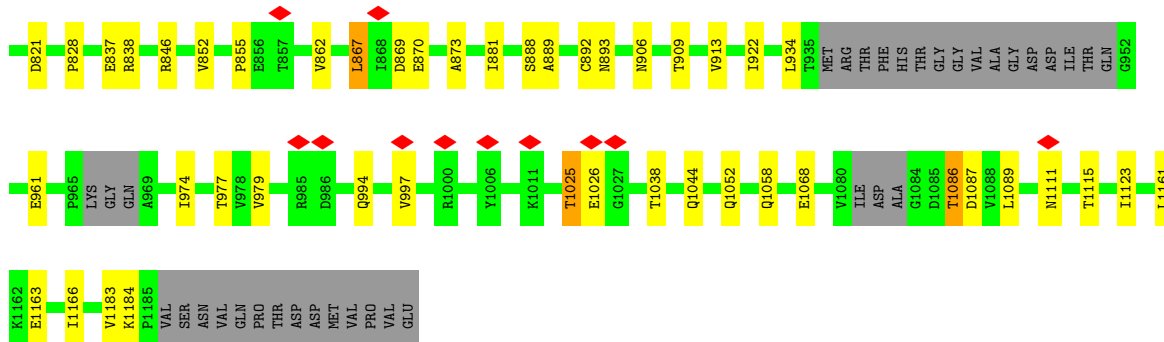


• Molecule 2: DNA-directed RNA polymerase subunit beta

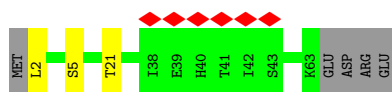
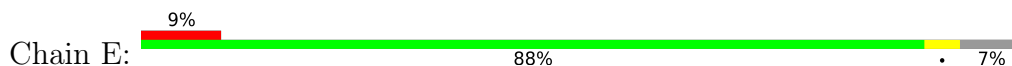


• Molecule 3: DNA-directed RNA polymerase subunit beta'

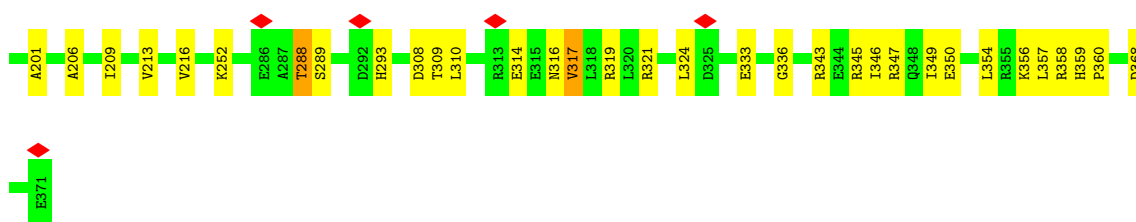
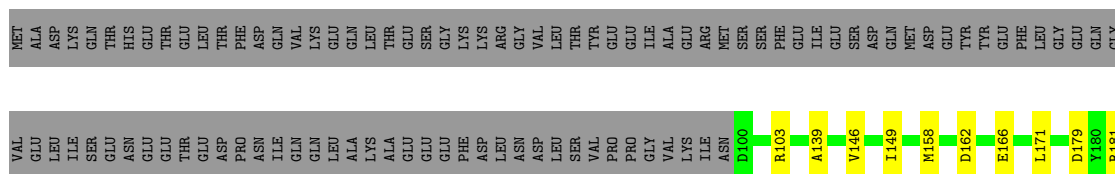




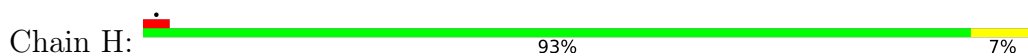
• Molecule 4: DNA-directed RNA polymerase subunit omega



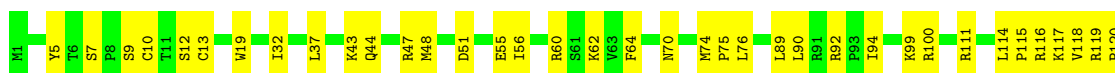
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA-directed RNA polymerase subunit epsilon



• Molecule 7: transcriptional regulator Spx







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59	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	0.152	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.011	Depositor
Map size ( $\text{\AA}$ )	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3069999, 1.3069999, 1.3069999	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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/1558	0.55	0/2132
1	B	0.32	0/1558	0.56	0/2138
1	I	0.31	0/530	0.59	0/705
2	C	0.37	0/8164	0.60	0/11137
3	D	0.37	0/7999	0.60	0/10896
4	E	0.30	0/407	0.55	0/550
5	F	0.32	0/2074	0.57	0/2804
6	H	0.34	0/550	0.63	0/740
7	G	0.34	0/1096	0.58	0/1478
8	J	0.65	0/1380	0.93	0/2132
9	K	0.68	0/1438	1.00	0/2216
10	L	0.24	0/779	0.40	0/1051
All	All	0.40	0/27533	0.64	0/37979

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1540	0	1395	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1538	0	1427	26	0
1	I	530	0	555	7	0
2	C	8041	0	7238	152	0
3	D	7891	0	7094	111	0
4	E	405	0	330	3	0
5	F	2047	0	1937	39	0
6	H	542	0	520	3	0
7	G	1077	0	1103	48	0
8	J	1225	0	664	61	0
9	K	1285	0	714	61	0
10	L	763	0	740	37	0
11	D	1	0	0	0	0
12	D	2	0	0	0	0
All	All	26887	0	23717	498	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 10.

All (498) 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)
9:K:33:DC:H2''	9:K:34:DC:C5	1.46	1.47
2:C:331:LEU:CD1	2:C:343:THR:HG23	1.64	1.26
8:J:36:DT:C6	8:J:37:DT:H72	1.73	1.24
2:C:681:ILE:CG2	2:C:693:ARG:HB2	1.74	1.16
9:K:21:DA:H2''	9:K:22:DA:OP1	1.44	1.15
2:C:681:ILE:HG21	2:C:693:ARG:CB	1.80	1.11
9:K:33:DC:C2'	9:K:34:DC:C5	2.33	1.10
2:C:331:LEU:HD13	2:C:343:THR:HG23	1.18	1.09
2:C:681:ILE:HG22	2:C:693:ARG:HB2	1.36	1.08
2:C:681:ILE:HB	2:C:693:ARG:O	1.51	1.07
5:F:308:ASP:HA	7:G:119:ARG:HH12	1.15	1.05
3:D:997:VAL:HG21	10:L:84:TYR:HB3	1.38	1.05
2:C:317:LYS:HA	2:C:317:LYS:HE2	1.36	1.05
9:K:17:DG:N2	9:K:17:DG:OP2	1.88	1.05
2:C:681:ILE:CG2	2:C:693:ARG:CB	2.36	1.04
4:E:2:LEU:N	4:E:5:SER:HG	1.57	1.03
9:K:22:DA:C2'	9:K:23:DT:H71	1.88	1.03
9:K:34:DC:H2''	9:K:35:DC:OP1	1.53	1.02
2:C:682:VAL:HG13	2:C:691:TRP:O	1.60	1.02
2:C:681:ILE:HG21	2:C:693:ARG:HB3	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:22:DA:H2'	9:K:23:DT:H71	1.37	1.01
7:G:118:VAL:HA	7:G:121:PHE:CD2	1.95	1.00
8:J:26:DT:H2''	8:J:27:DG:H5'	1.50	0.93
2:C:456:ALA:HB2	9:K:22:DA:OP1	1.70	0.92
9:K:61:DA:H2''	9:K:62:DC:C6	2.06	0.91
7:G:115:PRO:HB2	7:G:118:VAL:HG23	1.54	0.89
2:C:331:LEU:HD12	2:C:343:THR:HG23	1.53	0.89
8:J:52:DC:C2'	8:J:53:DA:C8	2.57	0.88
3:D:997:VAL:HG23	10:L:83:PRO:O	1.74	0.88
8:J:19:DG:H2''	8:J:20:DA:C8	2.08	0.87
5:F:308:ASP:HA	7:G:119:ARG:NH1	1.89	0.86
8:J:52:DC:H2''	8:J:53:DA:C8	2.09	0.86
5:F:308:ASP:CA	7:G:119:ARG:HH12	1.87	0.86
7:G:116:ARG:HG2	7:G:116:ARG:HH21	1.39	0.85
2:C:682:VAL:HA	2:C:692:VAL:HA	1.58	0.85
2:C:1144:ILE:O	2:C:1152:ILE:HG12	1.75	0.84
2:C:456:ALA:CB	9:K:22:DA:OP1	2.25	0.83
2:C:682:VAL:CG1	2:C:691:TRP:O	2.27	0.83
9:K:33:DC:H2''	9:K:34:DC:H5	1.36	0.83
2:C:293:THR:OG1	2:C:316:ASP:HB3	1.79	0.82
7:G:116:ARG:O	7:G:120:PRO:HD3	1.79	0.82
2:C:331:LEU:HD13	2:C:343:THR:CG2	2.07	0.82
9:K:21:DA:C2'	9:K:22:DA:OP1	2.22	0.81
2:C:1146:SER:HB3	2:C:1150:GLU:HB3	1.63	0.81
9:K:33:DC:H1'	9:K:34:DC:C6	2.16	0.81
9:K:51:DT:H2''	9:K:52:DT:H5''	1.61	0.81
8:J:39:DT:H2''	8:J:40:DA:C8	2.15	0.81
8:J:36:DT:C4	8:J:37:DT:O4	2.34	0.80
2:C:1145:LEU:HA	2:C:1150:GLU:O	1.82	0.80
2:C:317:LYS:HA	2:C:317:LYS:CE	2.03	0.79
7:G:117:LYS:O	7:G:120:PRO:HD2	1.82	0.79
8:J:52:DC:H2'	8:J:53:DA:C8	2.18	0.79
8:J:9:DA:H4'	8:J:10:DA:OP1	1.82	0.79
9:K:61:DA:H2''	9:K:62:DC:H6	1.42	0.79
2:C:455:ILE:HA	2:C:458:ILE:CG1	2.13	0.79
7:G:115:PRO:HB2	7:G:118:VAL:CG2	2.13	0.78
8:J:39:DT:H2''	8:J:40:DA:H8	1.48	0.77
3:D:1115:THR:CB	10:L:63:ASN:CG	2.53	0.76
8:J:39:DT:H2''	8:J:40:DA:H5'	1.68	0.76
2:C:317:LYS:HE2	2:C:317:LYS:CA	2.15	0.76
8:J:39:DT:C4	8:J:40:DA:N6	2.54	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:116:ARG:HG2	7:G:116:ARG:NH2	1.98	0.75
8:J:39:DT:C2'	8:J:40:DA:C8	2.70	0.75
8:J:36:DT:C6	8:J:37:DT:C7	2.64	0.74
3:D:852:VAL:HG12	3:D:862:VAL:HG22	1.69	0.73
8:J:25:DA:H2''	8:J:26:DT:OP2	1.89	0.73
10:L:51:LEU:HB3	10:L:54:ARG:HB3	1.71	0.72
8:J:19:DG:H2''	8:J:20:DA:H8	1.53	0.72
3:D:867:LEU:N	3:D:867:LEU:HD23	2.03	0.72
8:J:36:DT:N3	8:J:37:DT:C4	2.58	0.72
2:C:337:VAL:HG13	2:C:338:VAL:N	2.04	0.71
7:G:118:VAL:HA	7:G:121:PHE:CE2	2.26	0.71
9:K:33:DC:H2''	9:K:34:DC:C4	2.23	0.71
8:J:39:DT:C4	8:J:40:DA:C6	2.78	0.71
3:D:821:ASP:HB3	10:L:13:GLU:O	1.91	0.70
2:C:337:VAL:HG22	2:C:338:VAL:H	1.56	0.70
2:C:241:ARG:HH11	5:F:103:ARG:HH12	1.40	0.70
3:D:997:VAL:CG2	10:L:83:PRO:O	2.40	0.69
8:J:37:DT:H2'	8:J:37:DT:OP2	1.92	0.69
2:C:138:LEU:HD12	2:C:138:LEU:O	1.93	0.69
7:G:19:TRP:HH2	7:G:114:LEU:HD21	1.55	0.69
2:C:138:LEU:HD12	2:C:138:LEU:C	2.14	0.68
8:J:36:DT:C5	8:J:37:DT:H72	2.26	0.68
7:G:125:GLU:O	7:G:129:LEU:HD23	1.93	0.67
8:J:46:DA:OP1	8:J:48:DC:N4	2.28	0.67
2:C:684:ARG:H	2:C:691:TRP:HB2	1.59	0.67
3:D:561:THR:HG23	3:D:564:LYS:H	1.58	0.67
9:K:33:DC:C2'	9:K:34:DC:C6	2.78	0.67
3:D:1115:THR:CB	10:L:63:ASN:CB	2.73	0.66
7:G:7:SER:OG	7:G:10:CYS:SG	2.54	0.66
8:J:26:DT:C2'	8:J:27:DG:H5'	2.25	0.66
2:C:213:GLU:HB2	2:C:351:ALA:HB2	1.77	0.66
1:A:83:LYS:HD2	1:A:167:ASP:HB2	1.76	0.66
3:D:763:ILE:HG22	3:D:765:SER:H	1.60	0.66
3:D:323:LYS:HA	3:D:328:ARG:HD3	1.77	0.66
3:D:997:VAL:CG2	10:L:84:TYR:HB3	2.22	0.65
7:G:120:PRO:O	7:G:123:LEU:N	2.30	0.65
9:K:33:DC:H1'	9:K:34:DC:N1	2.11	0.65
9:K:22:DA:H2'	9:K:23:DT:C7	2.19	0.65
10:L:16:LEU:HD11	10:L:54:ARG:HH11	1.60	0.65
1:B:97:LEU:HB2	1:B:140:LEU:HB2	1.78	0.65
7:G:43:LYS:HD2	1:I:255:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1097:THR:HG23	2:C:1099:LYS:H	1.60	0.64
2:C:253:SER:HA	2:C:256:ASP:HB2	1.80	0.64
9:K:17:DG:C2'	9:K:18:DG:O5'	2.44	0.64
2:C:680:GLY:N	2:C:736:VAL:HG13	2.13	0.64
3:D:852:VAL:HG12	3:D:862:VAL:CG2	2.28	0.64
2:C:256:ASP:HA	2:C:260:PHE:HB2	1.79	0.64
2:C:680:GLY:HA2	2:C:736:VAL:H	1.64	0.63
1:B:106:THR:HG22	1:B:129:THR:HG23	1.80	0.63
2:C:931:ASN:ND2	2:C:970:GLN:OE1	2.31	0.63
8:J:39:DT:H2''	8:J:40:DA:C5'	2.29	0.62
8:J:39:DT:C2	8:J:40:DA:C5	2.87	0.62
3:D:1115:THR:HA	10:L:63:ASN:HB3	1.82	0.62
10:L:11:LEU:HD22	10:L:43:LEU:HD21	1.82	0.61
3:D:1115:THR:CA	10:L:63:ASN:HB3	2.30	0.61
2:C:516:PRO:HB2	3:D:780:THR:HG21	1.82	0.61
3:D:1115:THR:CB	10:L:63:ASN:OD1	2.48	0.61
2:C:337:VAL:HG13	2:C:338:VAL:H	1.65	0.61
3:D:1115:THR:CB	10:L:63:ASN:HB3	2.31	0.60
8:J:36:DT:C4	8:J:37:DT:C4	2.90	0.60
2:C:681:ILE:HB	2:C:693:ARG:C	2.21	0.60
9:K:33:DC:H2''	9:K:34:DC:C6	2.22	0.60
2:C:798:GLU:O	2:C:845:LYS:NZ	2.34	0.60
9:K:33:DC:O3'	9:K:34:DC:C6	2.54	0.60
1:B:188:VAL:HG12	1:B:190:ASN:H	1.67	0.60
3:D:65:TYR:HB2	3:D:82:VAL:HG11	1.83	0.59
8:J:10:DA:C2	8:J:11:DA:C6	2.90	0.59
8:J:19:DG:C2	8:J:20:DA:C6	2.90	0.59
8:J:46:DA:OP1	8:J:47:DG:N2	2.35	0.59
3:D:119:ASP:OD2	3:D:209:ARG:NH2	2.35	0.59
9:K:51:DT:H72	9:K:52:DT:H73	1.83	0.59
7:G:111:ARG:O	7:G:114:LEU:HG	2.02	0.59
9:K:33:DC:C1'	9:K:34:DC:C5	2.85	0.59
2:C:194:VAL:HG23	2:C:232:ALA:HB1	1.84	0.59
5:F:181:ARG:HD3	8:J:38:DA:N6	2.18	0.59
7:G:10:CYS:HB3	7:G:13:CYS:HB2	1.85	0.59
9:K:33:DC:C1'	9:K:34:DC:C6	2.85	0.59
5:F:308:ASP:CB	7:G:119:ARG:HH12	2.16	0.58
2:C:1146:SER:HB3	2:C:1150:GLU:CB	2.32	0.58
9:K:51:DT:C2'	9:K:52:DT:H5''	2.31	0.58
8:J:36:DT:H2''	8:J:37:DT:OP2	2.04	0.58
10:L:71:LEU:HB3	10:L:75:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:36:DT:C2	8:J:37:DT:C5	2.92	0.58
3:D:837:GLU:HG3	3:D:1052:GLN:HE21	1.69	0.57
4:E:2:LEU:N	4:E:5:SER:OG	2.32	0.57
2:C:1152:ILE:HG22	2:C:1154:MET:CB	2.33	0.57
9:K:61:DA:C2'	9:K:62:DC:C6	2.86	0.57
3:D:234:ILE:O	3:D:239:ARG:NH1	2.38	0.57
5:F:166:GLU:HG2	5:F:201:ALA:HB2	1.86	0.57
2:C:779:GLU:HA	2:C:782:VAL:HG12	1.86	0.57
3:D:426:PHE:HZ	3:D:442:VAL:HG11	1.68	0.57
3:D:754:PRO:HB3	3:D:785:LYS:HB2	1.86	0.57
7:G:44:GLN:OE1	7:G:47:ARG:NH2	2.37	0.57
1:B:34:THR:HG22	1:B:180:VAL:HG21	1.85	0.56
9:K:52:DT:H2''	9:K:53:DT:OP1	2.04	0.56
3:D:892:CYS:SG	3:D:893:ASN:N	2.79	0.56
1:B:53:VAL:HG11	1:B:140:LEU:HD12	1.87	0.56
7:G:5:TYR:HB2	7:G:94:ILE:HB	1.87	0.56
7:G:10:CYS:SG	7:G:92:ARG:HD2	2.45	0.56
9:K:17:DG:H21	9:K:17:DG:P	2.22	0.56
2:C:224:ASP:OD1	2:C:224:ASP:N	2.39	0.56
2:C:484:ARG:NH1	2:C:532:SER:O	2.38	0.56
2:C:843:VAL:HG11	2:C:909:VAL:HG21	1.86	0.56
2:C:213:GLU:HB3	2:C:361:ILE:HB	1.86	0.56
2:C:127:ILE:HD13	2:C:462:PHE:HB3	1.88	0.56
2:C:516:PRO:O	3:D:784:ARG:NH2	2.39	0.56
3:D:888:SER:OG	3:D:889:ALA:N	2.39	0.56
2:C:258:ARG:HA	2:C:262:PRO:HB3	1.88	0.55
3:D:124:ALA:HB1	3:D:149:LEU:HD21	1.87	0.55
3:D:934:LEU:HD12	3:D:1058:GLN:HG2	1.87	0.55
9:K:53:DT:H1'	9:K:54:DA:H5'	1.88	0.55
2:C:337:VAL:HG22	2:C:338:VAL:N	2.20	0.55
3:D:828:PRO:HB3	3:D:838:ARG:HA	1.89	0.55
2:C:56:GLU:HG3	2:C:60:GLY:HA2	1.87	0.55
1:B:114:HIS:NE2	1:B:118:VAL:O	2.39	0.55
9:K:33:DC:H1'	9:K:34:DC:C2	2.42	0.55
9:K:58:DC:H2'	9:K:59:DT:H72	1.89	0.55
2:C:1093:GLN:O	2:C:1097:THR:HB	2.07	0.55
10:L:10:GLU:O	10:L:14:MET:N	2.38	0.55
3:D:631:PHE:HB3	3:D:633:ILE:HG12	1.88	0.55
3:D:803:ARG:NH1	3:D:961:GLU:OE2	2.40	0.55
3:D:1115:THR:HA	10:L:63:ASN:CG	2.27	0.55
2:C:456:ALA:HB1	9:K:22:DA:OP1	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:326:ARG:HD2	3:D:330:ASN:HD22	1.72	0.54
3:D:234:ILE:HG22	3:D:258:TYR:HE2	1.72	0.54
3:D:997:VAL:HG21	10:L:84:TYR:CB	2.25	0.54
7:G:118:VAL:O	7:G:121:PHE:HB2	2.06	0.54
3:D:4:VAL:HG23	3:D:5:ASN:OD1	2.07	0.54
3:D:453:ASP:OD2	3:D:453:ASP:N	2.37	0.54
2:C:582:ASP:OD1	2:C:586:ALA:N	2.40	0.54
2:C:890:VAL:HG22	2:C:911:VAL:HG12	1.90	0.54
8:J:36:DT:C2	8:J:37:DT:C4	2.96	0.54
2:C:26:LEU:HD12	2:C:27:PRO:HD2	1.89	0.54
5:F:310:LEU:HD13	5:F:314:GLU:HG2	1.90	0.54
8:J:39:DT:N3	8:J:40:DA:C6	2.76	0.54
2:C:190:LEU:HG	2:C:194:VAL:HG11	1.89	0.54
2:C:680:GLY:N	2:C:736:VAL:CG1	2.71	0.54
9:K:34:DC:P	9:K:34:DC:H6	2.31	0.54
2:C:681:ILE:HG21	2:C:693:ARG:HB2	1.50	0.53
8:J:19:DG:N2	8:J:20:DA:C2	2.75	0.53
2:C:98:LEU:HB3	2:C:107:LYS:HB3	1.89	0.53
2:C:257:SER:O	2:C:264:ARG:NH2	2.33	0.53
3:D:1115:THR:HA	10:L:63:ASN:CB	2.37	0.53
7:G:10:CYS:CB	7:G:13:CYS:SG	2.97	0.53
8:J:39:DT:N3	8:J:40:DA:C5	2.76	0.53
7:G:47:ARG:NH1	7:G:48:MET:SD	2.82	0.53
8:J:36:DT:H2'	8:J:37:DT:C7	2.39	0.53
2:C:1144:ILE:HG13	2:C:1152:ILE:HB	1.90	0.53
7:G:56:ILE:HG13	7:G:90:LEU:HD22	1.90	0.53
8:J:18:DT:H2''	8:J:19:DG:C8	2.44	0.53
2:C:684:ARG:N	2:C:691:TRP:HB2	2.24	0.53
3:D:75:CYS:SG	3:D:76:ASP:N	2.82	0.53
3:D:260:ARG:HH12	3:D:305:VAL:HG11	1.74	0.53
2:C:212:GLY:HA2	2:C:361:ILE:HG13	1.90	0.52
5:F:181:ARG:HD3	8:J:38:DA:C6	2.44	0.52
2:C:434:ARG:NH2	2:C:434:ARG:O	2.43	0.52
3:D:257:LEU:HD13	3:D:295:LEU:HA	1.90	0.52
1:A:178:TYR:HB3	1:A:196:LEU:HD23	1.91	0.52
2:C:680:GLY:HA2	2:C:735:GLU:HA	1.92	0.52
10:L:28:LYS:HA	10:L:81:TRP:HZ2	1.75	0.52
2:C:546:PRO:HG2	2:C:613:VAL:HG11	1.90	0.52
2:C:331:LEU:HD12	2:C:343:THR:CG2	2.34	0.52
2:C:565:THR:OG1	2:C:566:ALA:N	2.43	0.52
5:F:309:THR:O	5:F:356:LYS:NZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:347:ARG:NH1	5:F:350:GLU:OE1	2.42	0.52
3:D:738:ALA:O	3:D:742:THR:OG1	2.26	0.52
5:F:336:GLY:O	5:F:343:ARG:NH2	2.43	0.52
8:J:26:DT:H2''	8:J:27:DG:H2'	1.92	0.52
1:I:296:LEU:HG	1:I:300:LYS:HE2	1.93	0.51
8:J:52:DC:C2'	8:J:53:DA:H8	2.16	0.51
3:D:666:LEU:HD11	3:D:716:LEU:HD13	1.92	0.51
3:D:855:PRO:HG3	3:D:881:ILE:HG23	1.92	0.51
2:C:769:TYR:OH	3:D:349:HIS:NE2	2.44	0.51
3:D:870:GLU:O	3:D:873:ALA:HB3	2.10	0.51
9:K:22:DA:H2''	9:K:23:DT:H71	1.89	0.51
2:C:247:THR:HG23	2:C:250:ASN:H	1.76	0.51
5:F:308:ASP:CB	7:G:119:ARG:NH1	2.73	0.51
8:J:36:DT:C5	8:J:37:DT:C7	2.92	0.51
5:F:345:ARG:O	5:F:345:ARG:NH1	2.44	0.51
8:J:36:DT:N1	8:J:37:DT:H72	2.20	0.51
2:C:387:TYR:HA	2:C:390:ASN:HD22	1.75	0.51
7:G:118:VAL:HA	7:G:121:PHE:HD2	1.67	0.51
2:C:121:ASP:N	2:C:121:ASP:OD1	2.44	0.51
2:C:486:LEU:HD11	2:C:531:LEU:HD12	1.92	0.50
2:C:620:SER:OG	2:C:621:ALA:N	2.43	0.50
3:D:977:THR:O	3:D:994:GLN:N	2.44	0.50
2:C:233:LEU:HA	2:C:236:ILE:HD12	1.93	0.50
2:C:676:CYS:CB	2:C:710:TYR:CZ	2.94	0.50
2:C:443:ILE:HD11	2:C:448:LEU:HD21	1.94	0.50
7:G:116:ARG:HH21	7:G:116:ARG:CG	2.14	0.50
5:F:359:HIS:HD2	5:F:360:PRO:HD2	1.75	0.50
7:G:70:ASN:O	7:G:74:MET:HB2	2.12	0.50
10:L:59:TYR:CE2	10:L:63:ASN:ND2	2.80	0.50
1:B:110:ALA:HB2	1:B:123:PRO:HB2	1.94	0.49
3:D:148:GLN:HE22	3:D:150:LEU:HB2	1.77	0.49
9:K:51:DT:C6	9:K:52:DT:H71	2.47	0.49
10:L:87:LEU:O	10:L:91:THR:HG23	2.13	0.49
3:D:331:LEU:HD22	3:D:1166:ILE:HG13	1.93	0.49
2:C:363:VAL:HG23	2:C:390:ASN:HD21	1.77	0.49
2:C:770:ASN:OD1	2:C:770:ASN:N	2.43	0.49
2:C:791:HIS:CE1	2:C:917:ARG:HH11	2.31	0.49
3:D:103:HIS:HD2	3:D:228:LEU:HD22	1.78	0.49
9:K:53:DT:C4	9:K:54:DA:C5	3.01	0.49
2:C:289:ARG:HB2	2:C:350:PHE:HB2	1.95	0.49
3:D:36:TYR:OH	3:D:37:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:39:DT:C2	8:J:40:DA:N7	2.81	0.49
10:L:72:SER:OG	10:L:73:ASP:N	2.45	0.49
1:B:167:ASP:OD1	1:B:167:ASP:N	2.46	0.49
2:C:41:LEU:O	2:C:69:TYR:OH	2.24	0.49
5:F:317:VAL:O	5:F:321:ARG:HB2	2.12	0.49
7:G:19:TRP:CH2	7:G:114:LEU:HD21	2.43	0.49
7:G:76:LEU:HD23	1:I:260:VAL:HG22	1.93	0.49
1:B:64:GLU:OE2	3:D:601:ASP:N	2.46	0.48
2:C:789:SER:OG	2:C:790:ILE:N	2.46	0.48
2:C:1006:GLU:HA	6:H:31:ARG:HG3	1.95	0.48
3:D:693:THR:HG23	3:D:696:GLU:H	1.78	0.48
3:D:1111:ASN:CG	10:L:74:GLN:HE21	2.15	0.48
9:K:17:DG:H2'	9:K:18:DG:O5'	2.12	0.48
3:D:253:ASP:HB2	3:D:313:LEU:HD22	1.94	0.48
2:C:575:ALA:HB2	2:C:608:VAL:HG21	1.95	0.48
9:K:33:DC:H1'	9:K:34:DC:C5	2.48	0.48
2:C:1146:SER:OG	2:C:1147:GLY:N	2.46	0.48
3:D:278:SER:HA	3:D:281:VAL:HG22	1.94	0.48
1:I:291:LEU:HD21	1:I:296:LEU:HB2	1.95	0.48
2:C:181:TYR:HA	2:C:191:PRO:HA	1.95	0.48
7:G:60:ARG:HD3	9:K:57:DG:H5''	1.93	0.48
8:J:11:DA:H1'	8:J:12:DA:H5'	1.94	0.48
2:C:975:HIS:HB3	2:C:1004:LEU:HD11	1.95	0.48
3:D:451:ASP:OD1	3:D:451:ASP:N	2.47	0.48
3:D:772:THR:OG1	3:D:773:VAL:N	2.46	0.48
3:D:1163:GLU:HA	3:D:1166:ILE:HG22	1.94	0.48
10:L:28:LYS:HA	10:L:81:TRP:CZ2	2.49	0.48
2:C:397:ASP:OD1	2:C:397:ASP:N	2.47	0.48
3:D:1115:THR:CA	10:L:63:ASN:CG	2.82	0.48
10:L:6:TYR:HB3	10:L:11:LEU:HG	1.95	0.48
2:C:180:VAL:H	2:C:221:LEU:HD21	1.79	0.48
2:C:184:ILE:HD11	2:C:195:LEU:HD21	1.96	0.48
3:D:53:GLY:H	3:D:88:ARG:HG3	1.79	0.48
5:F:158:MET:HG3	5:F:206:ALA:HB2	1.96	0.48
7:G:19:TRP:HH2	7:G:114:LEU:CD2	2.24	0.48
1:B:200:THR:OG1	1:B:201:ASP:N	2.47	0.47
2:C:332:TYR:HD2	2:C:346:SER:H	1.62	0.47
2:C:962:VAL:HG11	3:D:658:VAL:HG11	1.96	0.47
3:D:1044:GLN:NE2	3:D:1068:GLU:OE2	2.47	0.47
4:E:2:LEU:N	4:E:5:SER:O	2.47	0.47
3:D:5:ASN:OD1	3:D:5:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:51:DT:C7	9:K:52:DT:H73	2.44	0.47
8:J:18:DT:H2''	8:J:19:DG:H8	1.79	0.47
10:L:57:GLN:HA	10:L:60:THR:HG22	1.96	0.47
2:C:682:VAL:HG22	2:C:692:VAL:HG12	1.97	0.47
3:D:34:ILE:HG22	5:F:209:ILE:HD12	1.95	0.47
3:D:136:VAL:HG12	3:D:148:GLN:HE21	1.79	0.47
9:K:33:DC:C2'	9:K:34:DC:C4	2.92	0.47
10:L:71:LEU:HD23	10:L:71:LEU:HA	1.82	0.47
8:J:53:DA:H2	9:K:9:DT:H3	1.63	0.47
10:L:73:ASP:OD1	10:L:74:GLN:N	2.46	0.47
1:B:110:ALA:N	1:B:123:PRO:O	2.48	0.47
2:C:182:VAL:N	2:C:190:LEU:O	2.39	0.46
2:C:319:LEU:HA	2:C:320:PRO:HD3	1.50	0.46
3:D:92:MET:HG2	3:D:235:PRO:HD3	1.95	0.46
2:C:247:THR:OG1	2:C:249:GLU:OE1	2.24	0.46
2:C:672:ALA:HB1	2:C:746:PRO:HD2	1.97	0.46
2:C:680:GLY:HA2	2:C:736:VAL:N	2.31	0.46
1:A:11:THR:OG1	1:A:13:GLU:OE2	2.33	0.46
2:C:152:LYS:O	2:C:155:LYS:NZ	2.37	0.46
2:C:864:ILE:HD11	5:F:357:LEU:HB3	1.97	0.46
3:D:906:ASN:HB2	3:D:913:VAL:HG22	1.96	0.46
1:B:175:ARG:HG3	3:D:523:LEU:HD22	1.98	0.46
8:J:10:DA:N1	8:J:11:DA:N6	2.64	0.46
2:C:864:ILE:HA	5:F:354:LEU:HD11	1.98	0.46
5:F:308:ASP:CG	7:G:119:ARG:NH1	2.69	0.46
8:J:39:DT:C2'	8:J:40:DA:H5'	2.42	0.46
2:C:858:GLU:HA	2:C:861:LEU:HB2	1.97	0.46
3:D:1025:THR:OG1	3:D:1026:GLU:N	2.48	0.46
1:B:27:PRO:HB2	1:B:191:TYR:HD2	1.81	0.45
5:F:146:VAL:HA	5:F:149:ILE:HG22	1.97	0.45
3:D:253:ASP:N	3:D:253:ASP:OD1	2.46	0.45
8:J:36:DT:H2''	8:J:37:DT:C6	2.50	0.45
1:A:99:ILE:HG12	1:A:112:ILE:HG12	1.99	0.45
2:C:1138:LEU:HD21	3:D:105:TRP:CZ2	2.52	0.45
2:C:455:ILE:CA	2:C:458:ILE:CG1	2.89	0.45
3:D:179:LEU:HD12	3:D:223:PRO:HB2	1.98	0.45
1:A:15:SER:OG	1:A:16:ASP:N	2.50	0.45
1:B:58:ILE:HG13	1:B:138:VAL:HG13	1.98	0.45
3:D:137:THR:OG1	3:D:138:ASP:N	2.50	0.45
7:G:64:PHE:HB2	7:G:89:LEU:HD13	1.98	0.45
3:D:187:GLU:OE1	3:D:209:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:514:MET:HB2	3:D:537:VAL:HG13	1.97	0.45
3:D:751:MET:HE1	3:D:763:ILE:HG12	1.98	0.45
5:F:213:VAL:HA	5:F:216:VAL:HG12	1.99	0.45
7:G:62:LYS:NZ	9:K:59:DT:H72	2.31	0.45
9:K:32:DT:H2''	9:K:33:DC:C5	2.51	0.45
2:C:865:PHE:HA	5:F:358:ARG:HD3	1.99	0.45
1:B:59:ASP:OD1	1:B:59:ASP:N	2.50	0.45
1:B:72:VAL:HG23	1:B:73:GLU:HG3	1.99	0.45
2:C:467:LEU:HD23	2:C:467:LEU:HA	1.83	0.45
2:C:648:VAL:HG11	2:C:1039:LYS:HD2	1.99	0.45
5:F:179:ASP:OD1	5:F:179:ASP:N	2.38	0.45
5:F:308:ASP:OD1	5:F:308:ASP:O	2.35	0.45
1:I:293:ARG:HE	1:I:293:ARG:HB2	1.58	0.45
9:K:44:DA:H2''	9:K:45:DC:H5''	2.00	0.45
2:C:1010:SER:OG	2:C:1013:ALA:N	2.48	0.44
7:G:115:PRO:HG2	7:G:118:VAL:HG21	1.99	0.44
9:K:51:DT:C6	9:K:52:DT:C7	3.01	0.44
1:A:222:ASN:HA	1:A:225:VAL:HG12	2.00	0.44
2:C:861:LEU:HA	2:C:864:ILE:HG22	2.00	0.44
3:D:58:TRP:HZ3	3:D:71:LYS:HA	1.82	0.44
3:D:601:ASP:N	3:D:601:ASP:OD1	2.51	0.44
8:J:39:DT:H2'	8:J:40:DA:C8	2.52	0.44
1:B:22:LYS:HB2	1:B:22:LYS:HE3	1.78	0.44
1:B:173:VAL:HA	1:B:200:THR:HA	1.98	0.44
8:J:19:DG:N2	9:K:43:DC:N3	2.52	0.44
2:C:84:ARG:NH1	2:C:899:ASP:OD2	2.51	0.44
2:C:312:ARG:NH2	2:C:327:GLY:O	2.45	0.44
3:D:1115:THR:HA	10:L:63:ASN:ND2	2.32	0.44
2:C:88:TYR:HB3	2:C:126:ILE:HG23	1.99	0.44
2:C:98:LEU:N	2:C:107:LYS:O	2.42	0.44
10:L:71:LEU:CB	10:L:75:THR:HG23	2.46	0.44
1:A:70:GLY:O	1:A:131:GLY:N	2.46	0.44
3:D:1086:THR:OG1	3:D:1087:ASP:N	2.51	0.44
5:F:316:ASN:HD21	7:G:123:LEU:HB3	1.81	0.44
5:F:319:ARG:HA	5:F:324:LEU:HB2	1.98	0.44
8:J:19:DG:C2'	8:J:20:DA:C8	2.93	0.44
9:K:34:DC:C2'	9:K:35:DC:OP1	2.40	0.44
2:C:576:GLN:HE22	3:D:774:LEU:HD22	1.82	0.44
3:D:608:GLN:HE21	3:D:608:GLN:HB2	1.60	0.44
3:D:1123:ILE:HD13	3:D:1123:ILE:HA	1.88	0.44
3:D:1183:VAL:HG12	3:D:1184:LYS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:78:LEU:HB2	10:L:81:TRP:CZ3	2.52	0.44
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.87	0.43
3:D:694:GLU:O	3:D:698:TYR:HB2	2.18	0.43
3:D:257:LEU:HB3	3:D:295:LEU:HD12	2.00	0.43
9:K:39:DC:H2''	9:K:40:DG:C8	2.53	0.43
2:C:262:PRO:HB2	2:C:264:ARG:H	1.83	0.43
3:D:387:LYS:O	3:D:391:GLU:HB3	2.18	0.43
8:J:52:DC:H2'	8:J:53:DA:N7	2.33	0.43
3:D:737:ASN:OD1	3:D:740:ASN:N	2.50	0.43
5:F:345:ARG:HD3	8:J:12:DA:H2'	2.00	0.43
1:B:192:ASP:OD1	1:B:192:ASP:N	2.52	0.43
2:C:293:THR:HG1	2:C:316:ASP:HB3	1.79	0.43
2:C:445:PRO:HA	2:C:448:LEU:HB2	2.01	0.43
3:D:620:LEU:HA	3:D:623:ILE:HG22	1.99	0.43
10:L:37:LEU:HA	10:L:40:ILE:HG22	2.00	0.43
1:A:90:TYR:O	1:A:144:ARG:NH2	2.52	0.43
2:C:138:LEU:C	2:C:138:LEU:CD1	2.86	0.43
8:J:19:DG:H1	9:K:43:DC:H42	1.67	0.43
1:A:42:ARG:NH2	1:B:34:THR:OG1	2.51	0.43
3:D:509:ALA:HB1	3:D:535:THR:HA	2.01	0.43
7:G:99:LYS:HD3	7:G:100:ARG:HG2	2.00	0.43
3:D:14:LEU:H	3:D:221:ASN:ND2	2.16	0.43
3:D:748:ARG:HB2	3:D:763:ILE:HB	2.00	0.43
9:K:61:DA:H2''	9:K:62:DC:C5	2.51	0.43
3:D:104:ILE:HB	3:D:293:ASP:HB2	2.01	0.42
2:C:353:THR:HG22	2:C:354:ASP:H	1.83	0.42
2:C:213:GLU:HG2	2:C:361:ILE:HD12	2.01	0.42
2:C:681:ILE:HG22	2:C:693:ARG:CB	2.16	0.42
5:F:333:GLU:O	5:F:343:ARG:NH1	2.52	0.42
10:L:34:GLN:OE1	10:L:74:GLN:NE2	2.47	0.42
2:C:1049:HIS:NE2	2:C:1071:GLY:O	2.44	0.42
2:C:1062:GLN:NE2	3:D:330:ASN:OD1	2.52	0.42
7:G:74:MET:HA	7:G:75:PRO:HD3	1.89	0.42
9:K:53:DT:C5	9:K:54:DA:N7	2.87	0.42
2:C:939:LEU:HD13	2:C:940:PRO:HD2	2.00	0.42
7:G:32:ILE:HG22	7:G:37:LEU:HD21	2.00	0.42
8:J:36:DT:C2'	8:J:37:DT:OP2	2.68	0.42
2:C:180:VAL:HB	2:C:221:LEU:HD11	2.02	0.42
7:G:100:ARG:HE	7:G:100:ARG:HB3	1.51	0.42
9:K:61:DA:C2'	9:K:62:DC:C5	3.02	0.42
1:A:101:VAL:O	1:A:102:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:415:LEU:HD23	2:C:415:LEU:HA	1.90	0.42
3:D:390:ILE:HG22	3:D:397:VAL:HG21	2.00	0.42
7:G:47:ARG:HD3	1:I:252:THR:HG21	2.02	0.42
7:G:92:ARG:NH2	9:K:57:DG:N7	2.67	0.42
8:J:22:DC:H42	9:K:40:DG:H22	1.66	0.42
2:C:946:TYR:HA	2:C:952:PRO:HA	2.02	0.42
2:C:1152:ILE:HG22	2:C:1154:MET:H	1.84	0.42
1:I:269:ALA:HB2	1:I:288:VAL:HG13	2.00	0.42
1:B:187:GLN:HG2	1:B:188:VAL:HG23	2.01	0.42
2:C:111:VAL:HG21	2:C:449:ILE:HD11	2.01	0.42
2:C:576:GLN:HE22	3:D:774:LEU:HD13	1.84	0.42
2:C:1152:ILE:HG22	2:C:1154:MET:N	2.35	0.42
3:D:401:LEU:HA	3:D:404:VAL:HG12	2.02	0.42
2:C:761:VAL:HG23	2:C:955:ILE:HB	2.02	0.42
3:D:228:LEU:HD12	3:D:228:LEU:HA	1.81	0.42
3:D:846:ARG:HH22	3:D:888:SER:HB2	1.84	0.42
5:F:345:ARG:HH22	5:F:349:ILE:HD13	1.85	0.41
1:B:43:ILE:HG13	1:B:217:LEU:HD13	2.01	0.41
2:C:564:LEU:HD23	2:C:569:GLU:HG2	2.02	0.41
7:G:9:SER:HB3	8:J:3:DA:N7	2.35	0.41
8:J:24:DA:H2'	8:J:25:DA:H8	1.85	0.41
2:C:263:LYS:H	2:C:264:ARG:NH2	2.18	0.41
2:C:680:GLY:N	2:C:736:VAL:O	2.54	0.41
5:F:139:ALA:HA	5:F:171:LEU:HD21	2.00	0.41
5:F:288:THR:OG1	5:F:289:SER:N	2.53	0.41
6:H:5:VAL:HG11	6:H:37:LEU:HD21	2.02	0.41
8:J:36:DT:H2'	8:J:37:DT:H72	2.01	0.41
2:C:122:THR:O	2:C:483:LYS:NZ	2.42	0.41
3:D:326:ARG:HA	3:D:326:ARG:HD3	1.78	0.41
9:K:51:DT:H6	9:K:52:DT:H71	1.85	0.41
2:C:313:ARG:NE	2:C:315:LEU:O	2.47	0.41
2:C:1151:GLU:N	2:C:1151:GLU:CD	2.73	0.41
6:H:4:LYS:NZ	6:H:58:GLU:OE1	2.37	0.41
9:K:33:DC:O3'	9:K:34:DC:H6	2.01	0.41
9:K:52:DT:H2'	9:K:53:DT:C2	2.56	0.41
1:A:59:ASP:N	1:A:59:ASP:OD1	2.54	0.41
2:C:56:GLU:OE2	2:C:63:SER:OG	2.35	0.41
2:C:1152:ILE:CG2	2:C:1154:MET:CB	2.98	0.41
5:F:252:LYS:HE2	5:F:252:LYS:HB2	1.82	0.41
5:F:333:GLU:HA	5:F:343:ARG:HE	1.86	0.41
9:K:54:DA:C2	9:K:55:DA:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:25:PHE:CZ	3:D:91:ARG:HG2	2.56	0.41
3:D:382:ASN:HD21	5:F:368:ASP:HB2	1.86	0.41
3:D:537:VAL:HG12	3:D:538:ALA:H	1.85	0.41
1:B:183:THR:H	1:B:192:ASP:HA	1.84	0.41
2:C:140:ARG:HE	2:C:140:ARG:HB2	1.69	0.41
2:C:527:LEU:HD12	2:C:527:LEU:HA	1.90	0.41
2:C:1085:ALA:HB1	3:D:922:ILE:HG12	2.03	0.41
5:F:308:ASP:HB2	7:G:119:ARG:HH22	1.86	0.41
2:C:408:ARG:HE	2:C:408:ARG:HB2	1.72	0.40
8:J:58:DT:H2 <sup>7</sup>	8:J:59:DG:C8	2.56	0.40
1:B:43:ILE:HD13	1:B:43:ILE:HA	1.91	0.40
1:B:117:ASP:OD1	1:B:117:ASP:N	2.53	0.40
2:C:968:ILE:HD12	2:C:968:ILE:HA	1.95	0.40
3:D:367:LYS:HE2	3:D:367:LYS:HB3	1.81	0.40
3:D:662:ASP:OD2	3:D:724:ASN:ND2	2.55	0.40
5:F:336:GLY:HA2	5:F:346:ILE:HD12	2.02	0.40
9:K:34:DC:C6	9:K:34:DC:P	3.13	0.40
10:L:59:TYR:O	10:L:62:LEU:HG	2.21	0.40
1:A:26:GLU:HA	1:A:27:PRO:HA	1.91	0.40
3:D:767:PHE:HE1	3:D:771:LEU:HD11	1.86	0.40
3:D:1111:ASN:CG	10:L:74:GLN:NE2	2.74	0.40
7:G:51:ASP:N	7:G:55:GLU:OE2	2.42	0.40
5:F:319:ARG:O	5:F:324:LEU:N	2.42	0.40
2:C:434:ARG:HA	2:C:434:ARG:HD2	1.97	0.40
2:C:844:GLY:HA2	2:C:876:SER:HB3	2.03	0.40
2:C:928:ARG:HH11	2:C:928:ARG:HD3	1.74	0.40
3:D:974:ILE:HD12	3:D:974:ILE:HA	1.90	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	222/314 (71%)	207 (93%)	15 (7%)	0	100	100
1	B	218/314 (69%)	197 (90%)	21 (10%)	0	100	100
1	I	65/314 (21%)	65 (100%)	0	0	100	100
2	C	1127/1193 (94%)	1025 (91%)	99 (9%)	3 (0%)	41	76
3	D	1130/1199 (94%)	1014 (90%)	113 (10%)	3 (0%)	41	76
4	E	60/67 (90%)	55 (92%)	5 (8%)	0	100	100
5	F	270/371 (73%)	242 (90%)	28 (10%)	0	100	100
6	H	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
7	G	127/131 (97%)	123 (97%)	4 (3%)	0	100	100
10	L	90/173 (52%)	78 (87%)	12 (13%)	0	100	100
All	All	3376/4145 (81%)	3067 (91%)	303 (9%)	6 (0%)	50	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1153	GLU
3	D	5	ASN
3	D	869	ASP
3	D	572	PRO
2	C	337	VAL
2	C	320	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	145/273 (53%)	143 (99%)	2 (1%)	67	80
1	B	146/273 (54%)	145 (99%)	1 (1%)	84	90
1	I	59/273 (22%)	58 (98%)	1 (2%)	60	78
2	C	752/1026 (73%)	739 (98%)	13 (2%)	60	78
3	D	679/1027 (66%)	663 (98%)	16 (2%)	49	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	28/61 (46%)	27 (96%)	1 (4%)	35	60
5	F	192/329 (58%)	188 (98%)	4 (2%)	53	71
6	H	56/65 (86%)	56 (100%)	0	100	100
7	G	123/124 (99%)	120 (98%)	3 (2%)	49	69
10	L	82/159 (52%)	82 (100%)	0	100	100
All	All	2262/3610 (63%)	2221 (98%)	41 (2%)	61	76

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	111	ASP
1	B	220	HIS
2	C	24	LEU
2	C	138	LEU
2	C	161	THR
2	C	174	THR
2	C	193	THR
2	C	284	ARG
2	C	317	LYS
2	C	319	LEU
2	C	331	LEU
2	C	420	PHE
2	C	677	LYS
2	C	1003	THR
2	C	1053	THR
3	D	2	LEU
3	D	5	ASN
3	D	82	VAL
3	D	197	THR
3	D	301	ARG
3	D	470	ARG
3	D	711	VAL
3	D	772	THR
3	D	867	LEU
3	D	909	THR
3	D	979	VAL
3	D	1025	THR
3	D	1038	THR
3	D	1086	THR

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Mol	Chain	Res	Type
3	D	1089	LEU
3	D	1161	LEU
4	E	21	THR
5	F	162	ASP
5	F	288	THR
5	F	293	HIS
5	F	317	VAL
7	G	12	SER
7	G	122	GLN
7	G	129	LEU
1	I	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	B	220	HIS
2	C	100	ASN
2	C	280	HIS
2	C	287	ASN
2	C	390	ASN
2	C	576	GLN
2	C	644	GLN
3	D	148	GLN
3	D	221	ASN
3	D	478	ASN
3	D	608	GLN
3	D	781	HIS
3	D	1044	GLN
3	D	1052	GLN
3	D	1058	GLN
5	F	142	ASN
5	F	165	GLN
5	F	316	ASN
7	G	70	ASN

### 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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

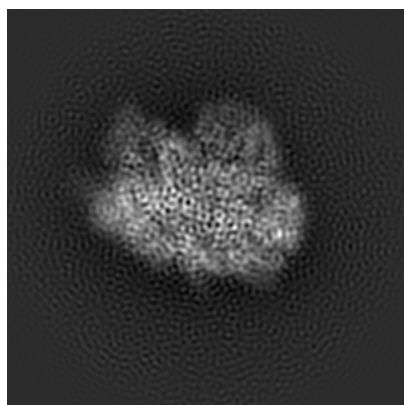
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31485. These allow visual inspection of the internal detail of the map and identification of artifacts.

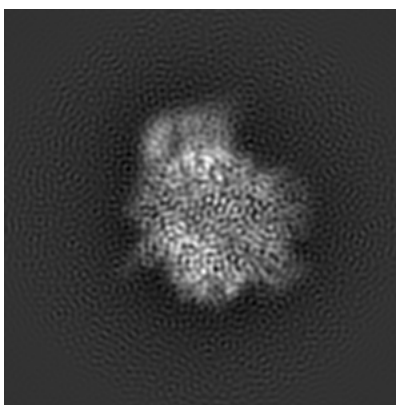
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

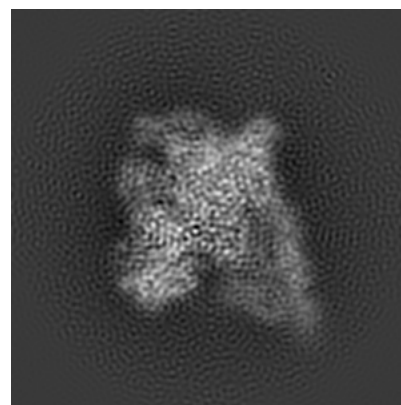
#### 6.1.1 Primary map



X



Y

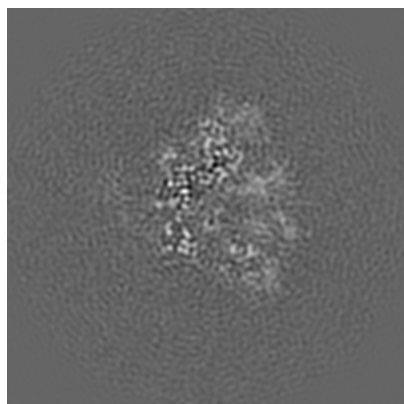


Z

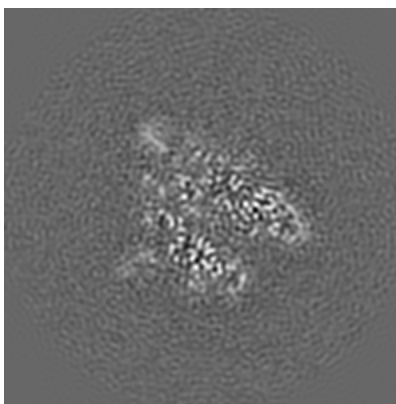
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

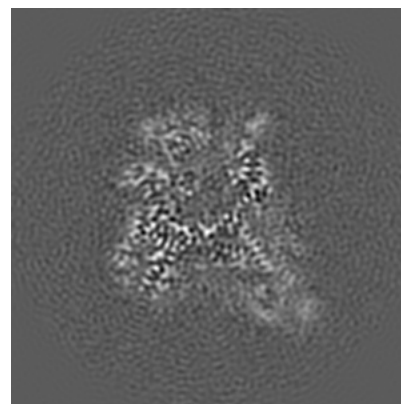
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

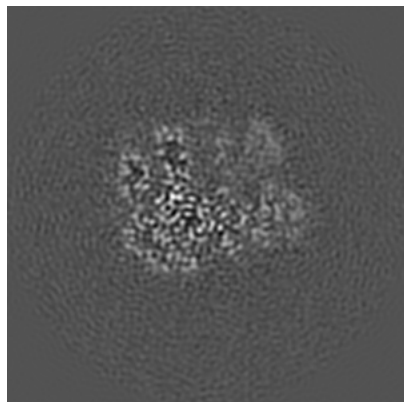


Z Index: 100

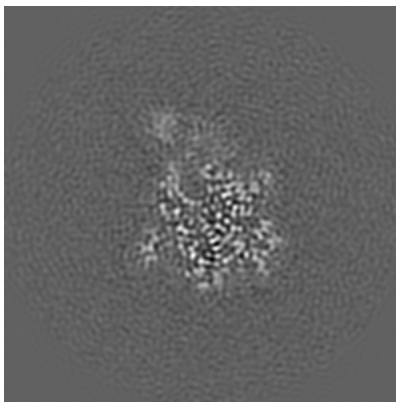
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

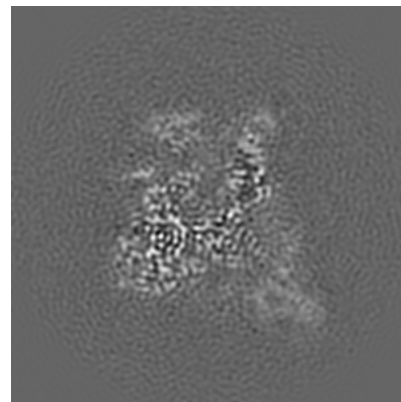
### 6.3.1 Primary map



X Index: 82



Y Index: 86

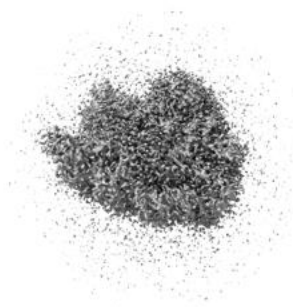


Z Index: 103

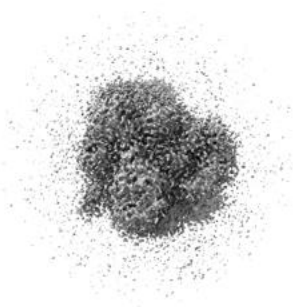
The images above show the largest variance slices of the map in three orthogonal directions.

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

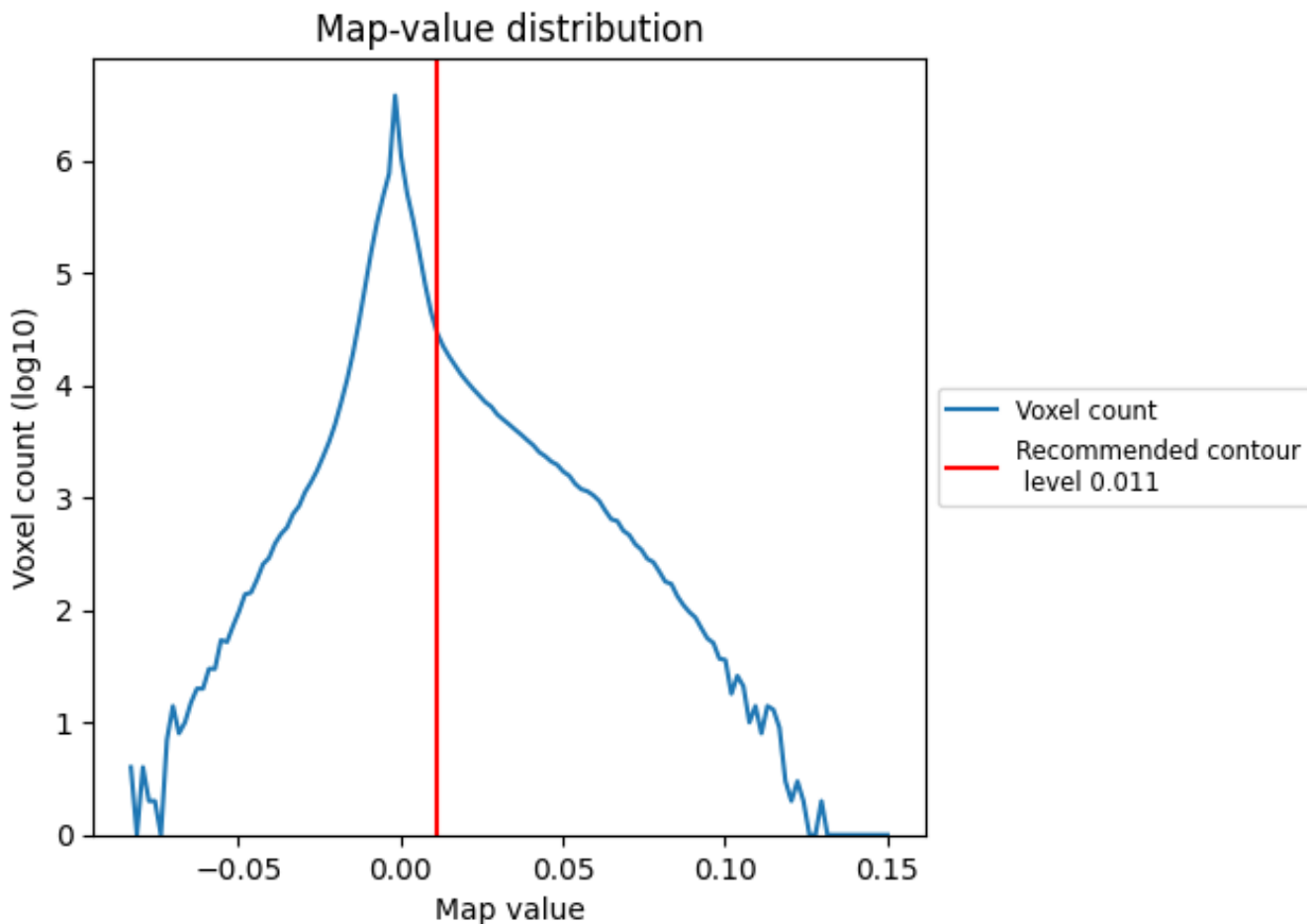
## 6.5 Mask visualisation

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.

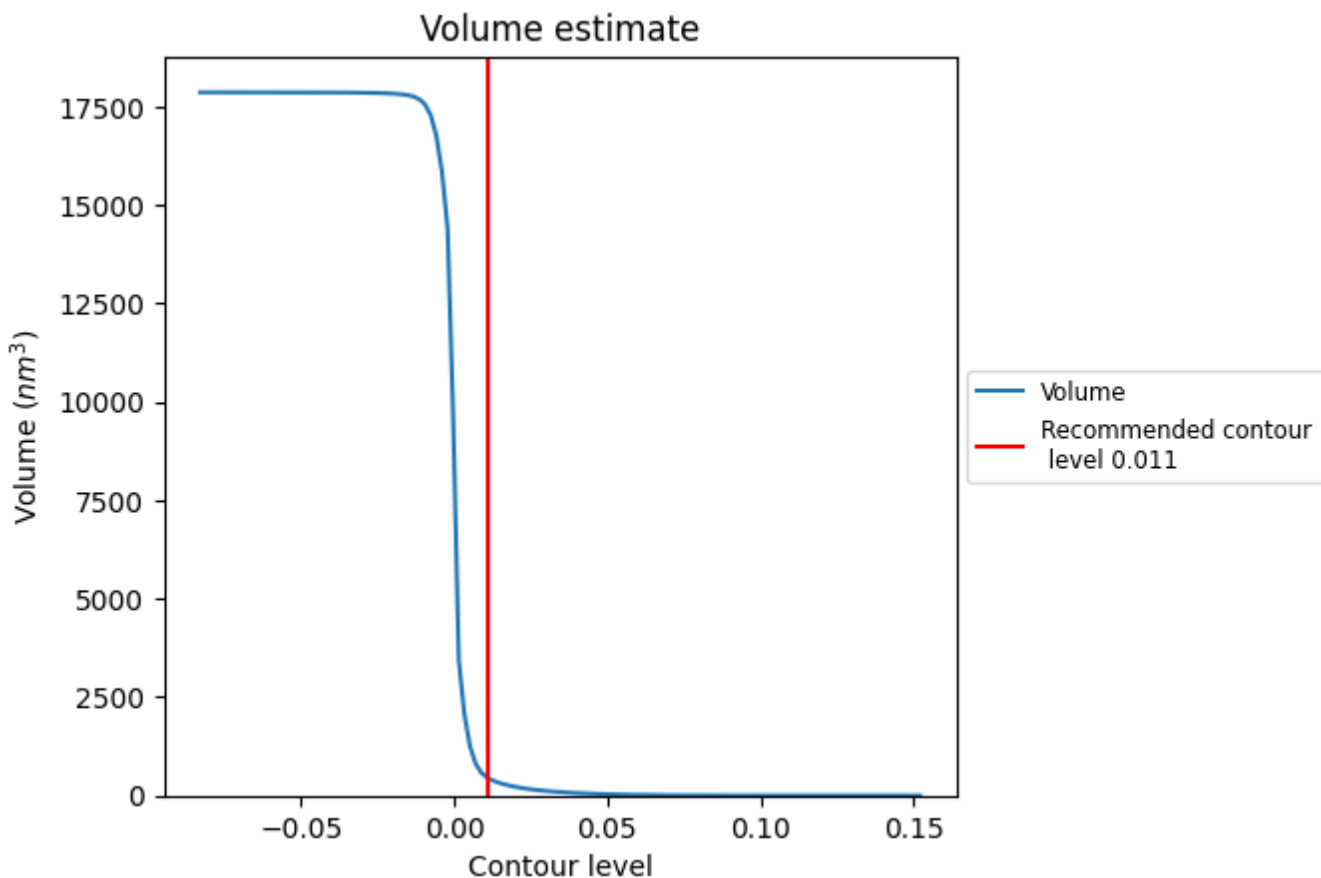
### 7.1 Map-value distribution [i](#)



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.



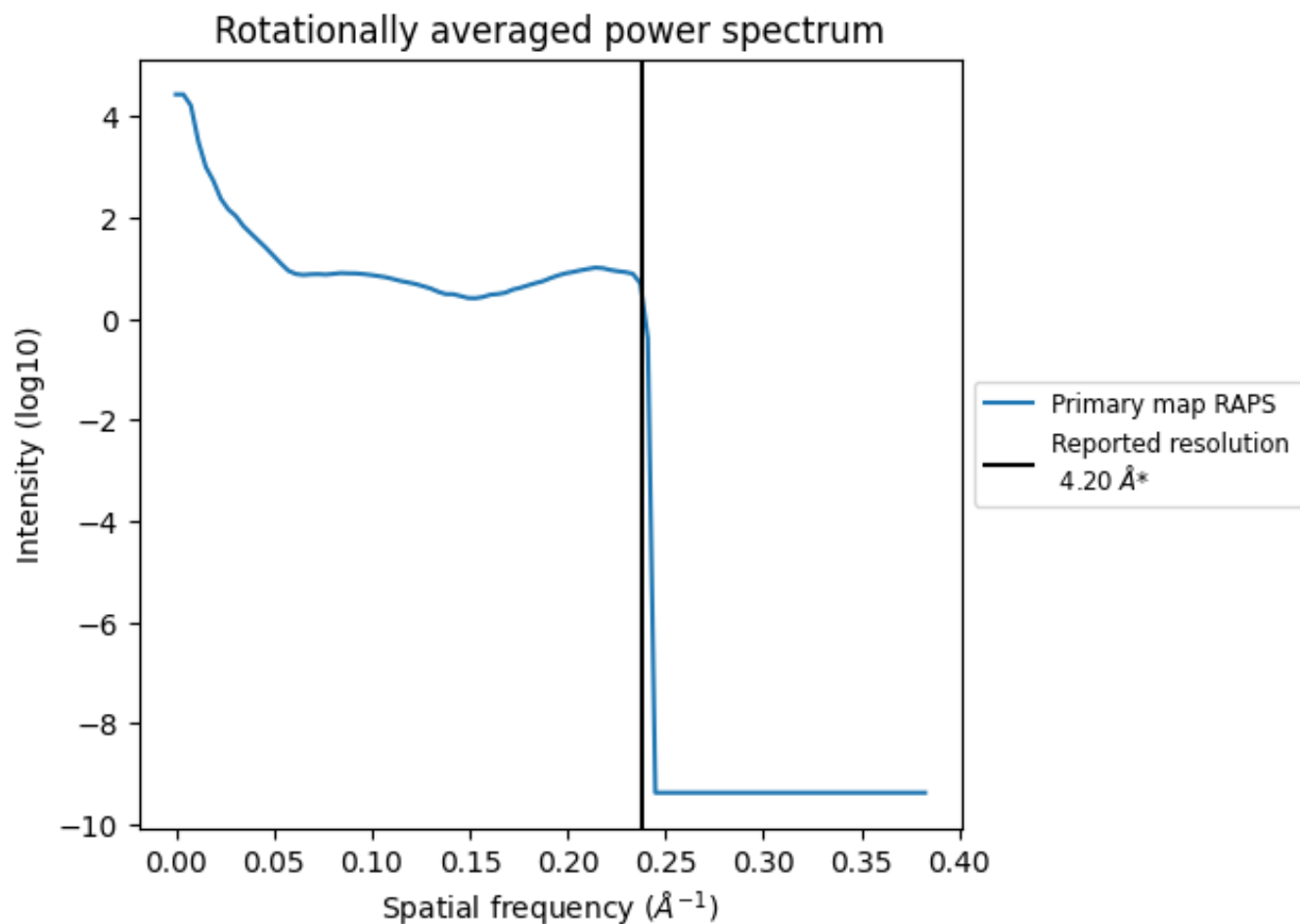
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 446  $\text{nm}^3$ ; this corresponds to an approximate mass of 403 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  $0.238 \text{\AA}^{-1}$

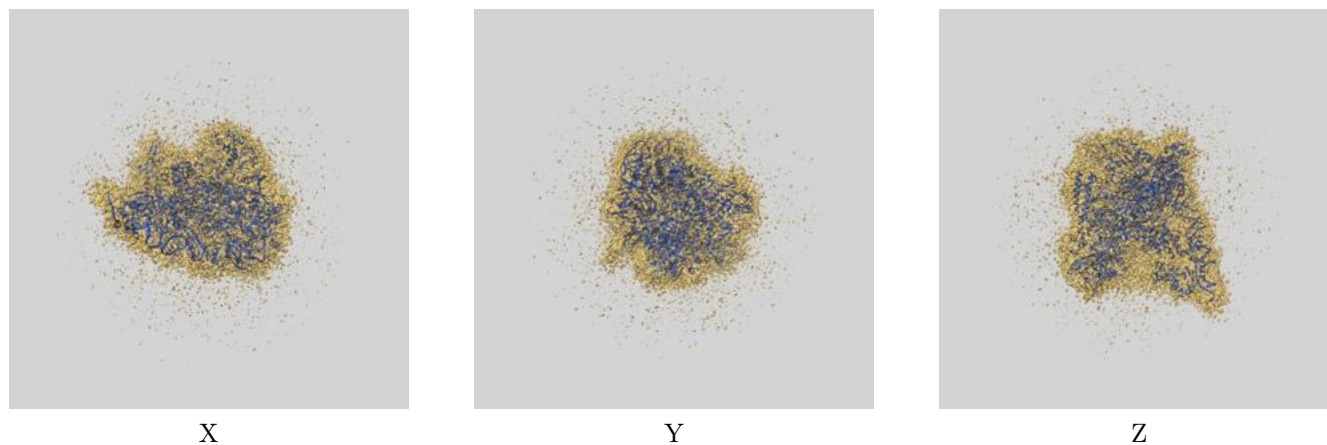
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

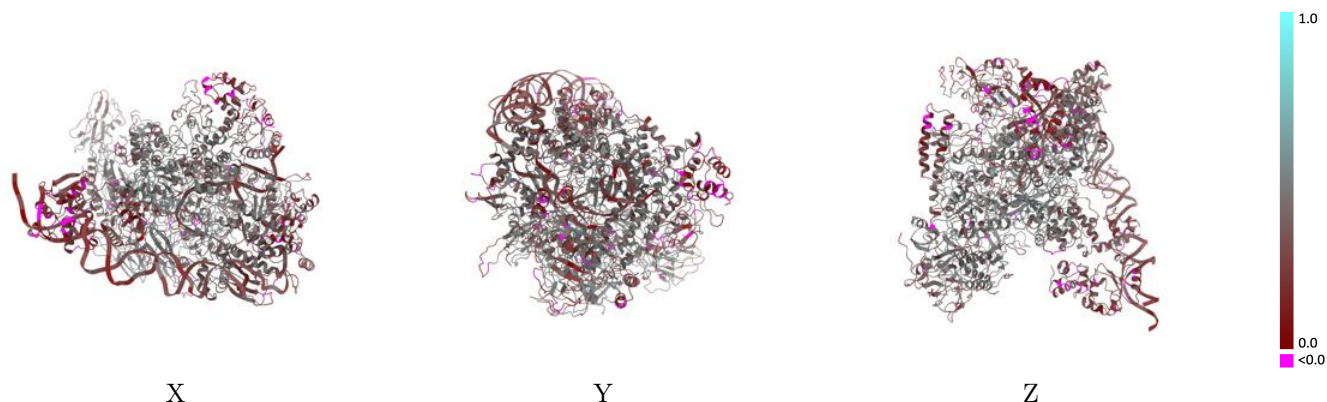
This section contains information regarding the fit between EMDB map EMD-31485 and PDB model 7F75. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



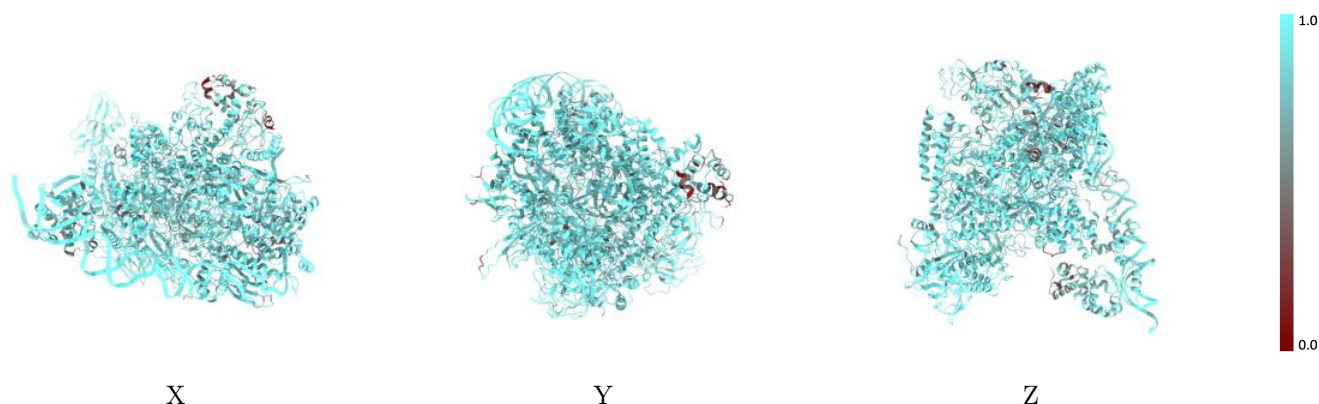
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



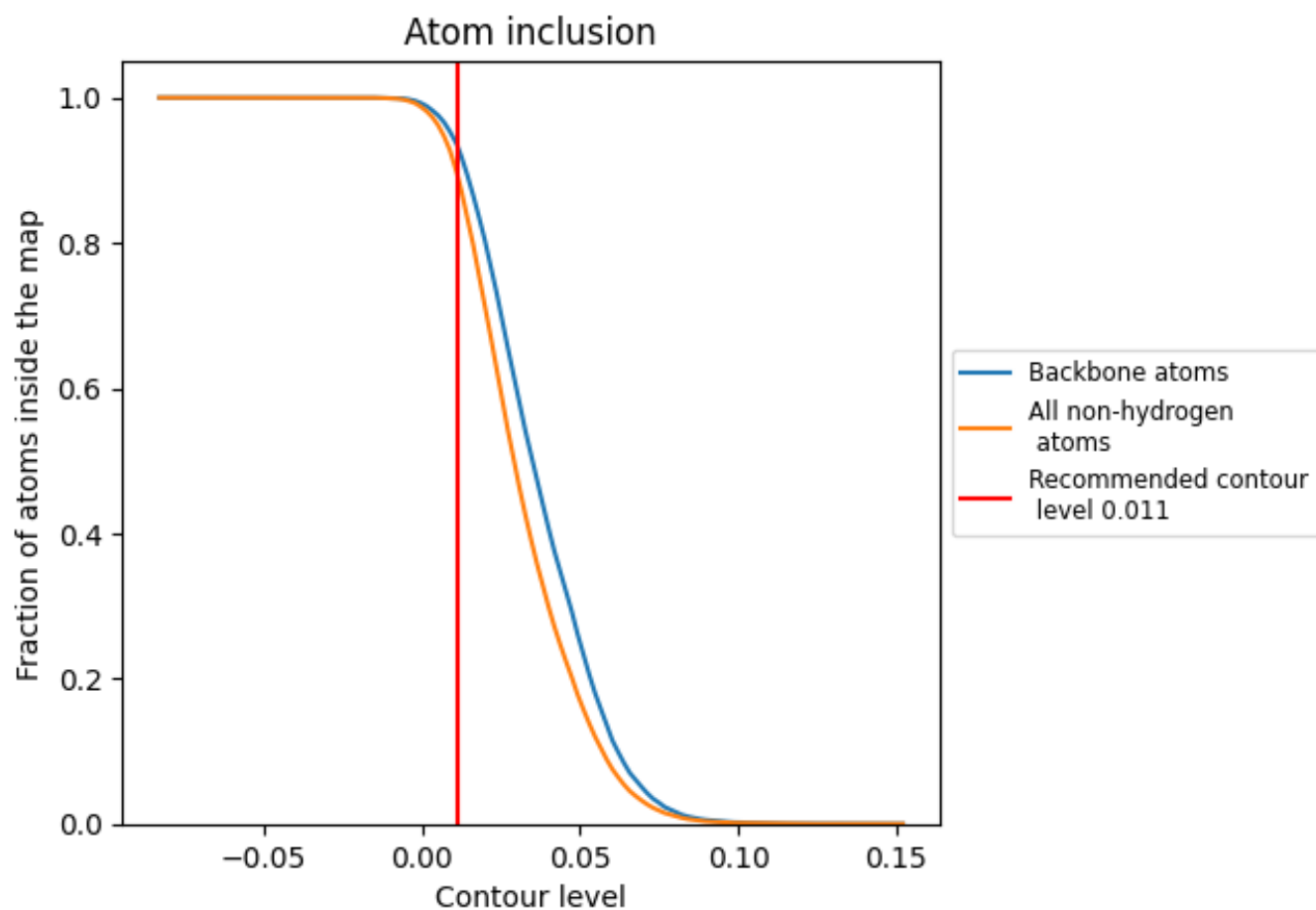
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8970	 0.3700
A	 0.9463	 0.4510
B	 0.9428	 0.4160
C	 0.9124	 0.4100
D	 0.9058	 0.3980
E	 0.8775	 0.3780
F	 0.9000	 0.3450
G	 0.8686	 0.2240
H	 0.8822	 0.4080
I	 0.7360	 0.1760
J	 0.9151	 0.2490
K	 0.9136	 0.2700
L	 0.5553	 0.1310

