



## Full wwPDB EM Validation Report ⓘ

Jun 9, 2026 – 05:13 pm BST

PDB ID : 9SS4 / pdb\_00009ss4  
EMDB ID : EMD-55176  
Title : pre-50S ribosomal subunit in rimM-KO with RsfS (-H68)  
Authors : Hassan, A.H.; Demo, G.  
Deposited on : 2025-09-25  
Resolution : 2.70 Å (reported)  
Based on initial model : 6WDE

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:

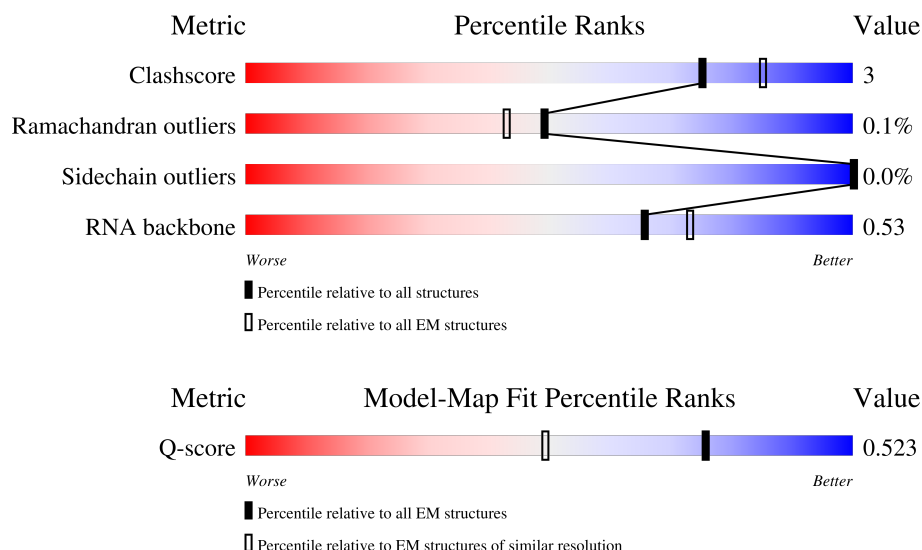
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

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







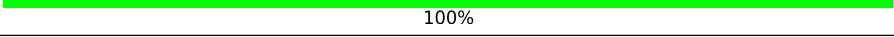


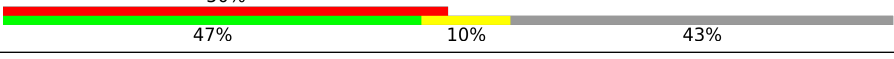
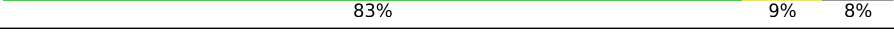

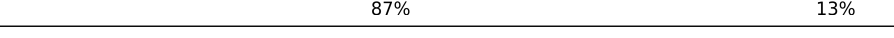
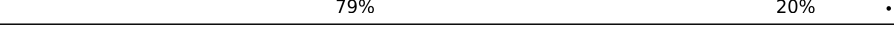




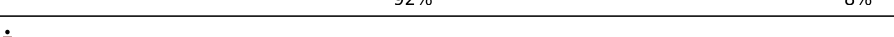

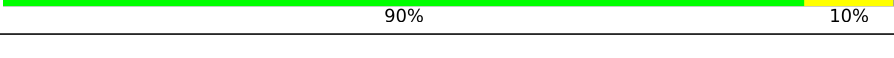

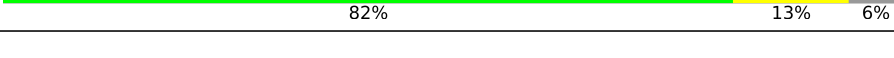
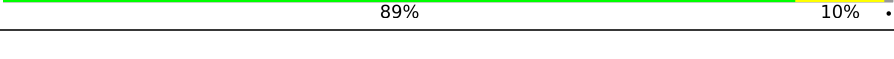

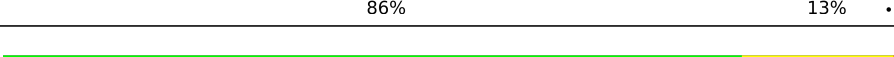

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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	B0	85	
2	B1	78	
3	B2	63	







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Mol	Chain	Length	Quality of chain
4	B3	58	
5	B4	70	
6	B5	57	
7	B6	55	
8	B7	46	
9	B8	65	
10	B9	38	
11	BA	234	
12	BB	273	
13	BC	209	
14	BD	201	
15	BE	179	
16	BF	177	
17	BG	87	
18	BI	149	
19	BK	142	
20	BM	142	
21	BN	123	
22	BO	144	
23	BP	136	
24	BQ	127	
25	BR	117	
26	BS	115	
27	BT	118	
28	BU	103	

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Mol	Chain	Length	Quality of chain
29	BV	110	 92%8%
30	BW	100	 88%5%7%
31	BX	104	 89%9%.
32	BY	94	 87%13%
33	D2	2903	 74%19%. .
34	D3	120	 75%20%5%
35	FS	105	 80%18%. .

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 91554 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 Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B0	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 2 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 3 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B2	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 4 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B3	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B4	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 7 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B6	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 8 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 9 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 10 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BA	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 12 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BB	251	Total	C	N	O	S	0	0
			1935	1196	394	338	7		

- Molecule 13 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BC	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BD	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 16 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BF	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 17 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BG	71	Total	C	N	O	S	0	0
			557	346	115	93	3		

- Molecule 18 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 19 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 20 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BM	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 21 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BN	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 22 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BO	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BP	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 24 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 25 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BR	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 26 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BS	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 28 is a protein called Large ribosomal subunit protein bL21.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	BU	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 29 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BV	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BW	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BX	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 32 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BY	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 33 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	D2	2808	Total	C	N	O	P	0	0
			60278	26892	11093	19486	2807		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D2	747	C	U	conflict	GB CP194060.1

- Molecule 34 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	D3	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	120	A	U	conflict	GB CP076697.1


- Molecule 35 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	FS	103	Total	C	N	O	S	0	0
			794	496	135	158	5		

### 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: Large ribosomal subunit protein bL27

Chain B0: 



- Molecule 2: Large ribosomal subunit protein bL28

Chain B1: 



- Molecule 3: Large ribosomal subunit protein uL29

Chain B2: 



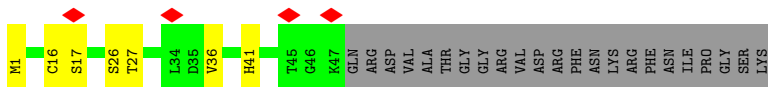
- Molecule 4: Large ribosomal subunit protein uL30

Chain B3: 



- Molecule 5: Large ribosomal subunit protein bL31A

Chain B4: 



- Molecule 6: Large ribosomal subunit protein bL32

[illegible]

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- Diagram illustrating the 128-bit key schedule. The key is represented as a sequence of 128 bits, grouped into 16 bytes. The bytes are labeled: MET, P1, K4, R7, K18, L28, R29, T33, L54, I58, and A64. The diagram shows the key schedule with the key being used in the first round and then being updated for subsequent rounds.

- 

- Chain BA: 



- Molecule 12: Large ribosomal subunit protein uL2

Chain BB:  83% 9% 8%



- Molecule 13: 50S ribosomal protein L3

Chain BC:  89% 11%




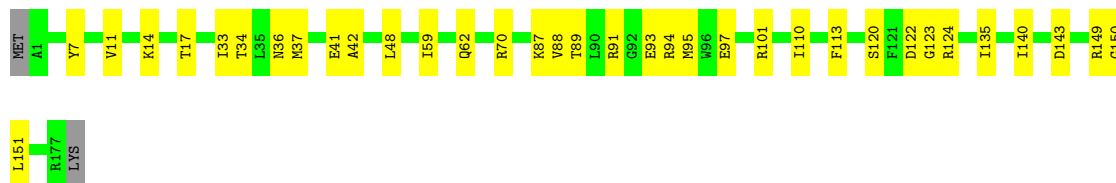
- Molecule 14: Large ribosomal subunit protein uL4

Chain BD:  87% 13%




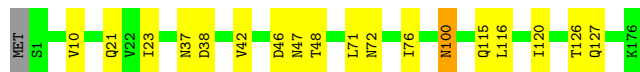
- Molecule 15: Large ribosomal subunit protein uL5

Chain BE:  79% 20%




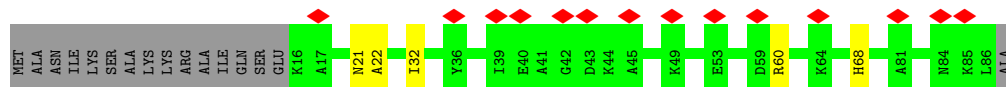
- Molecule 16: Large ribosomal subunit protein uL6

Chain BF:  89% 10% ..

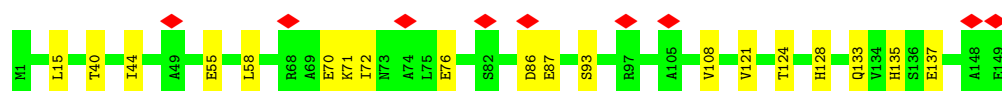
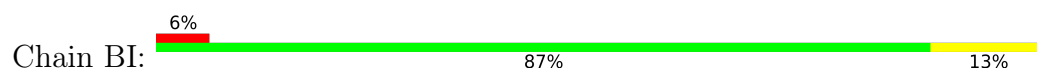


- Molecule 17: Small ribosomal subunit protein bS20

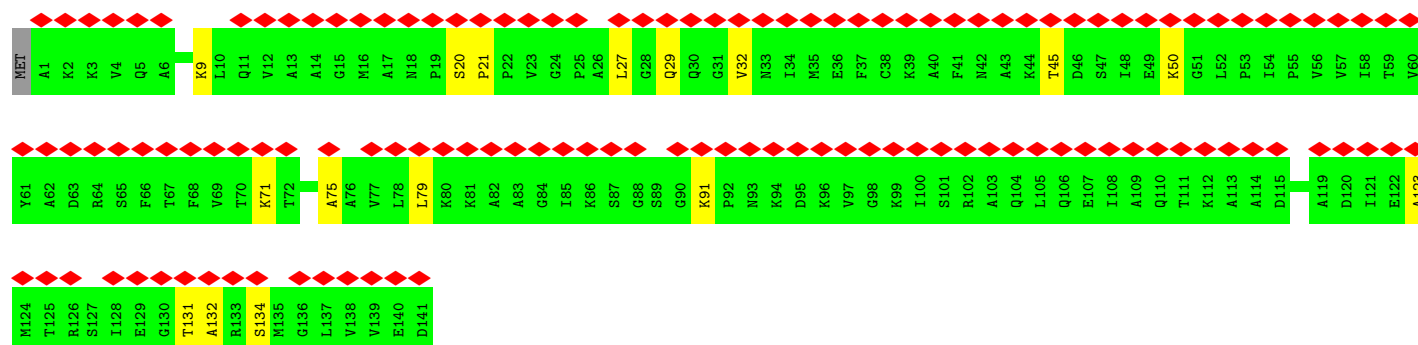
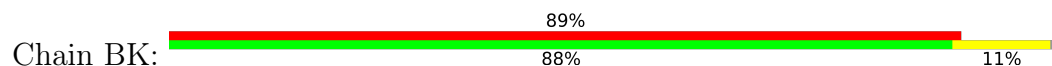
Chain BG:  16% 76% 6% 18%



- Molecule 18: Large ribosomal subunit protein bL9



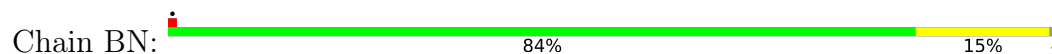
- Molecule 19: 50S ribosomal protein L11



- Molecule 20: Large ribosomal subunit protein uL13



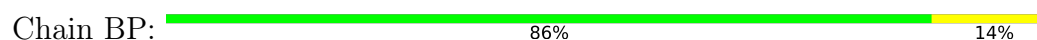
- Molecule 21: Large ribosomal subunit protein uL14




- Molecule 22: Large ribosomal subunit protein uL15



- Molecule 23: 50S ribosomal protein L16




- Molecule 24: Large ribosomal subunit protein bL17

Chain BQ:  82% 13% 6%




- Molecule 25: Large ribosomal subunit protein uL18

Chain BR:  89% 10% .




- Molecule 26: Large ribosomal subunit protein bL19

Chain BS:  86% 13% .




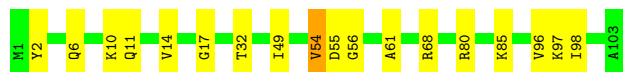
- Molecule 27: Large ribosomal subunit protein bL20

Chain BT:  86% 13% .



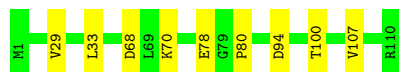
- Molecule 28: Large ribosomal subunit protein bL21

Chain BU:  83% 17% .



- Molecule 29: Large ribosomal subunit protein uL22

Chain BV:  92% 8%



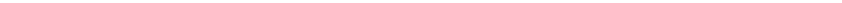
- Molecule 30: Large ribosomal subunit protein uL23

Chain BW:  88% 5% 7%



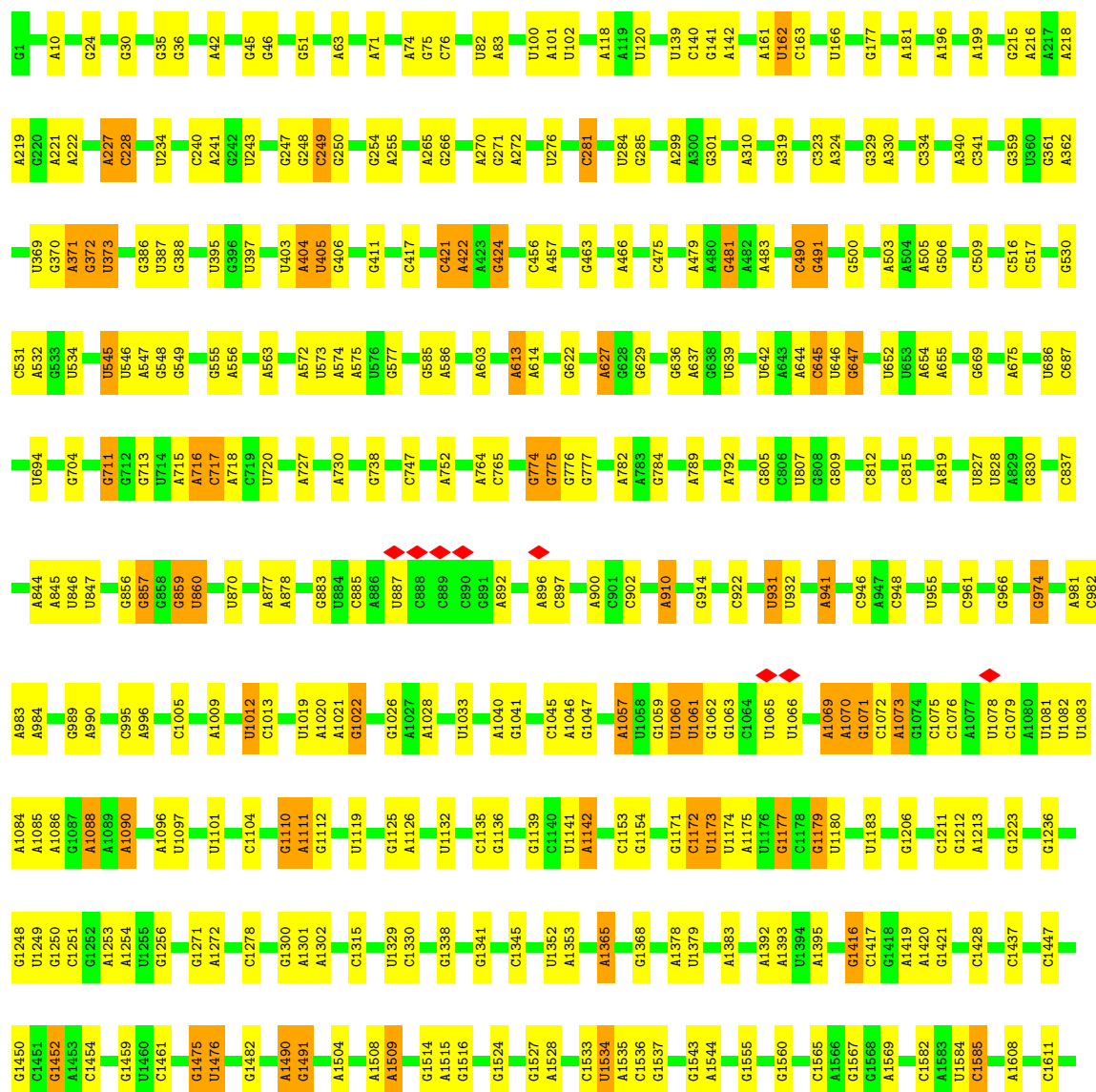
- Molecule 31: Large ribosomal subunit protein uL24

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid sequence: MET, A1, I11, K20, I38, N39, G56, D80, R81, K96, S97, I102, LYS. The 'A1' position has the highest information content, with 'A' being the most frequent residue.

- Chain BY:  87% 13%

Category	Count
M1	1
E35	1
L42	1
V47	1
S58	1
E59	1
V60	1
V64	1
K73	1
D76	1
V77	1
P81	1
Y82	1
K83	1
R93	1
A94	1

- Chain D2:  74% 19% ..







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	21.353	Depositor
Minimum map value	-6.538	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.971	Depositor
Recommended contour level	2	Depositor
Map size ( $\text{\AA}$ )	400.32, 400.32, 400.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.834, 0.834, 0.834	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	B0	0.17	0/582	0.32	0/769
2	B1	0.20	0/635	0.39	0/848
3	B2	0.20	0/510	0.40	0/677
4	B3	0.19	0/453	0.31	0/605
5	B4	0.14	0/371	0.32	0/496
6	B5	0.18	0/450	0.32	0/599
7	B6	0.16	0/416	0.31	0/554
8	B7	0.21	0/380	0.28	0/498
9	B8	0.21	0/513	0.34	0/676
10	B9	0.23	0/303	0.55	0/397
11	BA	0.14	0/1033	0.36	0/1387
12	BB	0.18	0/1967	0.34	0/2641
13	BC	0.19	0/1586	0.35	0/2134
14	BD	0.18	0/1571	0.34	0/2113
15	BE	0.16	0/1434	0.36	0/1926
16	BF	0.17	0/1343	0.36	0/1816
17	BG	0.14	0/563	0.36	0/747
18	BI	0.16	0/1122	0.37	0/1515
19	BK	0.16	0/1046	0.37	0/1410
20	BM	0.19	0/1152	0.29	0/1551
21	BN	0.19	0/947	0.38	0/1268
22	BO	0.18	0/1054	0.38	0/1403
23	BP	0.21	0/1093	0.42	0/1460
24	BQ	0.21	0/973	0.43	0/1301
25	BR	0.16	0/902	0.36	0/1209
26	BS	0.18	0/929	0.35	0/1242
27	BT	0.22	0/960	0.35	0/1278
28	BU	0.19	0/829	0.39	0/1107
29	BV	0.20	0/864	0.36	0/1156
30	BW	0.18	0/744	0.38	0/994
31	BX	0.17	0/787	0.37	0/1051
32	BY	0.19	0/766	0.36	0/1025
33	D2	0.21	0/67512	0.29	0/105322
34	D3	0.17	0/2872	0.27	0/4479

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	FS	0.15	0/803	0.38	0/1085
All	All	0.20	0/99465	0.31	0/148739

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	B0	575	0	592	8	0
2	B1	625	0	655	10	0
3	B2	509	0	543	13	0
4	B3	449	0	491	4	0
5	B4	364	0	366	4	0
6	B5	444	0	461	3	0
7	B6	409	0	440	3	0
8	B7	377	0	418	0	0
9	B8	504	0	574	7	0
10	B9	302	0	343	6	0
11	BA	1026	0	1092	17	0
12	BB	1935	0	2020	16	0
13	BC	1565	0	1616	17	0
14	BD	1552	0	1619	15	0
15	BE	1410	0	1447	29	0
16	BF	1323	0	1374	13	0
17	BG	557	0	595	4	0
18	BI	1111	0	1148	11	0
19	BK	1032	0	1088	12	0
20	BM	1129	0	1162	8	0
21	BN	938	0	1012	15	0
22	BO	1045	0	1117	12	0
23	BP	1074	0	1157	14	0
24	BQ	960	0	1000	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	BR	892	0	923	12	0
26	BS	917	0	965	10	0
27	BT	947	0	1022	12	0
28	BU	816	0	839	13	0
29	BV	857	0	922	6	0
30	BW	738	0	807	4	0
31	BX	779	0	834	7	0
32	BY	753	0	780	9	0
33	D2	60278	0	30320	225	0
34	D3	2568	0	1303	10	0
35	FS	794	0	793	13	0
All	All	91554	0	61838	465	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 (465) 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)
33:D2:2848:G:O2'	33:D2:2867:G:N2	2.08	0.87
27:BT:48:ASP:OD2	33:D2:534:U:O2'	1.93	0.86
33:D2:2125:G:O2'	33:D2:2126:A:O4'	1.93	0.85
33:D2:1061:U:O2'	33:D2:1070:A:O4'	1.95	0.83
33:D2:2326:C:O2'	33:D2:2327:A:OP1	1.97	0.83
33:D2:885:C:O2	33:D2:892:A:N6	2.13	0.82
21:BN:98:ARG:NH2	35:FS:98:TYR:O	2.13	0.81
19:BK:71:LYS:NZ	33:D2:1059:G:OP2	2.13	0.81
33:D2:481:G:O2'	33:D2:506:G:N2	2.14	0.80
35:FS:41:THR:OG1	35:FS:95:ARG:NH2	2.15	0.79
33:D2:475:C:O2	33:D2:479:A:N6	2.15	0.79
12:BB:86:ARG:NH2	33:D2:1817:G:OP1	2.16	0.78
23:BP:86:LYS:NZ	33:D2:955:U:OP1	2.16	0.78
33:D2:1969:A:O2'	33:D2:1972:G:N3	2.17	0.78
28:BU:80:ARG:NH2	33:D2:572:A:OP2	2.18	0.77
30:BW:18:GLU:OE2	33:D2:1392:A:N6	2.14	0.77
13:BC:128:ARG:NH2	33:D2:1995:U:OP1	2.18	0.77
27:BT:57:ARG:NH1	33:D2:1154:G:OP2	2.18	0.77
5:B4:1:MET:SD	15:BE:94:ARG:NH1	2.58	0.76
32:BY:35:GLU:OE2	32:BY:93:ARG:NH2	2.19	0.76
9:B8:4:LYS:NZ	33:D2:254:G:N7	2.33	0.75
22:BO:93:ASN:O	22:BO:94:THR:OG1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BE:122:ASP:O	33:D2:2302:U:O2'	2.03	0.74
22:BO:29:LYS:O	22:BO:30:THR:OG1	2.03	0.74
27:BT:5:ARG:NH2	33:D2:585:G:N7	2.35	0.74
19:BK:9:LYS:NZ	33:D2:1061:U:OP1	2.20	0.74
33:D2:2128:G:N2	33:D2:2161:C:O2'	2.21	0.74
15:BE:59:ILE:O	15:BE:101:ARG:NH2	2.21	0.74
12:BB:1:ALA:N	12:BB:19:VAL:O	2.20	0.74
3:B2:49:ASP:OD1	3:B2:52:ARG:NH1	2.20	0.73
14:BD:51:GLU:OE2	14:BD:88:ARG:NH2	2.22	0.73
23:BP:44:ARG:NH1	33:D2:2484:G:OP1	2.22	0.72
33:D2:545:U:O2	33:D2:548:G:O6	2.07	0.72
23:BP:6:ARG:NH1	33:D2:870:U:OP1	2.22	0.72
26:BS:38:ARG:NH1	26:BS:39:LEU:O	2.22	0.72
15:BE:97:GLU:OE2	15:BE:101:ARG:NH1	2.22	0.72
25:BR:111:ARG:NH1	25:BR:117:PHE:OXT	2.22	0.71
33:D2:240:C:OP2	33:D2:241:A:O2'	2.04	0.71
9:B8:33:THR:OG1	33:D2:2420:C:OP1	2.06	0.71
31:BX:80:ASP:OD1	31:BX:97:SER:OG	2.08	0.71
33:D2:2062:A:N7	33:D2:2503:A:N6	2.39	0.71
7:B6:5:ARG:NH1	33:D2:2285:C:OP2	2.24	0.70
14:BD:111:GLU:OE2	14:BD:115:GLN:NE2	2.25	0.70
21:BN:31:ARG:NH1	33:D2:1996:C:OP1	2.24	0.70
24:BQ:69:ARG:O	24:BQ:70:THR:OG1	2.04	0.70
10:B9:19:ARG:NE	33:D2:2756:U:OP2	2.24	0.69
10:B9:2:LYS:NZ	33:D2:2478:A:OP2	2.18	0.69
13:BC:133:THR:HG22	13:BC:134:HIS:H	1.56	0.69
33:D2:2139:U:O2	33:D2:2152:G:O6	2.11	0.69
33:D2:1173:U:O2'	33:D2:1177:G:N2	2.26	0.69
24:BQ:114:GLU:OE1	24:BQ:118:ARG:NH1	2.26	0.68
10:B9:4:ARG:O	10:B9:37:GLN:NE2	2.26	0.68
4:B3:11:SER:OG	33:D2:989:G:OP2	2.11	0.68
12:BB:70:LYS:O	12:BB:117:SER:OG	2.12	0.68
33:D2:2788:C:O2'	33:D2:2809:A:N3	2.25	0.68
33:D2:1490:A:O2'	33:D2:1491:G:OP1	2.11	0.68
12:BB:132:ARG:NH2	12:BB:186:ASP:OD2	2.27	0.68
15:BE:110:ILE:HD11	15:BE:113:PHE:HD1	1.59	0.67
16:BF:21:GLN:NE2	16:BF:37:ASN:O	2.28	0.67
33:D2:1508:A:O2'	33:D2:1509:A:O4'	2.05	0.67
4:B3:3:THR:OG1	4:B3:36:GLU:OE2	2.07	0.67
15:BE:120:SER:OG	33:D2:2303:G:O3'	2.13	0.66
22:BO:95:LEU:HD22	22:BO:100:ILE:HD11	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BC:77:ARG:NH1	13:BC:200:ASP:OD1	2.27	0.66
5:B4:16:CYS:SG	5:B4:17:SER:N	2.68	0.66
15:BE:124:ARG:NH2	33:D2:2315:G:N3	2.43	0.66
29:BV:94:ASP:OD2	33:D2:2013:A:O2'	2.11	0.66
2:B1:2:ARG:NH1	33:D2:1365:A:OP1	2.27	0.66
25:BR:117:PHE:O	33:D2:2377:A:O2'	2.07	0.66
27:BT:101:ASP:OD2	28:BU:2:TYR:OH	2.09	0.65
19:BK:75:ALA:HB3	19:BK:131:THR:HG21	1.78	0.65
33:D2:2163:A:O2'	33:D2:2171:A:OP2	2.09	0.65
14:BD:170:ARG:NH2	14:BD:179:SER:OG	2.29	0.65
2:B1:36:ARG:NH2	33:D2:2199:A:OP1	2.29	0.65
33:D2:177:G:OP2	33:D2:177:G:N2	2.23	0.65
12:BB:68:ARG:O	12:BB:188:ARG:NH1	2.30	0.64
10:B9:36:ARG:HG2	10:B9:37:GLN:H	1.62	0.64
10:B9:25:VAL:HG12	10:B9:35:GLN:HB2	1.78	0.64
24:BQ:106:ASP:OD2	33:D2:1649:G:O2'	2.08	0.64
33:D2:227:A:O2'	33:D2:228:C:O5'	2.14	0.64
32:BY:76:ASP:OD1	32:BY:77:VAL:N	2.30	0.64
33:D2:2104:C:N4	33:D2:2186:G:O6	2.31	0.64
1:B0:29:ALA:N	1:B0:60:ASP:OD1	2.31	0.63
15:BE:42:ALA:HA	15:BE:48:LEU:HD12	1.79	0.63
16:BF:23:ILE:HG21	16:BF:71:LEU:HD11	1.80	0.63
33:D2:704:G:O2'	33:D2:727:A:N6	2.32	0.63
33:D2:1939:U:O2'	33:D2:1940:U:O5'	2.14	0.63
9:B8:18:LYS:NZ	33:D2:652:U:OP2	2.26	0.63
33:D2:774:G:O2'	33:D2:775:G:O5'	2.16	0.63
25:BR:63:LYS:NZ	34:D3:51:G:OP1	2.20	0.62
11:BA:67:HIS:NE2	11:BA:187:GLU:OE2	2.33	0.62
23:BP:3:GLN:OE1	23:BP:92:TRP:NE1	2.33	0.62
34:D3:5:U:OP1	34:D3:61:G:O2'	2.15	0.62
11:BA:34:ALA:HB2	11:BA:216:THR:HG21	1.82	0.61
29:BV:80:PRO:O	29:BV:100:THR:OG1	2.13	0.61
33:D2:1315:C:O2'	33:D2:1392:A:N3	2.29	0.61
22:BO:91:ASP:OD1	22:BO:94:THR:OG1	2.19	0.61
30:BW:58:VAL:HG22	30:BW:85:VAL:HG12	1.83	0.61
18:BI:71:LYS:NZ	18:BI:76:GLU:OE2	2.33	0.61
20:BM:30:THR:HG21	33:D2:1005:C:O2'	2.00	0.61
33:D2:2143:C:O2	33:D2:2148:G:N2	2.34	0.61
3:B2:36:GLN:N	3:B2:36:GLN:OE1	2.34	0.61
18:BI:133:GLN:NE2	18:BI:135:HIS:O	2.34	0.61
33:D2:1779:U:OP2	33:D2:1784:A:N6	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BP:73:ILE:HD11	23:BP:93:VAL:HG22	1.83	0.60
13:BC:156:PHE:CD1	20:BM:81:ILE:HD13	2.36	0.60
17:BG:60:ARG:NE	33:D2:341:C:OP1	2.34	0.60
14:BD:162:ARG:NH2	33:D2:340:A:O2'	2.35	0.60
15:BE:62:GLN:NE2	34:D3:42:C:O2	2.34	0.60
21:BN:70:ARG:NH1	33:D2:2684:U:O4'	2.35	0.60
33:D2:270:A:N1	33:D2:369:U:O2'	2.33	0.60
22:BO:85:VAL:HG13	22:BO:86:GLU:H	1.67	0.59
19:BK:29:GLN:NE2	33:D2:1096:A:N1	2.49	0.59
16:BF:72:ASN:O	16:BF:76:ILE:HD12	2.03	0.59
24:BQ:49:GLU:OE2	24:BQ:95:THR:OG1	2.20	0.59
25:BR:94:ARG:NH1	25:BR:97:PHE:O	2.36	0.59
33:D2:1534:U:O2'	33:D2:1537:G:O6	2.12	0.59
1:B0:35:ARG:NH2	33:D2:2355:G:O2'	2.36	0.58
2:B1:60:LYS:NZ	33:D2:371:A:O2'	2.20	0.58
2:B1:64:ASP:OD2	2:B1:65:THR:N	2.36	0.58
12:BB:106:PRO:HD2	12:BB:109:LEU:HD22	1.85	0.58
15:BE:62:GLN:OE1	15:BE:94:ARG:NH2	2.36	0.58
33:D2:1447:C:O2'	33:D2:1544:A:N3	2.37	0.58
28:BU:17:GLY:O	28:BU:97:LYS:NZ	2.37	0.58
4:B3:23:LEU:HD11	4:B3:53:MET:CE	2.34	0.58
24:BQ:69:ARG:C	24:BQ:70:THR:HG1	2.07	0.58
15:BE:93:GLU:N	15:BE:93:GLU:OE1	2.34	0.58
21:BN:90:ASN:OD1	21:BN:91:SER:N	2.37	0.58
13:BC:26:VAL:HG22	13:BC:188:LEU:CD2	2.33	0.57
17:BG:68:HIS:NE2	33:D2:42:A:OP1	2.36	0.57
12:BB:224:MET:SD	12:BB:229:HIS:ND1	2.78	0.57
12:BB:35:LYS:NZ	33:D2:1353:A:O3'	2.37	0.57
26:BS:46:VAL:HG11	26:BS:49:ILE:HD11	1.86	0.57
33:D2:2438:U:O2'	33:D2:2440:C:OP1	2.22	0.57
33:D2:711:G:O6	33:D2:720:U:O2	2.22	0.57
33:D2:1009:A:N3	33:D2:1153:C:O2'	2.37	0.57
28:BU:14:VAL:HG21	28:BU:98:ILE:HD12	1.86	0.57
1:B0:25:GLU:OE2	33:D2:922:C:O2'	2.14	0.56
13:BC:151:THR:OG1	33:D2:2032:G:N2	2.37	0.56
11:BA:12:ARG:NH2	33:D2:2176:A:OP1	2.38	0.56
15:BE:36:ASN:ND2	33:D2:2312:U:O2	2.35	0.56
33:D2:370:G:O2'	33:D2:424:G:OP1	2.24	0.56
33:D2:1110:G:O2'	33:D2:1111:A:O4'	2.19	0.56
1:B0:36:GLN:OE1	1:B0:40:LYS:N	2.39	0.56
33:D2:2798:U:O2'	33:D2:2799:A:N7	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:4:LYS:NZ	3:B2:5:GLU:OE2	2.29	0.56
12:BB:70:LYS:NZ	12:BB:97:ASP:OD2	2.36	0.56
33:D2:642:U:O2'	33:D2:644:A:N7	2.32	0.56
14:BD:125:SER:O	14:BD:137:LYS:NZ	2.38	0.56
15:BE:135:ILE:HA	15:BE:140:ILE:HD11	1.88	0.56
33:D2:1528:A:OP2	33:D2:1543:G:N2	2.39	0.56
33:D2:2326:C:HO2'	33:D2:2327:A:P	2.25	0.56
33:D2:404:A:O2'	33:D2:405:U:O5'	2.18	0.55
16:BF:23:ILE:HD11	16:BF:42:VAL:HG11	1.87	0.55
33:D2:713:G:H21	33:D2:718:A:H62	1.54	0.55
33:D2:2469:A:N6	33:D2:2481:G:O2'	2.37	0.55
33:D2:2528:U:O2'	33:D2:2530:A:OP1	2.13	0.55
33:D2:1450:G:H21	33:D2:1452:G:H1	1.54	0.55
33:D2:2405:G:O2'	33:D2:2412:A:N6	2.34	0.55
26:BS:33:GLU:OE2	26:BS:38:ARG:NE	2.34	0.55
33:D2:716:A:O2'	33:D2:717:C:O4'	2.16	0.55
12:BB:16:VAL:HB	12:BB:203:VAL:HG22	1.89	0.55
17:BG:32:ILE:HD11	33:D2:613:A:C4	2.42	0.55
9:B8:29:ARG:NH1	33:D2:2394:C:OP2	2.40	0.55
27:BT:88:GLU:O	28:BU:11:GLN:NE2	2.39	0.54
33:D2:877:A:O2'	33:D2:900:A:N6	2.40	0.54
33:D2:2156:G:O6	33:D2:2157:G:N2	2.40	0.54
34:D3:12:C:O2'	34:D3:13:G:O5'	2.25	0.54
3:B2:2:LYS:HZ3	3:B2:6:LEU:HD22	1.72	0.54
11:BA:178:VAL:HG11	11:BA:216:THR:HG22	1.90	0.54
14:BD:117:ARG:NH2	14:BD:183:PHE:O	2.40	0.54
7:B6:28:THR:HG23	7:B6:29:LYS:HG2	1.88	0.54
31:BX:81:ARG:NH2	33:D2:301:G:OP2	2.36	0.54
1:B0:7:ARG:O	1:B0:10:ARG:NH2	2.40	0.54
2:B1:75:GLU:N	2:B1:75:GLU:OE1	2.40	0.54
20:BM:84:ILE:HG23	20:BM:84:ILE:O	2.08	0.54
22:BO:85:VAL:HG11	22:BO:90:VAL:HG12	1.90	0.54
33:D2:1071:G:H22	33:D2:1090:A:N6	2.06	0.54
33:D2:1712:U:OP2	33:D2:1713:A:O2'	2.25	0.54
33:D2:1730:C:O2	33:D2:1731:G:N1	2.41	0.54
33:D2:859:G:HO2'	33:D2:860:U:P	2.31	0.53
23:BP:12:MET:HA	33:D2:910:A:H62	1.73	0.53
25:BR:84:GLU:OE1	25:BR:84:GLU:N	2.36	0.53
18:BI:86:ASP:OD1	18:BI:87:GLU:N	2.42	0.53
24:BQ:86:ARG:NE	24:BQ:117:ASP:OD2	2.33	0.53
33:D2:1069:A:N7	33:D2:1073:A:N6	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:BN:61:VAL:HG23	21:BN:87:LEU:HD11	1.91	0.53
27:BT:91:ARG:NH2	33:D2:1153:C:OP1	2.42	0.53
33:D2:2646:C:OP2	33:D2:2732:G:O2'	2.24	0.53
5:B4:26:SER:OG	5:B4:27:THR:N	2.42	0.53
6:B5:12:ARG:NH2	33:D2:517:C:OP1	2.41	0.53
11:BA:47:ASN:ND2	11:BA:211:LYS:O	2.42	0.53
35:FS:30:LYS:NZ	35:FS:104:TRP:O	2.29	0.53
3:B2:13:GLU:HA	3:B2:16:THR:HG22	1.90	0.52
33:D2:2581:G:O2'	33:D2:2610:C:N4	2.36	0.52
11:BA:37:LYS:NZ	33:D2:2128:G:OP2	2.31	0.52
31:BX:96:LYS:O	31:BX:97:SER:OG	2.28	0.52
11:BA:215:SER:OG	11:BA:219:GLY:O	2.27	0.52
18:BI:72:ILE:HB	18:BI:108:VAL:HG12	1.92	0.52
33:D2:227:A:HO2'	33:D2:228:C:P	2.33	0.52
29:BV:29:VAL:O	29:BV:33:LEU:HD23	2.09	0.52
22:BO:78:ARG:NH2	33:D2:627:A:OP1	2.38	0.51
11:BA:7:ARG:NH2	11:BA:35:THR:O	2.43	0.51
18:BI:15:LEU:O	18:BI:15:LEU:HD23	2.10	0.51
20:BM:19:ASP:OD1	20:BM:20:ALA:N	2.43	0.51
23:BP:136:MET:HE1	32:BY:76:ASP:HA	1.92	0.51
11:BA:11:ILE:HG23	11:BA:33:LEU:HD22	1.93	0.51
27:BT:61:ILE:HD12	27:BT:75:TYR:OH	2.11	0.51
35:FS:48:VAL:HG23	35:FS:89:VAL:HG22	1.92	0.51
14:BD:168:ASP:OD1	14:BD:169:VAL:N	2.44	0.51
35:FS:74:SER:OG	35:FS:76:ASP:OD1	2.27	0.51
22:BO:41:ARG:NH2	33:D2:807:U:OP2	2.44	0.51
20:BM:39:LYS:NZ	33:D2:1009:A:OP1	2.43	0.51
20:BM:56:VAL:HB	20:BM:124:VAL:HG12	1.93	0.51
3:B2:2:LYS:NZ	3:B2:6:LEU:HD22	2.26	0.51
34:D3:30:C:H1'	34:D3:57:A:H61	1.76	0.51
35:FS:101:GLU:N	35:FS:101:GLU:OE1	2.44	0.51
16:BF:37:ASN:OD1	16:BF:38:ASP:N	2.42	0.50
29:BV:78:GLU:O	33:D2:24:G:O2'	2.27	0.50
33:D2:948:C:O2	33:D2:984:A:O2'	2.22	0.50
25:BR:9:ARG:NH2	33:D2:2296:U:OP2	2.43	0.50
14:BD:32:VAL:HG23	14:BD:178:VAL:HG12	1.93	0.50
35:FS:41:THR:HG1	35:FS:95:ARG:NH2	2.09	0.50
33:D2:586:A:N1	33:D2:809:G:O2'	2.44	0.50
3:B2:55:THR:HG21	33:D2:76:C:H1'	1.93	0.50
20:BM:68:LYS:NZ	33:D2:1022:G:O6	2.37	0.50
26:BS:1:SER:OG	26:BS:2:ASN:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BY:58:SER:O	32:BY:73:LYS:NZ	2.45	0.50
33:D2:219:A:N3	33:D2:234:U:O2'	2.40	0.50
15:BE:91:ARG:NH1	34:D3:43:C:O2	2.45	0.50
19:BK:134:SER:OG	33:D2:1088:A:N6	2.33	0.50
23:BP:97:GLN:N	23:BP:97:GLN:OE1	2.45	0.50
28:BU:85:LYS:NZ	33:D2:815:C:OP2	2.36	0.50
25:BR:93:ASP:OD1	25:BR:93:ASP:N	2.43	0.49
33:D2:774:G:HO2'	33:D2:775:G:P	2.35	0.49
33:D2:981:A:OP2	33:D2:982:C:N4	2.41	0.49
21:BN:70:ARG:HG2	21:BN:76:VAL:HG12	1.94	0.49
33:D2:1171:G:N1	33:D2:1179:G:O6	2.44	0.49
15:BE:36:ASN:ND2	33:D2:2313:C:O4'	2.45	0.49
18:BI:124:THR:O	18:BI:128:HIS:NE2	2.45	0.49
25:BR:111:ARG:NH2	33:D2:2376:A:N3	2.60	0.49
28:BU:61:ALA:HB1	28:BU:96:VAL:HG22	1.93	0.49
33:D2:577:G:O2'	33:D2:1254:A:OP1	2.31	0.49
28:BU:68:ARG:NH1	33:D2:1223:G:OP1	2.46	0.49
12:BB:40:GLY:O	12:BB:42:ARG:NH1	2.45	0.49
34:D3:40:U:N3	34:D3:44:G:OP2	2.37	0.49
2:B1:53:LYS:O	2:B1:57:VAL:HG23	2.13	0.49
28:BU:55:ASP:OD1	28:BU:56:GLY:N	2.45	0.49
12:BB:82:TYR:OH	33:D2:1567:G:OP2	2.28	0.49
33:D2:931:U:O4	33:D2:1183:U:O2'	2.26	0.49
33:D2:1213:A:N6	33:D2:1236:G:O2'	2.46	0.49
24:BQ:27:SER:OG	33:D2:1278:C:O2'	2.27	0.48
33:D2:1475:G:HO2'	33:D2:1514:G:H1	1.60	0.48
35:FS:51:ILE:HB	35:FS:89:VAL:HG21	1.94	0.48
13:BC:136:ASN:ND2	13:BC:139:SER:O	2.42	0.48
33:D2:675:A:N3	33:D2:2443:C:O2'	2.43	0.48
33:D2:1715:G:N2	33:D2:1744:A:OP2	2.43	0.48
33:D2:1490:A:HO2'	33:D2:1491:G:P	2.35	0.48
33:D2:1527:G:N1	33:D2:1544:A:OP2	2.42	0.48
33:D2:2291:U:OP1	33:D2:2380:C:O2'	2.30	0.48
11:BA:28:ALA:O	11:BA:32:GLU:N	2.46	0.48
19:BK:79:LEU:HD13	19:BK:132:ALA:HA	1.96	0.48
33:D2:271:G:O2'	33:D2:272:A:OP2	2.26	0.48
33:D2:2682:A:H61	33:D2:2728:U:H1'	1.78	0.48
1:B0:33:ILE:HG21	1:B0:76:ILE:HG21	1.95	0.47
26:BS:70:GLU:OE2	26:BS:100:ARG:NE	2.33	0.47
9:B8:7:ARG:NH1	33:D2:243:U:OP2	2.48	0.47
23:BP:54:THR:O	23:BP:58:LYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D2:2506:U:OP2	33:D2:2576:G:N1	2.46	0.47
33:D2:1715:G:O2'	33:D2:1716:U:O5'	2.32	0.47
14:BD:44:ARG:NH2	33:D2:1248:G:OP1	2.47	0.47
21:BN:40:LYS:HD2	21:BN:57:VAL:HG12	1.97	0.47
13:BC:83:ARG:NH1	33:D2:2637:U:OP1	2.47	0.47
15:BE:41:GLU:OE2	33:D2:2311:A:N6	2.47	0.47
33:D2:545:U:C2	33:D2:548:G:O6	2.68	0.47
14:BD:164:LEU:HB3	14:BD:167:VAL:HG22	1.97	0.47
15:BE:124:ARG:NE	33:D2:2315:G:O2'	2.35	0.47
34:D3:88:C:O2'	34:D3:89:U:O5'	2.30	0.47
14:BD:194:LYS:O	14:BD:198:GLU:OE1	2.33	0.47
33:D2:1172:C:O2'	33:D2:1173:U:O4'	2.31	0.47
33:D2:2638:G:HO2'	33:D2:2639:A:H8	1.61	0.47
13:BC:8:LYS:HB2	13:BC:201:LEU:HD11	1.96	0.47
15:BE:70:ARG:NH1	33:D2:2298:A:OP1	2.42	0.47
25:BR:31:THR:OG1	34:D3:29:A:OP2	2.33	0.47
2:B1:65:THR:O	2:B1:69:GLU:OE1	2.33	0.46
3:B2:51:ALA:O	3:B2:55:THR:HG23	2.16	0.46
22:BO:85:VAL:HG13	22:BO:86:GLU:N	2.30	0.46
33:D2:2110:G:N2	33:D2:2179:C:H42	2.13	0.46
28:BU:49:ILE:HG22	28:BU:54:VAL:H	1.80	0.46
31:BX:56:GLY:N	33:D2:483:A:O2'	2.49	0.46
33:D2:1833:C:N4	33:D2:1834:U:O4	2.48	0.46
33:D2:2581:G:N2	33:D2:2581:G:OP2	2.48	0.46
4:B3:23:LEU:HD11	4:B3:53:MET:HE2	1.97	0.46
26:BS:77:SER:OG	26:BS:79:VAL:HG12	2.15	0.46
28:BU:14:VAL:HG11	28:BU:98:ILE:CD1	2.45	0.46
33:D2:2595:G:N2	33:D2:2598:A:OP2	2.40	0.46
13:BC:59:ARG:NH2	33:D2:2831:G:OP2	2.48	0.46
25:BR:60:GLU:OE1	25:BR:60:GLU:N	2.39	0.46
33:D2:1416:G:O2'	33:D2:1417:C:O5'	2.26	0.46
13:BC:133:THR:HG22	13:BC:134:HIS:N	2.29	0.46
15:BE:150:GLY:O	15:BE:151:LEU:HD22	2.16	0.46
26:BS:32:VAL:O	26:BS:32:VAL:HG23	2.15	0.46
2:B1:65:THR:O	2:B1:68:ALA:HB3	2.16	0.46
24:BQ:2:ARG:O	24:BQ:2:ARG:HD3	2.16	0.46
35:FS:26:ASP:OD2	35:FS:28:GLN:NE2	2.49	0.46
2:B1:9:LYS:NZ	33:D2:397:U:OP2	2.47	0.46
6:B5:9:ARG:NH2	33:D2:516:C:OP1	2.48	0.46
23:BP:111:GLU:O	23:BP:115:GLU:OE1	2.33	0.46
33:D2:713:G:N2	33:D2:718:A:H62	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BC:114:LYS:NZ	33:D2:2681:C:OP2	2.43	0.45
14:BD:126:VAL:HG23	14:BD:156:ASN:HB3	1.98	0.45
15:BE:36:ASN:OD1	15:BE:37:MET:N	2.49	0.45
15:BE:89:THR:O	15:BE:89:THR:HG22	2.17	0.45
22:BO:91:ASP:OD1	22:BO:91:ASP:N	2.48	0.45
33:D2:713:G:H21	33:D2:718:A:N6	2.13	0.45
3:B2:17:GLU:HB2	3:B2:53:VAL:HG11	1.97	0.45
21:BN:61:VAL:HG21	21:BN:112:PHE:CE2	2.52	0.45
33:D2:299:A:N3	33:D2:319:G:O2'	2.35	0.45
33:D2:1582:C:O2'	33:D2:1585:C:N3	2.45	0.45
27:BT:3:VAL:HG21	33:D2:1249:U:H4'	1.98	0.45
30:BW:90:GLY:O	30:BW:91:GLN:NE2	2.50	0.45
33:D2:2522:U:O2'	33:D2:2647:U:OP1	2.20	0.45
33:D2:859:G:O2'	33:D2:860:U:P	2.74	0.45
3:B2:38:GLN:OE1	3:B2:38:GLN:N	2.45	0.45
11:BA:9:ARG:NH1	33:D2:2132:U:O2	2.49	0.45
11:BA:189:LEU:O	11:BA:193:LEU:HD13	2.16	0.45
5:B4:36:VAL:HG11	5:B4:41:HIS:ND1	2.32	0.45
12:BB:144:GLU:OE2	12:BB:150:GLY:N	2.50	0.45
14:BD:170:ARG:NH1	14:BD:176:ASP:OD1	2.41	0.45
18:BI:55:GLU:HG2	18:BI:58:LEU:HD12	1.98	0.45
25:BR:100:HIS:NE2	34:D3:37:C:O2	2.48	0.45
31:BX:38:ILE:HG23	31:BX:39:ASN:N	2.32	0.45
1:B0:67:VAL:HG22	1:B0:67:VAL:O	2.17	0.45
18:BI:40:THR:O	18:BI:44:ILE:HD12	2.16	0.45
13:BC:34:VAL:HG12	13:BC:50:VAL:HG12	1.99	0.44
11:BA:43:ASP:OD1	33:D2:2123:G:O2'	2.35	0.44
27:BT:69:ARG:NH2	33:D2:1012:U:OP2	2.48	0.44
33:D2:1338:G:O2'	33:D2:1393:A:N1	2.49	0.44
33:D2:1935:G:N2	33:D2:1964:G:O4'	2.46	0.44
15:BE:33:ILE:HD12	15:BE:95:MET:HG2	2.00	0.44
21:BN:38:ILE:HD13	21:BN:61:VAL:HG22	1.99	0.44
26:BS:83:ILE:HG22	26:BS:83:ILE:O	2.18	0.44
33:D2:1125:G:OP2	33:D2:1126:A:O2'	2.21	0.44
27:BT:4:LYS:NZ	33:D2:30:G:OP2	2.43	0.44
28:BU:32:THR:OG1	28:BU:61:ALA:O	2.21	0.44
19:BK:27:LEU:HD22	19:BK:32:VAL:HG21	2.00	0.44
28:BU:6:GLN:OE1	28:BU:10:LYS:N	2.51	0.44
6:B5:37:HIS:ND1	6:B5:38:LEU:O	2.51	0.44
12:BB:34:GLU:OE2	33:D2:1816:C:N4	2.26	0.44
24:BQ:90:ARG:NH2	33:D2:2880:C:O3'	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D2:1141:U:H4'	33:D2:1142:A:O4'	2.18	0.44
15:BE:143:ASP:OD1	15:BE:143:ASP:N	2.51	0.44
32:BY:42:LEU:HD13	32:BY:47:VAL:HG11	1.99	0.44
33:D2:1057:A:H62	33:D2:1086:A:H2'	1.82	0.44
33:D2:1081:U:N3	33:D2:1082:U:O4	2.50	0.44
18:BI:137:GLU:N	18:BI:137:GLU:OE1	2.51	0.43
33:D2:837:C:N3	33:D2:941:A:N6	2.65	0.43
35:FS:35:ASP:N	35:FS:84:ASP:O	2.41	0.43
2:B1:63:ILE:HD12	2:B1:63:ILE:H	1.83	0.43
3:B2:9:LYS:N	3:B2:12:GLU:OE2	2.42	0.43
21:BN:7:MET:HE1	21:BN:44:LYS:HG3	1.99	0.43
1:B0:39:THR:HG22	33:D2:2331:G:O2'	2.17	0.43
11:BA:217:THR:O	33:D2:2124:G:N2	2.52	0.43
16:BF:126:THR:HG22	16:BF:127:GLN:N	2.34	0.43
23:BP:20:LEU:HD13	32:BY:81:PRO:HG2	1.99	0.43
14:BD:61:ARG:NH1	14:BD:63:LYS:O	2.51	0.43
33:D2:645:C:H2'	33:D2:647:G:N7	2.34	0.43
33:D2:1730:C:O2'	33:D2:1731:G:O5'	2.32	0.43
21:BN:76:VAL:HG22	26:BS:72:VAL:HG22	2.00	0.43
33:D2:856:G:H2'	33:D2:857:G:C8	2.54	0.43
33:D2:1475:G:O2'	33:D2:1476:U:P	2.76	0.43
3:B2:43:LEU:HA	3:B2:46:VAL:HG12	2.01	0.43
16:BF:100:ASN:ND2	16:BF:115:GLN:OE1	2.52	0.43
31:BX:11:ILE:HD12	31:BX:20:LYS:O	2.19	0.43
33:D2:463:G:N2	33:D2:466:A:OP2	2.41	0.43
33:D2:1437:C:O2'	33:D2:1516:G:O2'	2.32	0.43
11:BA:8:MET:HE3	33:D2:2174:C:H4'	2.01	0.42
16:BF:116:LEU:HD13	16:BF:120:ILE:HG22	2.00	0.42
35:FS:37:MET:SD	35:FS:39:ILE:HD11	2.59	0.42
35:FS:76:ASP:OD1	35:FS:76:ASP:N	2.50	0.42
23:BP:42:THR:HG22	23:BP:93:VAL:HG12	2.00	0.42
29:BV:68:ASP:OD1	29:BV:70:LYS:NZ	2.48	0.42
15:BE:34:THR:OG1	15:BE:88:VAL:O	2.24	0.42
15:BE:87:LYS:NZ	33:D2:2314:A:OP1	2.53	0.42
21:BN:12:ASP:OD1	21:BN:14:SER:N	2.46	0.42
22:BO:76:GLU:OE1	33:D2:636:G:N1	2.42	0.42
27:BT:103:VAL:O	27:BT:106:THR:OG1	2.28	0.42
33:D2:83:A:N6	33:D2:101:A:N7	2.67	0.42
33:D2:372:G:O2'	33:D2:373:U:P	2.77	0.42
33:D2:966:G:O4'	33:D2:2267:A:N6	2.52	0.42
33:D2:1833:C:O2'	33:D2:1969:A:N6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D2:1930:G:N1	33:D2:1969:A:OP2	2.48	0.42
9:B8:28:LEU:HG	9:B8:28:LEU:O	2.20	0.42
12:BB:44:ASN:N	33:D2:1812:U:O2'	2.53	0.42
13:BC:56:LYS:NZ	33:D2:2830:C:OP1	2.53	0.42
32:BY:60:VAL:HG22	32:BY:73:LYS:HD3	2.01	0.42
33:D2:1028:A:N3	33:D2:2486:C:O2'	2.46	0.42
33:D2:247:G:OP2	33:D2:249:C:N4	2.48	0.42
33:D2:1636:U:O2'	33:D2:1760:C:O2'	2.29	0.42
20:BM:31:GLU:HG2	20:BM:142:ILE:HG21	2.01	0.42
33:D2:1475:G:O2'	33:D2:1476:U:OP2	2.36	0.42
33:D2:2110:G:OP1	33:D2:2118:U:N3	2.52	0.42
10:B9:30:GLU:N	10:B9:30:GLU:OE1	2.53	0.42
18:BI:70:GLU:O	18:BI:71:LYS:HE2	2.19	0.42
3:B2:56:LEU:HA	3:B2:59:GLU:HG3	2.01	0.42
19:BK:45:THR:OG1	19:BK:50:LYS:NZ	2.51	0.42
30:BW:58:VAL:HG13	30:BW:85:VAL:HG12	2.02	0.42
33:D2:2467:C:H2'	33:D2:2468:A:O4'	2.20	0.42
33:D2:2848:G:HO2'	33:D2:2867:G:H22	1.60	0.42
19:BK:20:SER:HB3	19:BK:21:PRO:HD3	2.02	0.42
19:BK:91:LYS:HE3	33:D2:1063:G:N2	2.34	0.42
23:BP:69:PRO:O	23:BP:70:ASP:OD1	2.37	0.42
35:FS:49:MET:SD	35:FS:50:SER:N	2.93	0.42
24:BQ:3:HIS:ND1	33:D2:2820:A:H4'	2.35	0.41
15:BE:14:LYS:O	15:BE:17:THR:OG1	2.27	0.41
15:BE:122:ASP:OD1	15:BE:123:GLY:N	2.53	0.41
19:BK:123:ALA:HB1	33:D2:1081:U:H4'	2.02	0.41
33:D2:1730:C:O2'	33:D2:1731:G:O4'	2.38	0.41
33:D2:2125:G:HO2'	33:D2:2126:A:C1'	2.24	0.41
33:D2:2299:U:O4	33:D2:2318:G:N2	2.53	0.41
7:B6:22:THR:OG1	7:B6:23:THR:N	2.53	0.41
21:BN:121:GLU:OE2	26:BS:65:ASN:ND2	2.53	0.41
33:D2:2177:C:O2'	33:D2:2178:C:O4'	2.35	0.41
21:BN:58:LEU:HD12	21:BN:87:LEU:O	2.21	0.41
33:D2:500:G:N1	33:D2:503:A:OP2	2.52	0.41
33:D2:629:G:N3	33:D2:639:U:O2'	2.53	0.41
22:BO:103:ILE:HD12	22:BO:103:ILE:H	1.85	0.41
33:D2:161:A:H3'	33:D2:162:U:H5''	2.02	0.41
33:D2:1019:U:H3	33:D2:1142:A:H62	1.69	0.41
16:BF:10:VAL:HG22	16:BF:47:ASN:O	2.21	0.41
25:BR:9:ARG:O	25:BR:12:THR:HG22	2.20	0.41
33:D2:281:C:H42	33:D2:359:G:H1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BF:126:THR:HG22	16:BF:127:GLN:H	1.86	0.41
32:BY:83:LYS:NZ	33:D2:1119:U:OP1	2.52	0.41
13:BC:45:TYR:HH	33:D2:2636:C:HO2'	1.63	0.41
19:BK:131:THR:OG1	33:D2:1060:U:O4	2.34	0.41
9:B8:54:LEU:O	9:B8:58:ILE:HD12	2.20	0.41
13:BC:35:THR:HG21	13:BC:79:LEU:HD22	2.03	0.41
15:BE:37:MET:HE3	15:BE:149:ARG:HD2	2.03	0.41
16:BF:100:ASN:ND2	16:BF:100:ASN:C	2.78	0.41
18:BI:93:SER:OG	18:BI:121:VAL:HG23	2.21	0.41
21:BN:28:SER:OG	33:D2:2566:A:N1	2.45	0.41
23:BP:26:VAL:O	23:BP:26:VAL:HG13	2.20	0.41
27:BT:82:LEU:HD22	27:BT:87:VAL:HG21	2.01	0.41
11:BA:4:LEU:HD21	11:BA:8:MET:HB2	2.01	0.41
11:BA:217:THR:HB	33:D2:2124:G:H21	1.86	0.41
15:BE:7:TYR:HA	15:BE:11:VAL:HG12	2.03	0.41
33:D2:2637:U:H2'	33:D2:2638:G:O4'	2.21	0.41
13:BC:3:GLY:C	13:BC:4:LEU:HD12	2.45	0.40
16:BF:46:ASP:OD1	16:BF:48:THR:N	2.54	0.40
24:BQ:72:ASP:OD1	24:BQ:73:ASN:N	2.54	0.40
33:D2:974:G:H8	33:D2:990:A:H62	1.67	0.40
33:D2:1937:A:N7	33:D2:1939:U:O2'	2.54	0.40
17:BG:21:ASN:OD1	17:BG:22:ALA:N	2.54	0.40
29:BV:107:VAL:O	29:BV:107:VAL:HG13	2.22	0.40
32:BY:64:VAL:O	32:BY:64:VAL:HG13	2.22	0.40
12:BB:258:SER:O	12:BB:258:SER:OG	2.36	0.40
14:BD:127:GLU:OE1	14:BD:127:GLU:N	2.48	0.40
16:BF:100:ASN:ND2	16:BF:100:ASN:O	2.48	0.40
33:D2:421:C:HO2'	33:D2:422:A:P	2.43	0.40
33:D2:1833:C:HO2'	33:D2:1969:A:N6	2.19	0.40
31:BX:11:ILE:HD12	31:BX:20:LYS:C	2.46	0.40
33:D2:490:C:O2'	33:D2:491:G:P	2.80	0.40
33:D2:2808:G:H4'	33:D2:2809:A:O5'	2.22	0.40
24:BQ:22:ARG:HG3	24:BQ:70:THR:HA	2.04	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	B0	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
2	B1	75/78 (96%)	75 (100%)	0	0	100	100
3	B2	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
4	B3	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
5	B4	45/70 (64%)	43 (96%)	2 (4%)	0	100	100
6	B5	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
7	B6	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
8	B7	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
9	B8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
10	B9	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
11	BA	130/234 (56%)	120 (92%)	10 (8%)	0	100	100
12	BB	247/273 (90%)	236 (96%)	11 (4%)	0	100	100
13	BC	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
14	BD	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	24	48
15	BE	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
16	BF	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
17	BG	69/87 (79%)	67 (97%)	2 (3%)	0	100	100
18	BI	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
19	BK	139/142 (98%)	126 (91%)	13 (9%)	0	100	100
20	BM	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
21	BN	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
22	BO	141/144 (98%)	126 (89%)	15 (11%)	0	100	100
23	BP	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
24	BQ	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
25	BR	114/117 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BS	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
27	BT	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
28	BU	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	12	32
29	BV	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
30	BW	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
31	BX	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
32	BY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
35	FS	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
All	All	3628/3904 (93%)	3431 (95%)	195 (5%)	2 (0%)	49	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	BU	54	VAL
14	BD	83	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B0	57/63 (90%)	57 (100%)	0	100	100
2	B1	67/68 (98%)	67 (100%)	0	100	100
3	B2	55/55 (100%)	55 (100%)	0	100	100
4	B3	48/48 (100%)	48 (100%)	0	100	100
5	B4	43/62 (69%)	43 (100%)	0	100	100
6	B5	47/48 (98%)	47 (100%)	0	100	100
7	B6	45/49 (92%)	45 (100%)	0	100	100
8	B7	38/38 (100%)	38 (100%)	0	100	100
9	B8	51/52 (98%)	51 (100%)	0	100	100
10	B9	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	BA	110/181 (61%)	110 (100%)	0	100	100
12	BB	202/218 (93%)	202 (100%)	0	100	100
13	BC	164/164 (100%)	164 (100%)	0	100	100
14	BD	165/165 (100%)	165 (100%)	0	100	100
15	BE	148/150 (99%)	148 (100%)	0	100	100
16	BF	137/138 (99%)	136 (99%)	1 (1%)	76	90
17	BG	54/66 (82%)	54 (100%)	0	100	100
18	BI	114/114 (100%)	114 (100%)	0	100	100
19	BK	109/110 (99%)	109 (100%)	0	100	100
20	BM	116/116 (100%)	116 (100%)	0	100	100
21	BN	103/104 (99%)	103 (100%)	0	100	100
22	BO	102/103 (99%)	102 (100%)	0	100	100
23	BP	109/109 (100%)	109 (100%)	0	100	100
24	BQ	100/103 (97%)	100 (100%)	0	100	100
25	BR	86/87 (99%)	86 (100%)	0	100	100
26	BS	99/100 (99%)	99 (100%)	0	100	100
27	BT	89/90 (99%)	89 (100%)	0	100	100
28	BU	84/84 (100%)	84 (100%)	0	100	100
29	BV	93/93 (100%)	93 (100%)	0	100	100
30	BW	80/84 (95%)	80 (100%)	0	100	100
31	BX	83/85 (98%)	83 (100%)	0	100	100
32	BY	78/78 (100%)	78 (100%)	0	100	100
35	FS	89/91 (98%)	89 (100%)	0	100	100
All	All	2999/3150 (95%)	2998 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	BF	100	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B0	42	HIS
9	B8	25	HIS
11	BA	160	GLN
14	BD	9	GLN
14	BD	94	GLN
14	BD	97	ASN
14	BD	136	GLN
18	BI	43	ASN
19	BK	30	GLN
21	BN	5	GLN
21	BN	93	GLN
25	BR	98	GLN
27	BT	43	GLN
28	BU	86	GLN
29	BV	9	HIS
30	BW	91	GLN
35	FS	57	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	D2	2806/2903 (96%)	444 (15%)	20 (0%)
34	D3	119/120 (99%)	20 (16%)	3 (2%)
All	All	2925/3023 (96%)	464 (15%)	23 (0%)

All (464) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	D2	10	A
33	D2	35	G
33	D2	36	G
33	D2	45	G
33	D2	46	G
33	D2	51	G
33	D2	63	A
33	D2	71	A
33	D2	74	A
33	D2	75	G
33	D2	82	U
33	D2	100	U
33	D2	102	U
33	D2	118	A

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Mol	Chain	Res	Type
33	D2	120	U
33	D2	139	U
33	D2	140	C
33	D2	141	G
33	D2	142	A
33	D2	162	U
33	D2	163	C
33	D2	166	U
33	D2	181	A
33	D2	196	A
33	D2	199	A
33	D2	215	G
33	D2	216	A
33	D2	218	A
33	D2	221	A
33	D2	222	A
33	D2	228	C
33	D2	248	G
33	D2	249	C
33	D2	250	G
33	D2	255	A
33	D2	265	A
33	D2	266	G
33	D2	276	U
33	D2	281	C
33	D2	284	U
33	D2	285	G
33	D2	310	A
33	D2	323	C
33	D2	324	A
33	D2	329	G
33	D2	330	A
33	D2	334	C
33	D2	361	G
33	D2	362	A
33	D2	371	A
33	D2	372	G
33	D2	373	U
33	D2	386	G
33	D2	387	U
33	D2	388	G
33	D2	395	U

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Mol	Chain	Res	Type
33	D2	403	U
33	D2	404	A
33	D2	405	U
33	D2	406	G
33	D2	411	G
33	D2	417	C
33	D2	422	A
33	D2	424	G
33	D2	456	C
33	D2	457	A
33	D2	481	G
33	D2	491	G
33	D2	505	A
33	D2	509	C
33	D2	530	G
33	D2	531	C
33	D2	532	A
33	D2	545	U
33	D2	546	U
33	D2	547	A
33	D2	549	G
33	D2	556	A
33	D2	563	A
33	D2	573	U
33	D2	574	A
33	D2	575	A
33	D2	603	A
33	D2	613	A
33	D2	614	A
33	D2	622	G
33	D2	627	A
33	D2	637	A
33	D2	645	C
33	D2	646	U
33	D2	647	G
33	D2	654	A
33	D2	655	A
33	D2	669	G
33	D2	686	U
33	D2	687	C
33	D2	694	U
33	D2	711	G

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Mol	Chain	Res	Type
33	D2	715	A
33	D2	716	A
33	D2	717	C
33	D2	730	A
33	D2	738	G
33	D2	747	C
33	D2	752	A
33	D2	764	A
33	D2	765	C
33	D2	775	G
33	D2	776	G
33	D2	777	G
33	D2	782	A
33	D2	784	G
33	D2	789	A
33	D2	792	A
33	D2	805	G
33	D2	812	C
33	D2	819	A
33	D2	827	U
33	D2	828	U
33	D2	830	G
33	D2	844	A
33	D2	845	A
33	D2	846	U
33	D2	847	U
33	D2	857	G
33	D2	860	U
33	D2	878	A
33	D2	883	G
33	D2	887	U
33	D2	896	A
33	D2	897	C
33	D2	902	C
33	D2	910	A
33	D2	914	G
33	D2	932	U
33	D2	941	A
33	D2	946	C
33	D2	961	C
33	D2	974	G
33	D2	983	A

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Mol	Chain	Res	Type
33	D2	995	C
33	D2	996	A
33	D2	1012	U
33	D2	1013	C
33	D2	1021	A
33	D2	1022	G
33	D2	1026	G
33	D2	1033	U
33	D2	1040	A
33	D2	1041	G
33	D2	1045	C
33	D2	1046	A
33	D2	1047	G
33	D2	1057	A
33	D2	1060	U
33	D2	1061	U
33	D2	1062	G
33	D2	1065	U
33	D2	1066	U
33	D2	1069	A
33	D2	1070	A
33	D2	1071	G
33	D2	1072	C
33	D2	1073	A
33	D2	1075	C
33	D2	1076	C
33	D2	1078	U
33	D2	1079	C
33	D2	1083	U
33	D2	1084	A
33	D2	1085	A
33	D2	1088	A
33	D2	1090	A
33	D2	1097	U
33	D2	1101	U
33	D2	1104	C
33	D2	1110	G
33	D2	1111	A
33	D2	1112	G
33	D2	1132	U
33	D2	1135	C
33	D2	1136	G

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Mol	Chain	Res	Type
33	D2	1139	G
33	D2	1142	A
33	D2	1172	C
33	D2	1173	U
33	D2	1174	U
33	D2	1175	A
33	D2	1177	G
33	D2	1179	G
33	D2	1180	U
33	D2	1206	G
33	D2	1211	C
33	D2	1212	G
33	D2	1250	G
33	D2	1251	C
33	D2	1253	A
33	D2	1256	G
33	D2	1271	G
33	D2	1272	A
33	D2	1300	G
33	D2	1301	A
33	D2	1302	A
33	D2	1329	U
33	D2	1330	C
33	D2	1341	G
33	D2	1345	C
33	D2	1352	U
33	D2	1365	A
33	D2	1368	G
33	D2	1378	A
33	D2	1379	U
33	D2	1383	A
33	D2	1395	A
33	D2	1416	G
33	D2	1419	A
33	D2	1420	A
33	D2	1421	G
33	D2	1428	C
33	D2	1452	G
33	D2	1454	C
33	D2	1459	G
33	D2	1461	C
33	D2	1475	G

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Mol	Chain	Res	Type
33	D2	1476	U
33	D2	1482	G
33	D2	1490	A
33	D2	1491	G
33	D2	1504	A
33	D2	1509	A
33	D2	1515	A
33	D2	1524	G
33	D2	1533	C
33	D2	1534	U
33	D2	1535	A
33	D2	1536	C
33	D2	1555	G
33	D2	1560	G
33	D2	1565	C
33	D2	1569	A
33	D2	1584	U
33	D2	1585	C
33	D2	1608	A
33	D2	1611	C
33	D2	1646	C
33	D2	1647	U
33	D2	1648	U
33	D2	1654	A
33	D2	1664	A
33	D2	1674	G
33	D2	1715	G
33	D2	1716	U
33	D2	1730	C
33	D2	1731	G
33	D2	1732	C
33	D2	1733	G
33	D2	1735	A
33	D2	1738	G
33	D2	1744	A
33	D2	1758	U
33	D2	1764	C
33	D2	1773	A
33	D2	1776	G
33	D2	1780	A
33	D2	1791	A
33	D2	1800	C

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Mol	Chain	Res	Type
33	D2	1801	A
33	D2	1802	A
33	D2	1808	A
33	D2	1812	U
33	D2	1816	C
33	D2	1829	A
33	D2	1833	C
33	D2	1937	A
33	D2	1938	A
33	D2	1940	U
33	D2	1941	C
33	D2	1945	G
33	D2	1955	U
33	D2	1962	C
33	D2	1965	C
33	D2	1967	C
33	D2	1969	A
33	D2	1970	A
33	D2	1971	U
33	D2	1972	G
33	D2	1991	U
33	D2	1993	U
33	D2	1997	C
33	D2	2022	U
33	D2	2023	C
33	D2	2027	G
33	D2	2031	A
33	D2	2033	A
33	D2	2043	C
33	D2	2052	A
33	D2	2055	C
33	D2	2056	G
33	D2	2060	A
33	D2	2061	G
33	D2	2062	A
33	D2	2069	G
33	D2	2093	G
33	D2	2096	C
33	D2	2098	U
33	D2	2109	U
33	D2	2110	G
33	D2	2111	U

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Mol	Chain	Res	Type
33	D2	2112	G
33	D2	2113	U
33	D2	2114	A
33	D2	2115	G
33	D2	2118	U
33	D2	2119	A
33	D2	2120	G
33	D2	2125	G
33	D2	2130	U
33	D2	2133	G
33	D2	2134	A
33	D2	2135	A
33	D2	2137	U
33	D2	2144	G
33	D2	2145	C
33	D2	2151	U
33	D2	2157	G
33	D2	2159	G
33	D2	2162	G
33	D2	2164	C
33	D2	2165	C
33	D2	2166	U
33	D2	2167	U
33	D2	2171	A
33	D2	2172	U
33	D2	2173	A
33	D2	2177	C
33	D2	2178	C
33	D2	2182	U
33	D2	2186	G
33	D2	2187	U
33	D2	2188	U
33	D2	2189	U
33	D2	2191	A
33	D2	2193	G
33	D2	2198	A
33	D2	2199	A
33	D2	2203	U
33	D2	2204	G
33	D2	2212	A
33	D2	2213	U
33	D2	2225	A

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Mol	Chain	Res	Type
33	D2	2226	C
33	D2	2238	G
33	D2	2239	G
33	D2	2250	G
33	D2	2279	G
33	D2	2283	C
33	D2	2286	G
33	D2	2287	A
33	D2	2297	A
33	D2	2303	G
33	D2	2305	U
33	D2	2307	G
33	D2	2309	A
33	D2	2311	A
33	D2	2325	G
33	D2	2327	A
33	D2	2331	G
33	D2	2334	U
33	D2	2345	G
33	D2	2350	C
33	D2	2361	G
33	D2	2382	G
33	D2	2383	G
33	D2	2385	C
33	D2	2392	A
33	D2	2402	U
33	D2	2406	A
33	D2	2407	A
33	D2	2423	U
33	D2	2424	C
33	D2	2425	A
33	D2	2429	G
33	D2	2430	A
33	D2	2435	A
33	D2	2441	U
33	D2	2447	G
33	D2	2448	A
33	D2	2475	C
33	D2	2476	A
33	D2	2497	A
33	D2	2498	C
33	D2	2502	G

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Mol	Chain	Res	Type
33	D2	2503	A
33	D2	2504	U
33	D2	2505	G
33	D2	2508	G
33	D2	2518	A
33	D2	2529	G
33	D2	2547	A
33	D2	2566	A
33	D2	2567	G
33	D2	2572	A
33	D2	2573	C
33	D2	2576	G
33	D2	2582	G
33	D2	2585	U
33	D2	2602	A
33	D2	2603	G
33	D2	2609	U
33	D2	2610	C
33	D2	2613	U
33	D2	2629	U
33	D2	2630	G
33	D2	2655	G
33	D2	2682	A
33	D2	2689	U
33	D2	2690	U
33	D2	2714	G
33	D2	2733	A
33	D2	2744	G
33	D2	2748	A
33	D2	2757	A
33	D2	2764	A
33	D2	2765	A
33	D2	2778	A
33	D2	2779	U
33	D2	2797	U
33	D2	2798	U
33	D2	2800	A
33	D2	2807	U
33	D2	2808	G
33	D2	2809	A
33	D2	2818	U
33	D2	2820	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
33	D2	2833	U
33	D2	2849	U
33	D2	2867	G
33	D2	2868	A
33	D2	2872	A
33	D2	2873	A
33	D2	2880	C
33	D2	2884	U
33	D2	2887	A
33	D2	2903	U
34	D3	3	C
34	D3	4	C
34	D3	9	G
34	D3	12	C
34	D3	13	G
34	D3	23	G
34	D3	25	U
34	D3	35	C
34	D3	42	C
34	D3	44	G
34	D3	52	A
34	D3	67	G
34	D3	87	U
34	D3	88	C
34	D3	89	U
34	D3	90	C
34	D3	105	G
34	D3	108	A
34	D3	109	A
34	D3	120	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	D2	227	A
33	D2	372	G
33	D2	404	A
33	D2	421	C
33	D2	490	C
33	D2	555	G
33	D2	715	A
33	D2	774	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
33	D2	859	G
33	D2	931	U
33	D2	1020	A
33	D2	1475	G
33	D2	1490	A
33	D2	1663	G
33	D2	1715	G
33	D2	1730	C
33	D2	2326	C
33	D2	2333	A
33	D2	2391	G
33	D2	2808	G
34	D3	3	C
34	D3	66	A
34	D3	88	C

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.



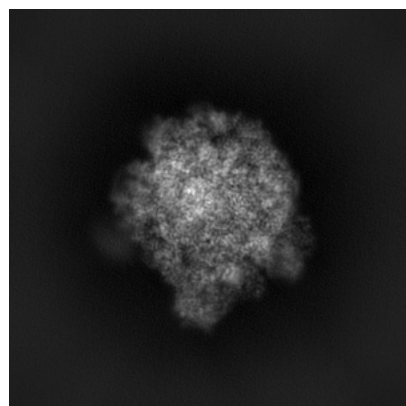
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55176. These allow visual inspection of the internal detail of the map and identification of artifacts.

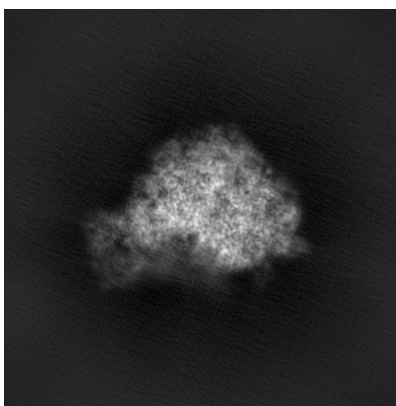
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

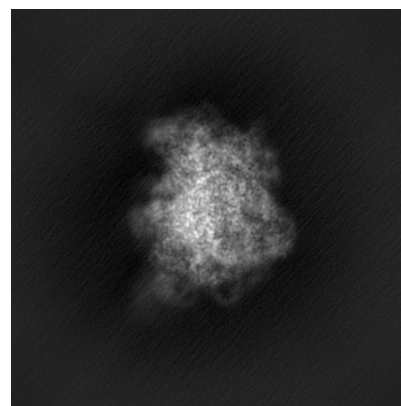
#### 6.1.1 Primary map



X

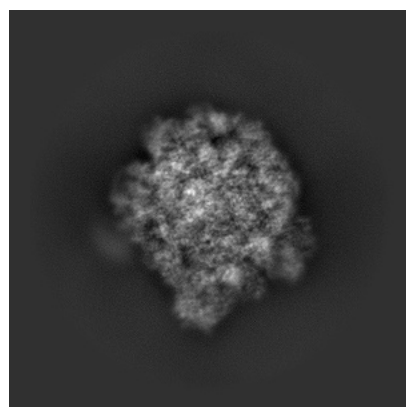


Y

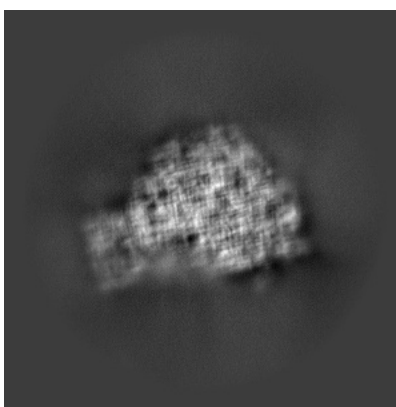


Z

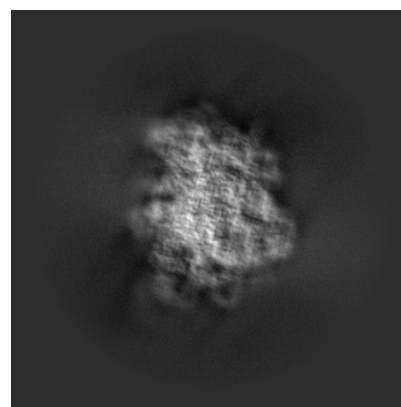
#### 6.1.2 Raw map



X



Y

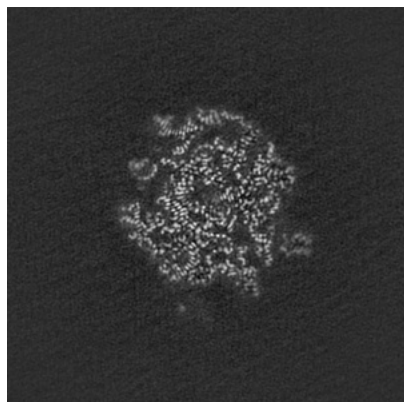


Z

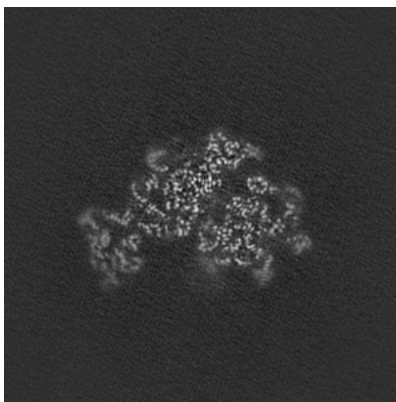
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

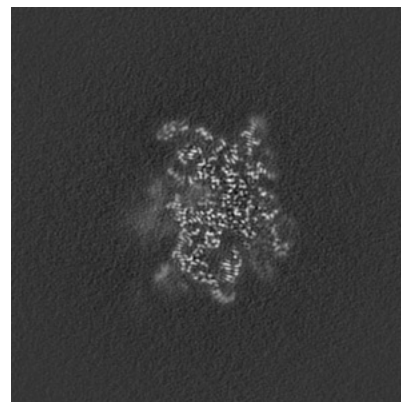
### 6.2.1 Primary map



X Index: 240

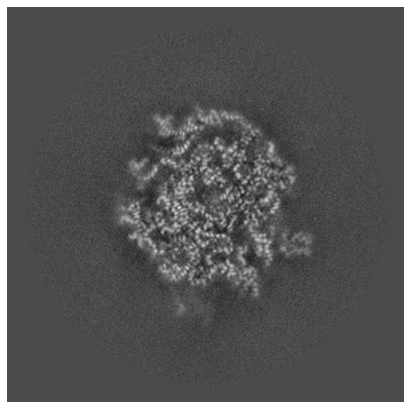


Y Index: 240

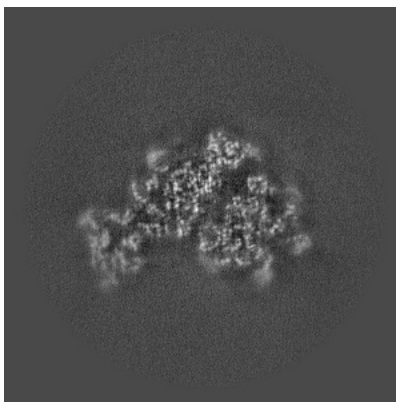


Z Index: 240

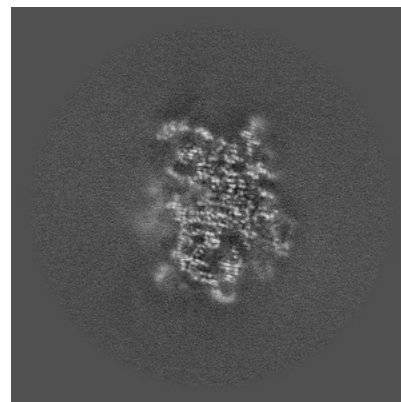
### 6.2.2 Raw map



X Index: 240



Y Index: 240

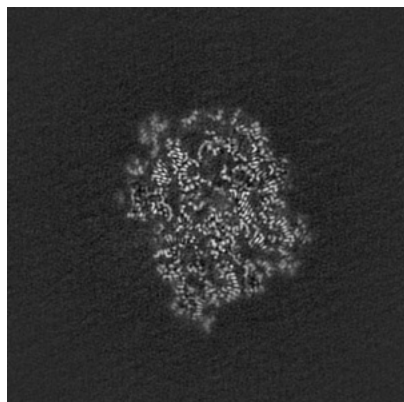


Z Index: 240

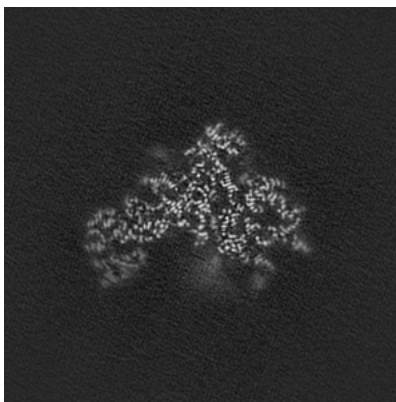
The images above show central slices of the map in three orthogonal directions.

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

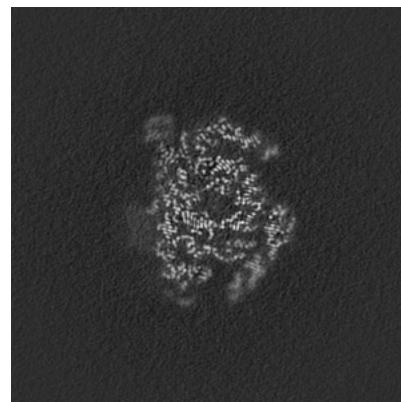
### 6.3.1 Primary map



X Index: 224

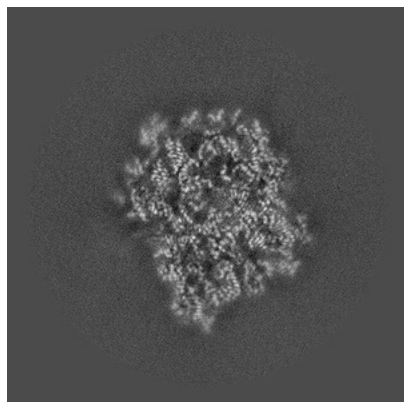


Y Index: 227

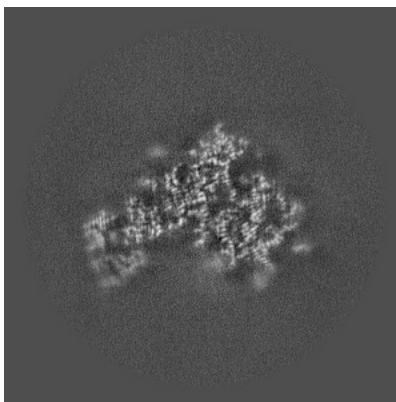


Z Index: 262

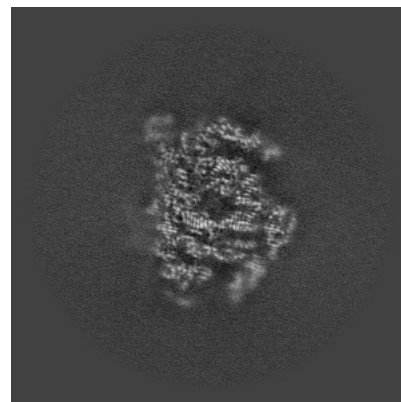
### 6.3.2 Raw map



X Index: 223



Y Index: 231

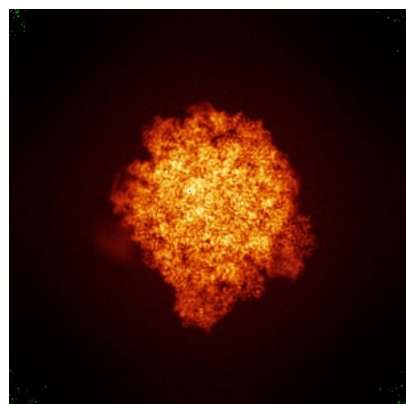


Z Index: 262

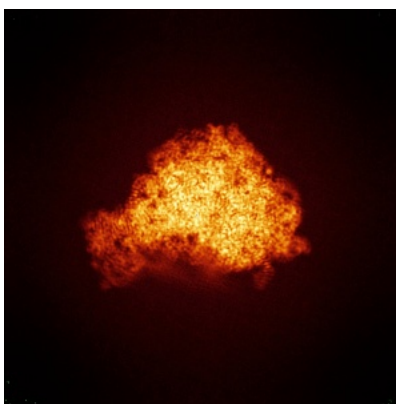
The images above show the largest variance slices of the map in three orthogonal directions.

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

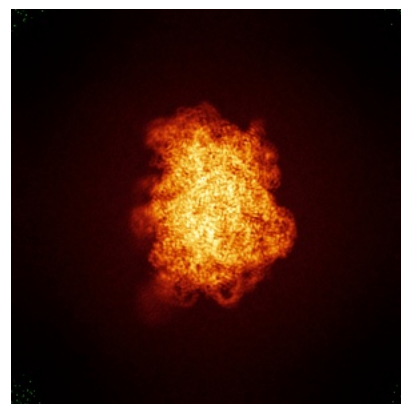
### 6.4.1 Primary map



X

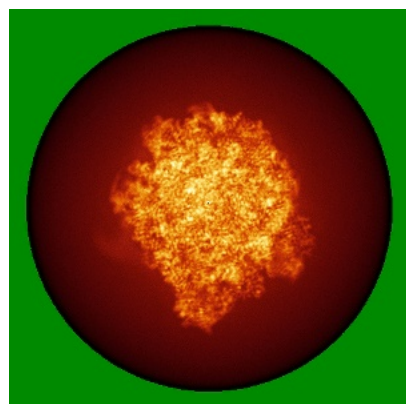


Y

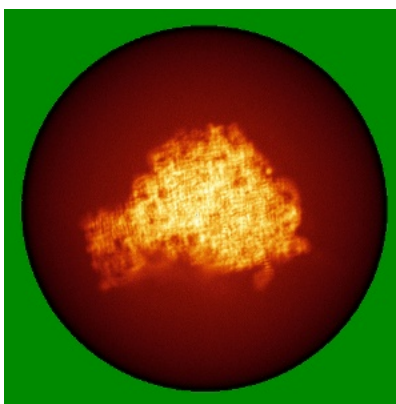


Z

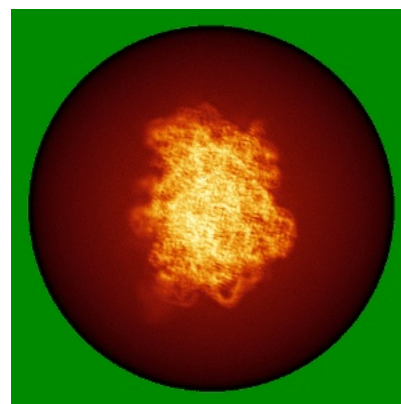
### 6.4.2 Raw map



X



Y

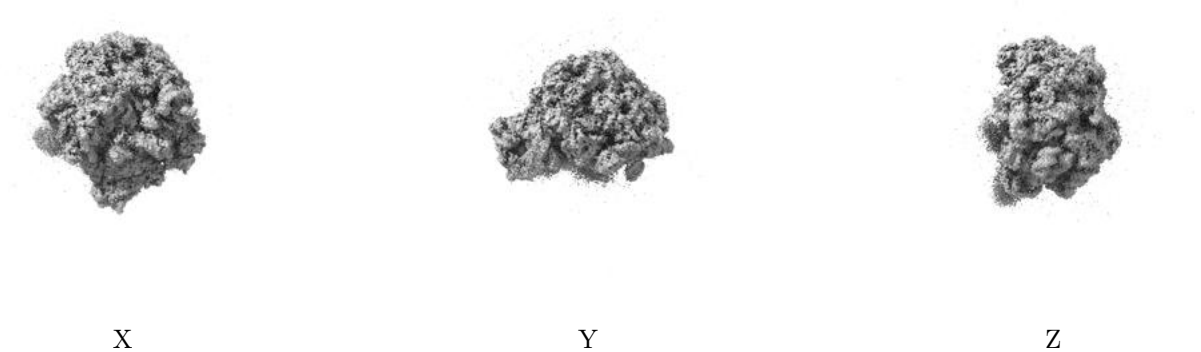


Z

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

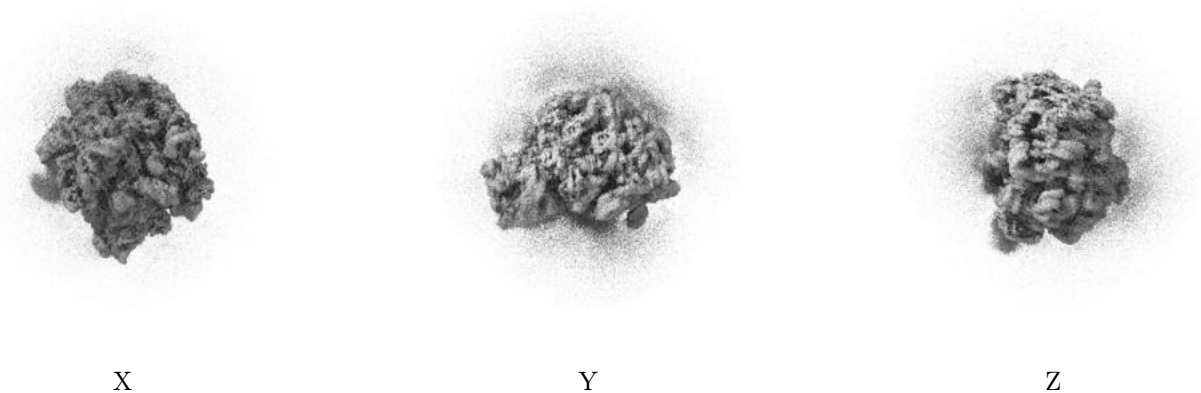
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

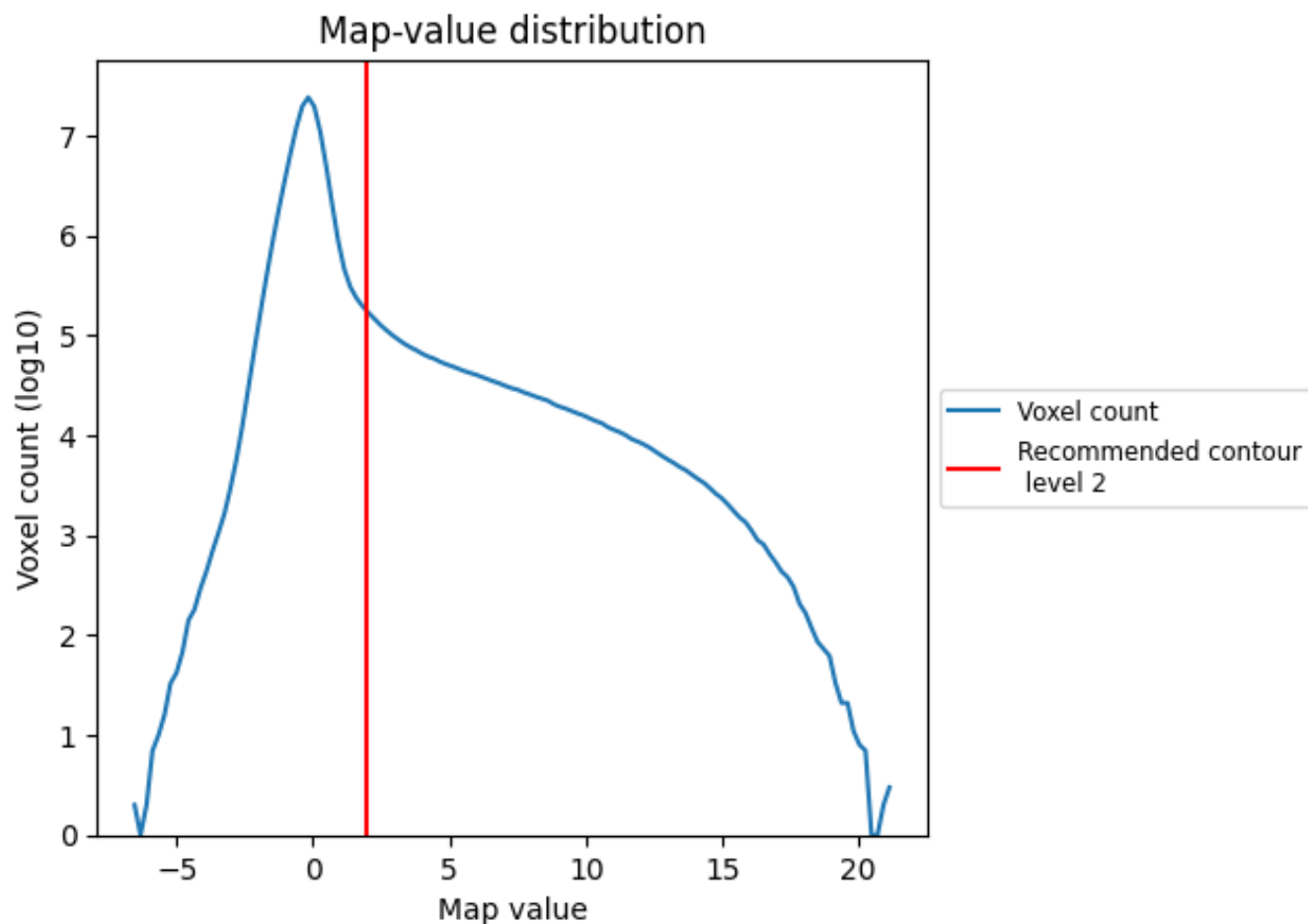
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

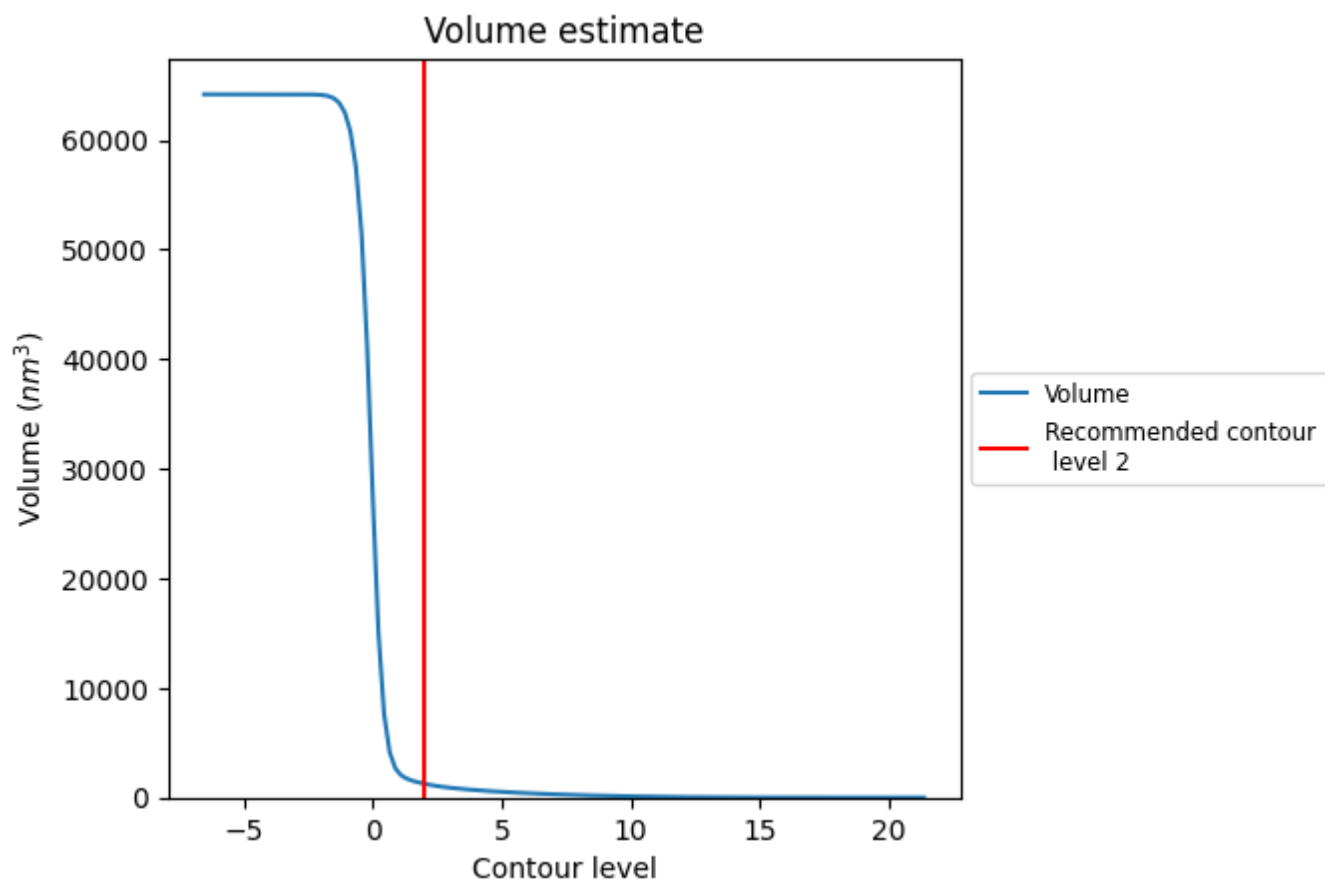
This section contains the results of statistical analysis of the map.

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



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

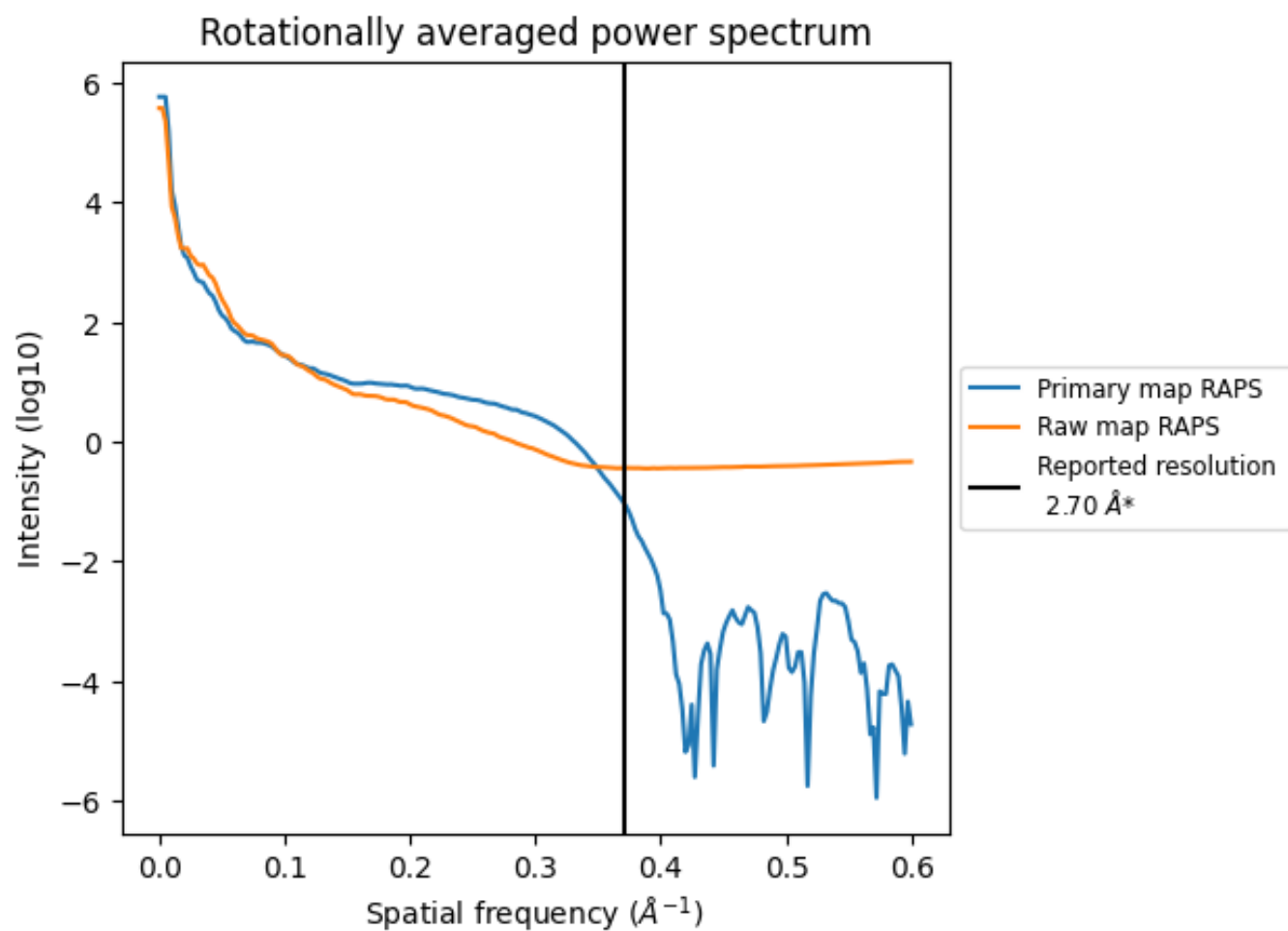
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1257 nm<sup>3</sup>; this corresponds to an approximate mass of 1135 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



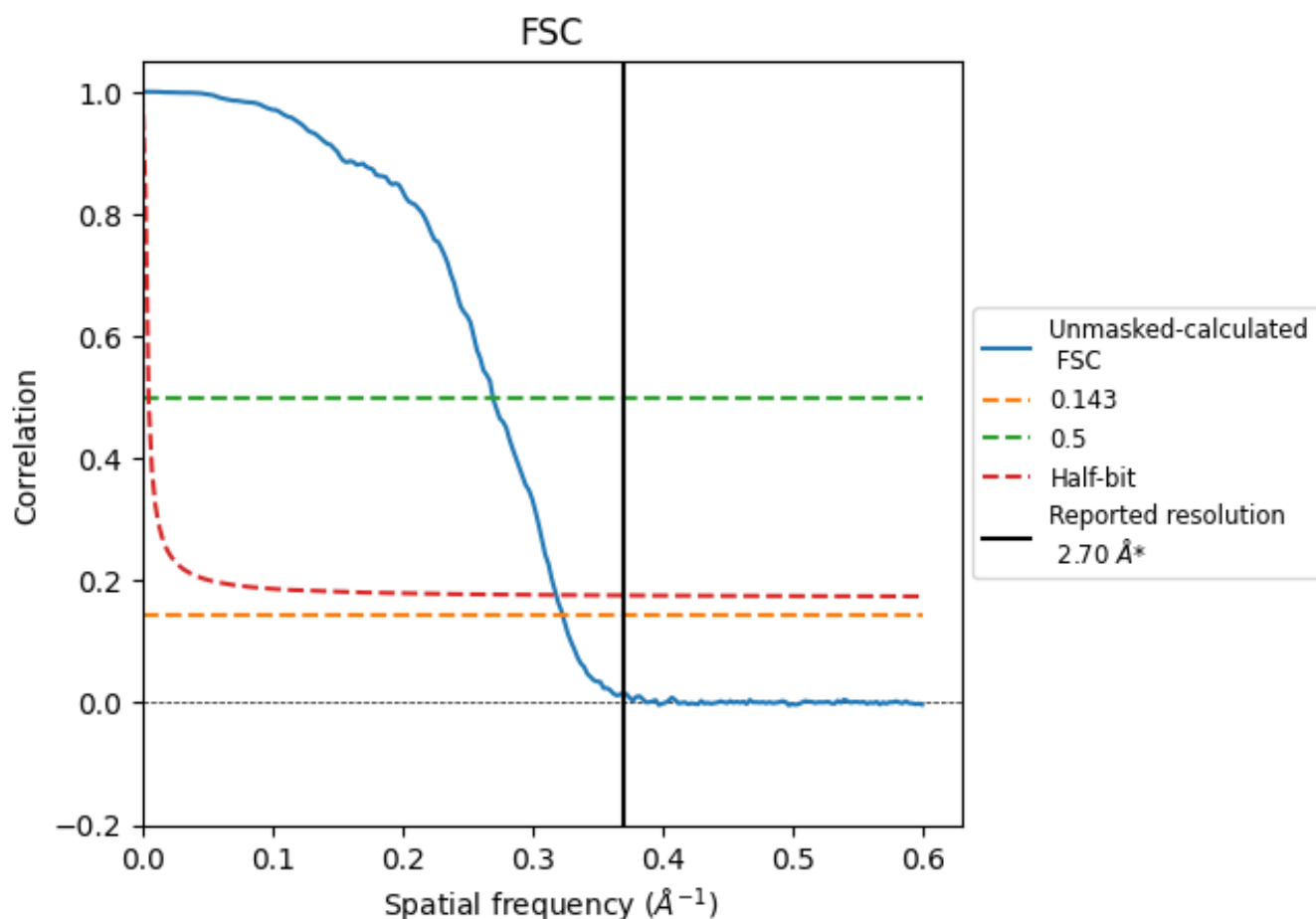
\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.370 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

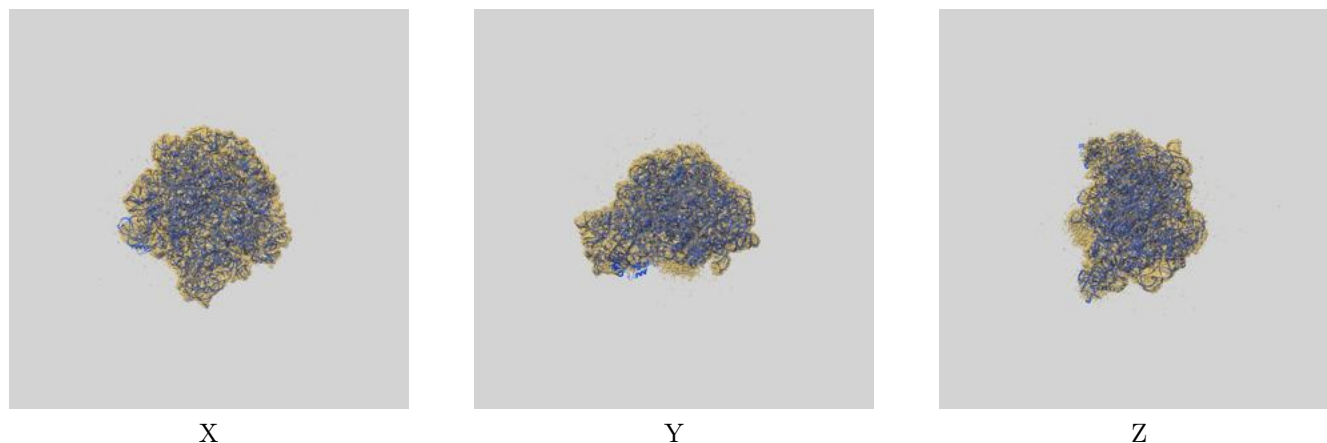
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.09	3.71	3.14

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.7 by more than 10 %

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

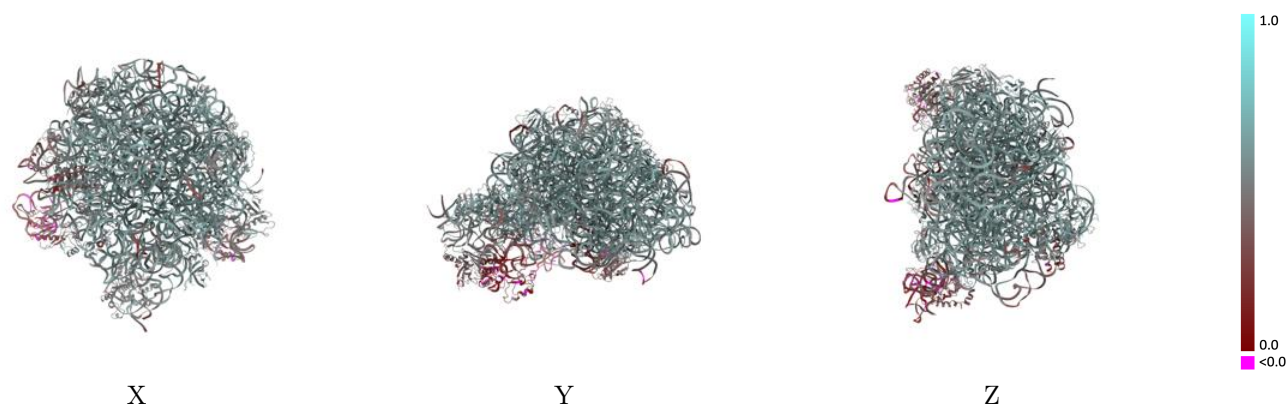
This section contains information regarding the fit between EMDB map EMD-55176 and PDB model 9SS4. Per-residue inclusion information can be found in section 3 on page 11.

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



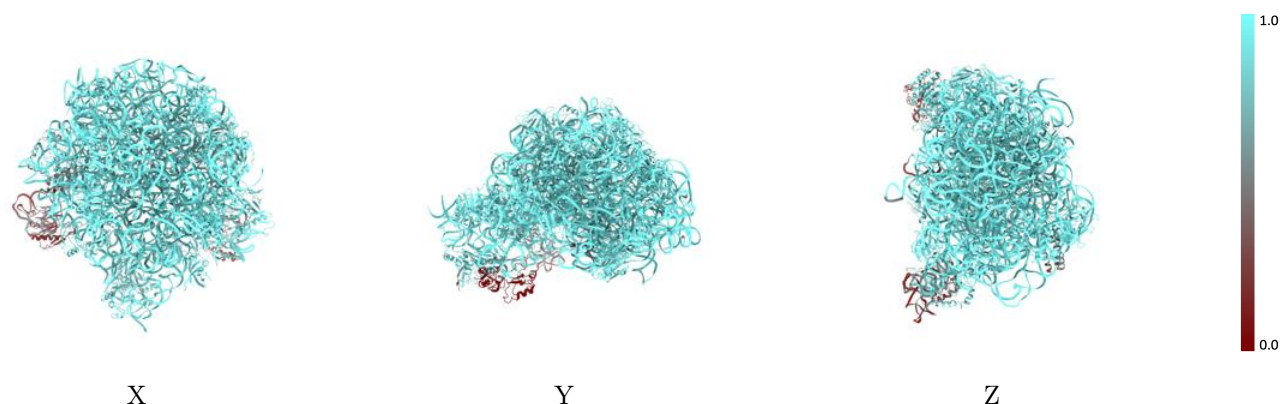
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



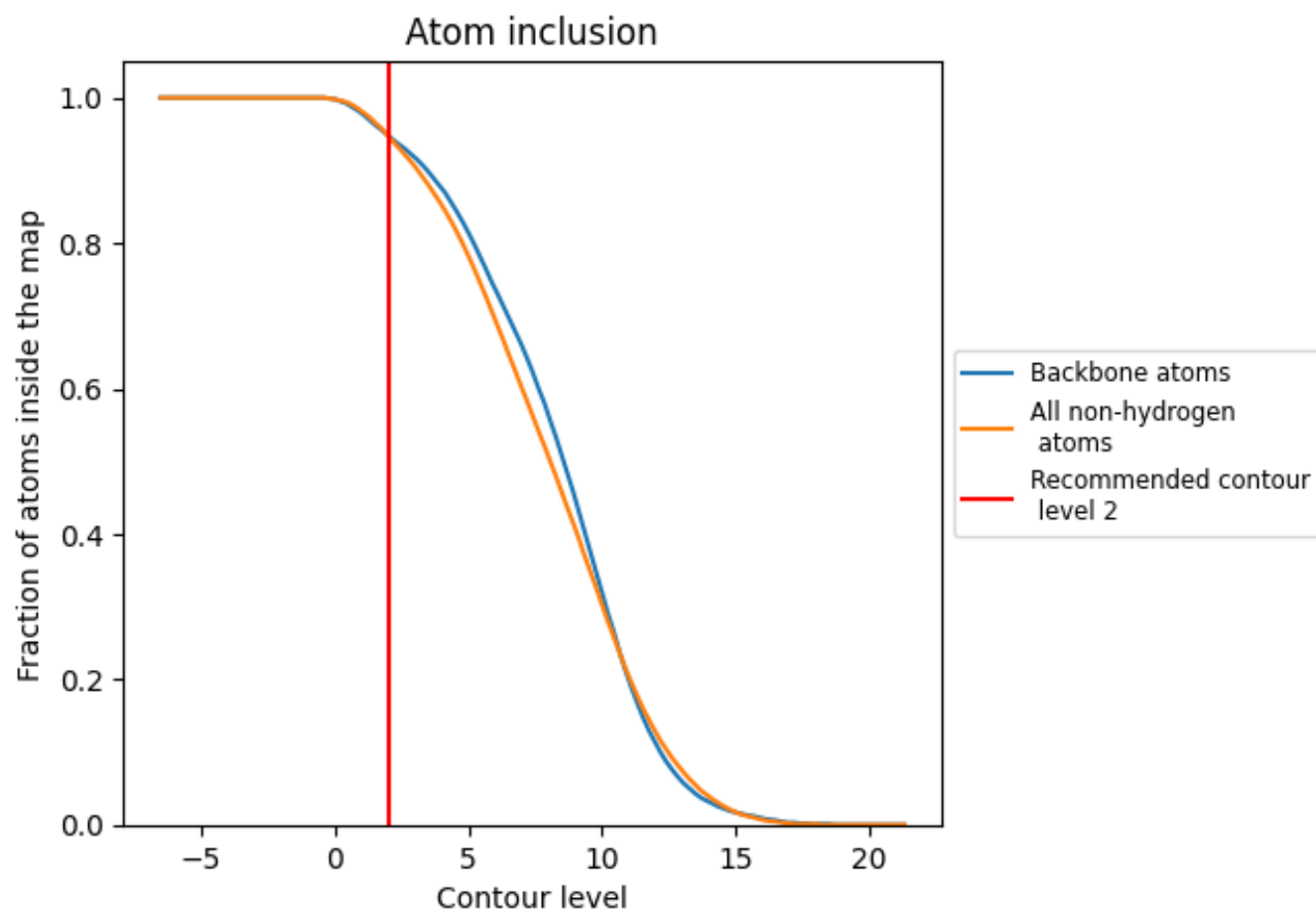
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).









































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 95% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.5230
B0	 0.9880	 0.5760
B1	 0.9850	 0.5620
B2	 0.9640	 0.4940
B3	 0.9910	 0.5700
B4	 0.7920	 0.3680
B5	 0.9930	 0.5720
B6	 0.9850	 0.5490
B7	 0.9940	 0.5890
B8	 0.9920	 0.5830
B9	 0.9760	 0.5440
BA	 0.1630	 0.1970
BB	 0.9940	 0.5710
BC	 0.9880	 0.5690
BD	 0.9820	 0.5370
BE	 0.9200	 0.4150
BF	 0.9570	 0.5030
BG	 0.6320	 0.3250
BI	 0.8020	 0.3580
BK	 0.1160	 0.2000
BM	 0.9880	 0.5770
BN	 0.9550	 0.5420
BO	 0.9730	 0.5540
BP	 0.9890	 0.5610
BQ	 0.9950	 0.5740
BR	 0.9750	 0.4910
BS	 0.9640	 0.5290
BT	 0.9950	 0.5780
BU	 0.9770	 0.5520
BV	 0.9800	 0.5650
BW	 0.9770	 0.5420
BX	 0.9870	 0.5340
BY	 0.9700	 0.5360
D2	 0.9690	 0.5340
D3	 0.9970	 0.5200
FS	 0.8570	 0.3830

